

CCP2021



XXXII IUPAP Conference on Computational Physics

2-5 August 2021, ~~Coventry, England~~ *online*



Preface

CCP2021 is the 32nd conference in a series of meetings on computational physics that have been held annually and under the auspices of the International Union for Pure and Applied Physics (IUPAP) for more than 20 years now. The conference has a tradition of following a triannual cycle between the European, American and Asian/Pacific (plus maybe more frequently in the future also: African) regions, according to which it should have been held in Coventry in 2020. While preparations were well advanced, the meeting was called off in April 2020 due to the restrictions relating to the coronavirus pandemic. We were quite confident back then that the meeting could be held face-to-face in 2021, but the virus proved to be more persistent than we had envisaged, such that CCP2021 will be held entirely online. While we are rather disappointed that we cannot welcome you to Coventry in person, we are also excited about the new opportunities afforded by the online format: it is more inclusive, more ecological, more diverse, and more family friendly than any CCP conference before! At the same time, thanks to the many and varied contributions, we are glad to be able to present an excellent representation of where computational physics stands in the summer of 2021.

We are grateful for the kind sponsorship of a number of prestigious academic bodies, and leading publishing and software houses (listed on page 12). We thank you for participating and we warmly welcome you (virtually) to the ancient city of Coventry.

Coventry/Chemnitz, July 2021

Damien Foster
Nikolaos G. Fytas
Charo del Genio
Ran Holtzman
Susanne Horn
Abhishek Kumar
Alban Potherat
Martin Weigel (chair)
Taras Yavors'kii

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Previous CCP conferences

2019 Hong Kong (CN)

2018 Davies (US)

2017 Paris (FR)

2016 Pretoria (ZA)

2015 Guhawati (IN)

2014 Boston (US)

2013 Moscow (RU)

2012 Kobe (JP)

2011 Gatlinburg (US)

2010 Trondheim (NO)

2009 Kaohsiung (TW)

2008 Ouro Preto (BR)

2007 Brussels (BE)

2006 Gyeongju (KR)

2005 Los Angeles (US)

2004 Genova (IT)

2003 Beijing (CN)

2002 Dan Diego (US)

2001 Aachen (DE)

2000 Brisbane (AU)

1999 Atlanta (US)

1998 Grenada (ES)

1997 Santa Cruz (US)

International Advisory Board

Joan Adler, Technion
Nithaya Chetty, Wits U, Johannesburg
Mei-Yin Chou, Academia Sinica
Bismarck Vaz da Costa, UFMG, Belo Horizonte
Yuan Ping Feng, NUS, Singapore
Suklyun Hong, Sejong U
Andrew Horsfield, Imperial
Trevis Humble, ORNL
Barry Klein, UC Davis
Georg Kresse, U Vienna
David Landau, UGA, Athens
Hai-Qing Lin, CSRC, Beijing
Richard Liska, TU Prague
Priya Mahadevan, Bose Centre, Kolkata
Regina Maphanga, CSIR, Pretoria
Sitangshu Bikas Santra, IIT Guwahati
Lev Shchur, Landau Institute
Laurette Tuckerman, ESPCI
Roser Valentí U Frankfurt
Daniel Vizman, UVT, Timisoara
Rodolphe Vuilleumier, ENS, Paris
Xiaoqun Wang, SJTU, Shanghai
Renata Wentzcovitch, Columbia U
Junyi Zhu, CU Hong Kong

Program Committee

Statistical mechanics and complex systems

Wolfhard Janke, U Leipzig (chair)

Youjin Deng, USTC Hefei

Jonathan Machta, UMass Amherst

Lev Shchur, Landau Institute

Soft matter, biophysics

Julia Yeomans, U Oxford (chair)

Anna Balazs, U Pittsburgh

Changbong Hyeon, KIAS, Seoul

Materials and nano-science

Luca Ghiringhelli, FHI, Berlin (chair)

Francesca Baletto, King's College London

Silvana Botti, U Jena

Bryan Goldsmith, U Michigan, Ann Arbor

James Kermode, U Warwick

Sergey Levchenko, Skolkovo, Moscow

Fluid dynamics

Greg Sheard, Monash (chair)

Bruno Carmo, U Sao Paulo

Wisam Al Saadi, Australian College of Kuwait

Quantum many-body physics

Anders Sandvik, Boston U (chair)
Sylvain Capponi, U Toulouse
Kedar Damle, TIFR Mumbai
Chisa Hotta, U Tokyo
Shiwei Zhang, Flatiron Institute

Quantum computing

Stephen Jordan, Microsoft (chair)
David Gosset, U Waterloo
Artur Izmaylov, U Toronto
Bei Zeng, U Guelph

Lattice field theory

Constantina Alexandrou, Cyprus Institute (chair)
Gert Aarts, Swansea
Karl Jansen, DESY Zeuthen
Aida X. El-Khadra, U Illinois, Urbana-Champaign

Astrophysics, gravitation, cosmology

Raphael Hirschi, U Keele (chair)

Novel hardware and software

Massimo Bernaschi, NRC, Rome (chair)
Valeri Halyo, U Princeton
Victor Martin-Mayor, U Complutense, Madrid

Computational physics education

Joan Adler, Technion (chair)
Amy Graves, Swarthmore College

Machine learning and algorithms

Lenka Zdeborova, Paris (chair)

Chiara Cammarota, King's College London

Alexander Hartmann, U Oldenburg

Ehsan Katami, San Jose State U

Maria Schuld, KwaZulu-Natal

Pan Zhang, CAS, Beijing

Geophysics and porous media

Steve Tobias, U Leeds (chair)

Emmanuel Dormy, CNRS, Paris

Geoff Vallis, U Exeter

Local Organizing Committee

Damien Foster
Nikolaos G. Fytas
Charo del Genio
Ran Holtzman
Susanne Horn
Abhishek Kumar
Alban Potherat
Martin Weigel (chair)
Taras Yavors'kii

Sponsors



Conference Schedule: Timetable

GMT+1	Monday Aug 2			Tue Aug 3			Wed Aug 4			Thur Aug 5		
9:00												
9:15												
9:30			Opening			Plenary 4: Woods			Plenary 8: Wang			Parallel
9:45												Parallel
10:00			Plenary 1: Rillich			Plenary 5: Polmann			Plenary 9: Draxl			Backup
10:15												MS4
10:30												
10:45												
11:00			Plenary 2: Barkley			Plenary 6: Davies			Plenary 10: Saxe			Plenary 12: Berthier
11:15												
11:30						Plenary 7: Tucumalai			Plenary 11: Naarang			Plenary 13: Shaikina
11:45			Plenary 3: Csanyi									
12:00												
12:15												
12:30												
12:45												
13:00			Poster 1: SP, MS, FD, LA, HS, AS			Cultural presentations			Poster 2: SM, QC, ED, GP, ML			
13:15												
13:30												
13:45	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel
14:00												
14:15	SP1	MS1	FD1	AS1	GP1	QP1	LA1	SP3	MS3	LA2	HS1	
14:30												
14:45												
15:00												
15:15												
15:30												
15:45												
16:00	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel	Parallel
16:15												
16:30	SP2	MS2	FD2		QC1	QP2	ML1	SP4	MS3	QP3	ED1	
16:45												
17:00												
17:15												
17:30												
17:45												
18:00			Poster 1: SP, MS, FD, LA, HS, AS			YSP Award Session			Poster 2: SM, QC, ED, GP, ML			
18:15												
18:30												
18:45												
18:00												

(SP) Statistical physics & complex systems
 (SM) Soft matter, biophysics
 (MS) Materials and nano-science
 (FD) Fluid dynamics
 (QP) Quantum many-body physics
 (QC) Quantum computing
 (LA) Lattice field theory
 (AS) Astrophysics, gravitation, cosmology
 (HS) Novel hardware and software
 (ED) Computational physics education
 (ML) Machine Learning and algorithms
 (GP) Geophysics and porous media

Conference Schedule: Overview

Day 1: Monday, 02 August 2021

09:15 - 09:45		– Conference Opening (Audimax) –
09:45 – 10:30	Audimax	Plenary Session 1
11:00 – 12:30	Audimax	Plenary Session 2
12:45 - 13:30		– Poster Session 1 (Poster Rooms 1-3) –
13:45 – 15:30	Lecture Hall 1	Parallel Session: Statistical physics and complex systems 1
13:45 – 15:30	Lecture Hall 2	Parallel Session: Materials and non-science 1
13:45 – 15:30	Lecture Hall 3	Parallel Session: Fluid dynamics 1
13:45 – 15:30	Lecture Hall 4	Parallel Session: Astrophysics, gravitation, cosmology 1
16:00 – 17:45	Lecture Hall 1	Parallel Session: Statistical physics and complex systems 2
16:00 – 17:45	Lecture Hall 2	Parallel Session: Materials and non-science 2
16:00 – 17:45	Lecture Hall 3	Parallel Session: Fluid dynamics 2
16:00 - 17:45		– (Lecture Hall 4) –
18:00 - 19:00		– Poster Session 1 (Poster Rooms 1-3) –

Day 2: Tuesday, 03 August 2021

09:00 – 10:30	Audimax	Plenary Session 3
11:00 – 12:30	Audimax	Plenary Session 4
12:45 – 13:30		– Cultural Presentations (Audimax) –
13:45 – 15:30	Lecture Hall 1	Parallel Session: Soft matter and biophysics 1
13:45 – 15:30	Lecture Hall 2	Parallel Session: Quantum many-body physics 1
13:45 – 15:30	Lecture Hall 3	Parallel Session: Geophysics and porous media 1
13:45 – 15:30	Lecture Hall 4	Parallel Session: Lattice field theory 1
16:00 – 17:45	Lecture Hall 1	Parallel Session: Soft matter and biophysics 2
16:00 – 17:45	Lecture Hall 2	Parallel Session: Quantum many-body physics 2
16:00 – 17:45	Lecture Hall 3	Parallel Session: Quantum computing 1
16:00 – 17:45	Lecture Hall 4	Parallel Session: Machine learning and algorithms 1
18:00 – 19:00		– IUPAP Young Scientist Prize Award Session (Audimax) –

Day 3: Wednesday, 04 August 2021

09:00 – 10:30	Audimax	Plenary Session 5
11:00 – 12:30	Audimax	Plenary Session 6
12:45 – 13:30		– Poster Session 2 (Poster Rooms 1-3) –
13:45 – 15:30	Lecture Hall 1	Parallel Session: Statistical physics and complex systems 3
13:45 – 15:30	Lecture Hall 2	Parallel Session: Materials and non-science 3
13:45 – 15:30	Lecture Hall 3	Parallel Session: Lattice field theory 2
13:45 – 15:30	Lecture Hall 4	Parallel Session: Novel hardware and software 1
16:00 – 17:45	Lecture Hall 1	Parallel Session: Statistical physics and complex systems 4
16:00 – 17:45	Lecture Hall 2	Parallel Session: Soft matter and biophysics 3
16:00 – 17:45	Lecture Hall 3	Parallel Session: Quantum many-body physics 3
16:00 – 17:45	Lecture Hall 4	Parallel Session: Computational physics education 1
18:00 – 19:00		– Poster Session 2 (Poster Rooms 1-3) –

Day 4: Thursday, 05 August 2021

09:00 – 10:45	Lecture Hall 1	Parallel Session: Soft matter and biophysics 4
09:00 - 10:45		– Backup (Lecture Hall 2) –
09:00 – 10:45	Lecture Hall 3	Parallel Session: Machine learning and algorithms 2
09:00 – 10:45	Lecture Hall 4	Parallel Session: Materials and non-science 4
11:00 – 12:30	Audimax	Plenary Session 7
13:30 – 15:30	Audimax	Plenary Session 8
15:00 - 15:30		– Announcement of CCP2022 and Closing Remarks (Audimax) –

Conference Schedule: Session Details

Monday, 02 August 09:45–10:30 GMT+1: Audimax

Plenary Session 1

(Chairs: Abhishek Kumar, Martin Weigel)

09:45 – **Annalisa** Universe(s) in a box
 10:30 **Pillepich**

Monday, 02 August 11:00–12:30 GMT+1: Audimax

Plenary Session 2

(Chairs: Charo del Genio, Abhishek Kumar)

11:00 – **Dwight** Universality and rare events in the subcritical
 11:45 **Barkley** route to turbulence
 11:45 – **Gabor Csanyi** Machine learned force fields: status and chal-
 12:30 lenges

Monday, 02 August 12:45–13:30 GMT+1: Poster Rooms 1-3

Poster Session 1

12:45 – **Dao Duc Anh** Elucidating atomic-scale phenomena with
 13:30 transmission electron microscopy: a study of
 gold nanocontact (17)
 12:45 – **Yusuke** Molecular-Dynamics Simulation of Liquid Sul-
 13:30 **Suzumura** fur by Artificial Neural Network Potentials
 (18)
 12:45 – **Mykhailo** Confinement effects on packings of disco-
 13:30 **Tatochenko** rectangles in slit pores (24)
 12:45 – **Arsha** Study of velocity auto-correlation function of a
 13:30 **Noushad** confined Brownian particle (49)

- 12:45 – **Erik Shalenov** The capture cross sections at the electron collisions with hydrogen atom in non Maxwellian dense semiclassical plasma (58)
13:30
- 12:45 – **Takashi** A charge-momentum-energy-conserving alternative numerical method for the Vlasov–Maxwell system (84)
13:30 **Shiroto**
- 12:45 – **Kazue Kudo** Compressed sensing using an Ising machine (105)
13:30
- 12:45 – **Masaru Kato** Molecular + Field Dynamics Method for Vortex Dynamics in a Superconductor (124)
13:30
- 12:45 – **Tsuyoshi** Orthogonal and antiparallel vortex tubes and energy cascades in quantum turbulence (130)
13:30 **Kadokura**
- 12:45 – **Hideaki Miura** Statistical properties of Hall MHD turbulence with a high magnetic Prandtl number (132)
13:30
- 12:45 – **Alexandros** Crossover Phenomena in the 2D Random-Bond Blume-Capel Model (156)
13:30 **Vasilopoulos**
- 12:45 – **Samiran Das** Weakly relativistic effect in the formation of ion-acoustic solitary waves in dusty plasma (172)
13:30
- 12:45 – **Argyro Mainou** Scaling of the Random-Field Ising Model in Two Dimensions (190)
13:30
- 12:45 – **Yoshitaka** Phenomenological simulation on intermediate states in a type-I superconducting wire (197)
13:30 **Mizuhara**
- 12:45 – **Togo Aoki** Molecular Dynamics Simulation on Vortex Dynamics in a Dirty Superconductor (209)
13:30
- 12:45 – **Nikolaos Fytas** Universality aspects of the two-dimensional spin-1 Baxter-Wu model in a crystal field (233)
13:30
- 12:45 – **Shoichi** DFT-NEGF Study of Electron Transfer Property in Graphene Nanoribbon Double Barrier System (235)
13:30 **Sakamoto**

12:45 – 13:30	Daigo Mugita	Efficiency of equilibration with three event-based algorithms in hard disk melting (242)
12:45 – 13:30	Ranna Masheyeva	Automated Complex for Investigation of the Dusty Plasma Properties (245)
12:45 – 13:30	Ryuhei Sato	Molecular Dynamic Study of the Relationship between Li-ion Migration and Disordering of Hydride Complexes in $\text{LiCB}_9\text{H}_{10}$ (246)
12:45 – 13:30	Yoshifumi Nakamura	QCD software development and performance of Fugaku and ARM architectures (247)
12:45 – 13:30	Michail Akritidis	Geometrical clusters of the multi-replica Ising model (256)
12:45 – 13:30	Denis Gessert	The Role of Resampling in Population Annealing (262)
12:45 – 13:30	Paul Ebert	Population annealing with weighted averages: A case study for the Ising model (269)
12:45 – 13:30	Hiroataka Banno	Diffusional characteristics of Newtonian Event-Chain Monte Carlo in hard disk systems (278)
12:45 – 13:30	Dimitar Vlaykov	Convective non-locality: the impact of boundary layers on the convection dynamics in 2D stellar hydrodynamic simulations (287)
12:45 – 13:30	Sarun Phibanchon	The unstable analysis of soliton compression in Silicon photonic crystal (294)
12:45 – 13:30	Lambert Muenster	Percolation Properties of Spin Glasses (298)
12:45 – 13:30	Kaito Kitaya	Molecular dynamics study on the nano-scale β -type Stirling engine (305)
12:45 – 13:30	Mitsuyoshi Tomiya	Numerical Analysis of Electronic state of CNT/BNNT Heterojunction (307)
12:45 – 13:30	Edwin Mapasha	Li on a C-H divacancy in graphane (328)

- 12:45 – **Manoj Kumar** Critical properties of the three-dimensional
13:30 three-state random-field Potts model (357)
- 12:45 – **Janett Prehl** Structural and dynamical properties of ran-
13:30 domised mixed labyrinth fractals (400)

Monday, 02 August 13:45–15:30 GMT+1: Lecture Hall 4

Parallel Session: Astrophysics, gravitation, cosmology 1

(Chairs: Raphael Hirschi)

- 13:45 – **Sean Couch** Understanding Massive Stellar Death: Predic-
14:15 **(invited)** tive Simulation of Core-collapse Supernovae
- 14:15 – **Thomas** Multi-dimensional, fully compressible, time-
14:45 **Guillet** implicit simulations of hydrodynamical pro-
(invited) cesses in stars
- 14:45 – **Keiya** Predicting the expansion of supernova shell for
15:00 **Hirashima** high-resolution galaxy simulations using deep
learning
- 15:00 – **Koki Otaki** The formation of dark matter deficient galax-
15:15 ies through galaxy collisions
- 15:15 – **Federico** 3D hydrodynamic simulations of massive stars
15:30 **Rizzuti** with the PROMPI code

Monday, 02 August 13:45–15:30 GMT+1: Lecture Hall 3

Parallel Session: Fluid dynamics 1

(Chairs: Greg Sheard, Sijo Sebastian)

- 13:45 – **Susanne Horn** Tornado-Like Vortices in the Quasi-
14:15 **(invited)** Cyclostrophic Regime of Coriolis-Centrifugal
Convection
- 14:15 – **Sijo Sebastian** Solitary waves in a multi-ion plasma
14:30
- 14:30 – **Soichiro** Plasma Propagation via Radiation Transfer in
14:45 **Suzuki** Millimeter-wave Discharge under Subcritical
Condition

- 14:45 – **Masayuki** Coupling Simulation on Two-dimensional Ax-
15:00 **Takahashi** isymmetric Beaming Propulsion System
- 15:00 – **Tomo-Hiko** Kinetic simulation of multi-scale turbulence in-
15:15 **Watanabe** teractions and diffusion in magnetized plasma

Monday, 02 August 13:45–15:30 GMT+1: Lecture Hall 2

Parallel Session: Materials and non-science 1

(Chairs: Francesca Baletto)

- 13:45 – **Boris Kozinsky** Towards ex-machina computations of trans-
14:15 **(invited)** port and transformations in complex materials
- 14:15 – **Nobuhiko** Optical Properties of OLED Materials by
14:30 **Akino** TDDFT
- 14:30 – **James Boust** *Ab initio* theory of Nd₂Fe₁₄B-based hard mag-
14:45 netic materials
- 14:45 – **Hyeon-Deuk** Anomalous Properties of Condensed Hydro-
15:00 **Kim** gen Systems under Extreme Thermodynamic
Conditions Revealed by the Non-Empirical Ab
Initio Molecular Dynamic Simulation Method
- 15:00 – **Martin Matas** Role of the M choice in Hf(M)SiBCN
15:15 (M = Y, Ho, Ta, Mo) thin films: DFT, ab-
initio molecular dynamics and experiment

Monday, 02 August 13:45–15:30 GMT+1: Lecture Hall 1

Parallel Session: Statistical physics and complex systems 1

(Chairs: Wolfhard Janke, Yuko Okamoto)

- 13:45 – **Lev Shchur** Acceptance rate is a thermodynamic function
14:00 in local Monte Carlo algorithms
- 14:00 – **Nir Schreiber** Changeover phenomenon in randomly colored
14:15 Potts models
- 14:15 – **Tasrief** Phase diagram of the polyhedral spin models
14:30 **Surungan** on square lattice with diluted bonds

14:30 – 14:45	Thomas Prellberg	Entropy of Dense Trails on the Square Lattice
14:45 – 15:00	Evgeni Burovski	Ising model on an (interacting) SAW
15:00 – 15:15	Francesco Parisen Toldin	Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class
15:15 – 15:30	Alfred Farris	Replica exchange Wang-Landau sampling of long HP lattice protein sequences

Monday, 02 August 16:00–17:45 GMT+1: Lecture Hall 3

Parallel Session: Fluid dynamics 2

(Chairs: Greg Sheard)

16:00 – 16:30	Justin Leontini (invited)	Gas transport in human airways during high-frequency ventilation
16:30 – 16:45	Ryoji Matsumoto	Global Three-Dimensional Radiation Magneto-hydrodynamic Simulations of State Transitions in Black Hole Accretion Flows
16:45 – 17:00	Evan Rajbhandari	Optimal Design Under Uncertainty of a 3D Resistive Magneto-hydrodynamic Generator with Ion-Slip
17:00 – 17:15	Anthony Rouquier	Quasi-static magneto-hydrodynamic convection in a rotating cylinder

Monday, 02 August 16:00–17:45 GMT+1: Lecture Hall 2

Parallel Session: Materials and non-science 2

(Chairs: James Kermode)

16:00 – 16:30	Laura Ratcliff (invited)	Simulating Disordered Supramolecular Materials for Organic Electronics using Linear Scaling Density Functional Theory
16:30 – 16:45	Gus Hart	Speeding up DFT with generalized regular k-point grids

16:45 – 17:00	Jeremy Jorgensen	Quadratic algorithm for computing the band energy and estimating its error
17:00 – 17:15	Uyen Lieu	Inverse Design of Two-dimensional Self-assembly of Patchy Particles
17:15 – 17:30	Hiroshi Shinaoka	Sparse sampling approach to efficient ab initio calculations at finite temperature

Monday, 02 August 16:00–17:45 GMT+1: Lecture Hall 1

Parallel Session: Statistical physics and complex systems 2

(Chairs: Jonathan Machta, Stefan Schnabel)

16:00 – 16:15	Geet Rakala	Fully-packed anisotropic hard-core plates on a cubic lattice.
16:15 – 16:30	Dipanjan Mandal	Phase transitions in a system of hard plates on the three dimensional cubic lattice
16:30 – 16:45	Ozan Ericok	On the topology and geometry of the configuration spaces of hard disks
16:45 – 17:00	Henrik Christiansen	Phase-ordering kinetics and persistence of the two-dimensional long-range Ising model at zero temperature
17:00 – 17:15	Wolfhard Janke	Aging in the Two-Dimensional Long-Range Ising Model with Power-Law Interactions
17:15 – 17:30	Sourav Chattopadhyay	Thermally driven dynamic phase transitions in site diluted Ising ferromagnet
17:30 – 17:45	Antonio Astillero	Parallel computation in GPU of the dynamic critical exponent of the three-dimensional Heisenberg model

Monday, 02 August 18:00–19:00 GMT+1: Poster Rooms 1-3***Poster Session 1*****Tuesday, 03 August 09:00–10:30 GMT+1: Audimax*****Plenary Session 3******(Chairs: Ran Holtzman, Nikolaos Fytas)***

- 09:00 – **Andy Woods** Dynamics Of Bubble And Particle Plumes
09:45
- 09:45 – **Frank** Exploring Topological Phases of Matter on
10:30 **Pollmann** Quantum Processors

Tuesday, 03 August 11:00–12:30 GMT+1: Audimax***Plenary Session 4******(Chairs: Charo del Genio, Susanne Horn)***

- 11:00 – **Christine** Solving the quandary of the quark with High
11:45 **Davies** Performance Computing
- 11:45 – **Dave** Sub-diffusive glassy dynamics to super-
12:30 **Thirumalai** diffusion in an evolving cell colony

Tuesday, 03 August 13:45–15:30 GMT+1: Lecture Hall 3***Parallel Session: Geophysics and porous media 1******(Chairs: Steven Tobias)***

- 13:45 – **Valerio** Dynamical landscape and multistability of a
14:15 **Lucarini** climate model
(invited)
- 14:15 – **Ludivine** Rotating convection in a penny shaped cylin-
14:45 **Oruba** der: from numerical models of idealized config-
(invited) urations to tropical cyclones
- 14:45 – **Jemma** Compatible finite element methods and
15:15 **Shipton** parallel-in-time schemes for numerical weather
(invited) prediction
- 15:00 – **Marco Dentz** Energy dissipated through Haines jumps in
15:15 disordered media

Tuesday, 03 August 13:45–15:30 GMT+1: Lecture Hall 4***Parallel Session: Lattice field theory 1****(Chairs: Christine Davies, Biagio Lucini)*

- | | | |
|------------------|------------------------------------------|-------------------------------------------------------------------------------------|
| 13:45 –
14:15 | Gert Aarts
(invited) | Lattice QCD at nonzero temperature and density |
| 14:15 –
14:45 | Vera Guelpers
(invited) | Lattice QCD calculations for Muon g-2 |
| 14:45 –
15:00 | Issaku
Kanamori | General purpose lattice QCD code set
Bridge++ 2.0 for high performance computing |
| 15:00 –
15:15 | Biagio Lucini | Efficient computations of continuous action densities of states for lattice models |

Tuesday, 03 August 13:45–15:30 GMT+1: Lecture Hall 2***Parallel Session: Quantum many-body physics 1****(Chairs: Chisa Hotta, Kedar Damle)*

- | | | |
|------------------|------------------------------------------------------|----------------------------------------------------------------------------------------------|
| 13:45 –
14:15 | Naoki
Kawashima
(invited) | How to carry out the generic real-space renormalization group program |
| 14:15 –
14:45 | Philippe
Corboz
(invited) | Tensor network study of $\text{SrCu}_2(\text{BO}_3)_2$ under pressure |
| 14:45 –
15:00 | Tsuyoshi
Okubo | Tensor network approach to the magnetization of frustrated square lattice Heisenberg systems |
| 15:00 –
15:15 | Syngye Todo | Novel approaches for tensor renormalization group method - ATRG and BTRG |
| 15:15 –
15:30 | Atsuthi Iwaki | Thermal Pure Quantum Matrix Product States |

Tuesday, 03 August 13:45–15:30 GMT+1: Lecture Hall 1***Parallel Session: Soft matter and biophysics 1****(Chairs: Cristian Micheletti, Julia Yeomans)*

13:45 – 14:15	Ronojoy Adhikari (invited)	PyStokes: phoresis and Stokesian hydrodynamics in Python
14:15 – 14:30	Juliane U. Klamser	Continuous-time limit of kinetic Monte Carlo for Active-Matter systems
14:30 – 14:45	Siddhartha Mukherjee	Active turbulence, a Lévy walk away from inertial
14:45 – 15:00	Sagarika Adhikary	Collective Pattern Formation in a Binary Mixture of Self-Propelled Particles
15:00 – 15:15	Subhajit Paul	Effect of Vicsek-like Activity on the Dynamics of a Flexible Polymer
15:15 – 15:30	Leonardo Santos Lopes	Vicsek model with Malthusian Dynamics

Tuesday, 03 August 16:00–17:45 GMT+1: Lecture Hall 4***Parallel Session: Machine learning and algorithms 1****(Chairs: Ehsan Khatami)*

16:00 – 16:30	Juan Carrasquilla (invited)	Neural autoregressive toolbox for many-body physics
16:30 – 17:00	Lei Wang (invited)	Fermi Flow: Ab-initio study of fermions at finite temperature
17:00 – 17:15	Dimitrios Bachtis	Quantum field theories, Markov random fields and machine learning
17:15 – 17:30	Emanuele Guidotti	An Explainable Probabilistic Classifier for Categorical Data Inspired to Quantum Physics

Tuesday, 03 August 16:00–17:45 GMT+1: Lecture Hall 3***Parallel Session: Quantum computing 1****(Chairs: Artur Izmaylov, Stephen Jordan)*

- 16:00 – **Martin** Quantum resource estimation at scale
16:30 **Roetteler**
(invited)
- 16:30 – **Christopher** How hard will it be to simulate many-body
17:00 **White**
(invited)
- 17:00 – **Miles** Simulating Near-Term Quantum Computers
17:30 **Stoudenmire** with Approximate Tensor Network Algorithms
(invited)
- 17:30 – **Nobuyasu Ito** Simulation of quantum computer on the Fu-
17:45 gaku computer

Tuesday, 03 August 16:00–17:45 GMT+1: Lecture Hall 2***Parallel Session: Quantum many-body physics 2****(Chairs: Mario Motta, Sylvain Capponi)*

- 16:00 – **Hui Shao** Recent Development of the Stochastic Analytic
16:30 **(invited)** Continuation Method
- 16:30 – **Emanuel Gull** Nevanlinna Analytic Continuation
16:45
- 16:45 – **Andreas** Quantum Monte-Carlo simulations of highly
17:00 **Honecker** frustrated magnets in a cluster basis
- 17:00 – **Zheng Zhou** Simulating Rokhsar-Kivelson quantum critical
17:15 point in a realistic quantum Ising model
- 17:15 – **Masafumi** Numerical sign problem and the tempered Lef-
17:30 **Fukuma** schetz thimble method
- 17:30 – **Lev Barash** A new method for calculating elements of ma-
17:45 trix functions with application to the exponential of a transverse-field Ising model

Tuesday, 03 August 16:00–17:45 GMT+1: Lecture Hall 1***Parallel Session: Soft matter and biophysics 2****(Chairs: Julia Yeomans, Julia Yeomans)*

- | | | |
|---------|-----------------------------------------|------------------------------------------------------------------------------------------------------|
| 16:00 – | Cristian Micheletti
(invited) | Designing molecular knots |
| 16:30 – | Suman Majumder | Knot are Generic Stable Phases in Semiflexible Polymers |
| 16:45 – | Hiroshi Noguchi | Non-equilibrium dynamics of fluid membranes: traveling wave, Turing pattern, and membrane undulation |
| 17:00 – | Emma Wood | Mesoscopic modelling of highly ordered mesophases of board-shaped polymers |
| 17:15 – | Zoriana Danel | Dilute solution of ring and star polymers in confined geometries: theory and simulations |

Wednesday, 04 August 09:00–10:30 GMT+1: Audimax***Plenary Session 5****(Chairs: Damien Foster, Ran Holtzman)*

- | | | |
|---------|----------------------|-----------------------------------------------------------------------------------------------------------------------|
| 09:00 – | Zhijun Wang | Topology and symmetry in materials |
| 09:45 – | Claudia Draxl | Excitations in solids: theoretical approaches, benchmarks, limitations, and perspectives towards exascale performance |

Wednesday, 04 August 11:00–12:30 GMT+1: Audimax***Plenary Session 6****(Chairs: Nikolaos Fytas, Martin Weigel)*

- | | | |
|---------|-----------------------|----------------------------------------------------------------------------------------|
| 11:00 – | Andrew Saxe | Dynamics of learning in simple neural networks through the lens of statistical physics |
| 11:45 – | Prineha Narang | Computational Physics Approaches to Dynamics and Transport in Quantum Matter |

Wednesday, 04 August 12:45–13:30 GMT+1: Poster Rooms 1-3**Poster Session 2**

- 12:45 – **Minh Quyet Ha** Application of evidence theory to recommend solvent mixtures for chemical exfoliation of graphite (14)
13:30
- 12:45 – **Evgenii Brikov** The experience of using of versions of binary correlation function approximations by proposed sets of functions for purposes of the structural quasicrystal analysis and model computations by means of variational principle of a functional of the equilibrium free energy of simple liquids (25)
13:30
- 12:45 – **Yoshihiro Matsumura** Microscopic insights into dynamic disorder in the conformational changes of the protein (51)
13:30
- 12:45 – **Saturnin Yoca Enzonga** Radiative-rate calculations of erbium-like ions Lu IV, Hf V and Ta VI of interest in fusion (63)
13:30
- 12:45 – **Rico Pohle** Dynamics of spin-1 magnets from numerical simulations (67)
13:30
- 12:45 – **Ayori Mitsutake** Dynamical analysis for protein folding simulations using relaxation mode analysis (82)
13:30
- 12:45 – **Motokuni Nakajima** Molecular dynamics simulation for LIM2 domain mutants in FHL1 protein (86)
13:30
- 12:45 – **Kengo Moribayashi** Application of plasma simulation and theory to heavy ion cancer therapy (87)
13:30
- 12:45 – **Kunio Ishida** Dynamics of photoinduced entanglement generation between remote electron-phonon systems (88)
13:30
- 12:45 – **Piotr Kuterba** Molecular Dynamics simulations of ring polymers in a slit geometry of two parallel walls. (98)
13:30

12:45 – 13:30	Hiroaki Onishi	Excitation and transport of bound magnon clusters in frustrated ferromagnetic chain (100)
12:45 – 13:30	DuongNguyen Nguyen	Active learning in discovery SmFe _{12-x-y} A _x B _y magnets A, B as Mo, Zn, Co, Cu, Ti, Al, Ga (101)
12:45 – 13:30	Daisuke Suzuki	Thermodynamic folding transition of a small protein molecule (112)
12:45 – 13:30	Yoshiki Ishii	Molecular Modeling of Ionic Liquids and their Analogues via Self-Consistent Scheme with MD and DFT Methods (122)
12:45 – 13:30	Djenabou Bayo	Machine Learning the 2D Percolation Transitions (127)
12:45 – 13:30	Burak Çivitcioğlu	Machine Learning Methods applied to the 2D Ising Model (128)
12:45 – 13:30	Kazutomo Kawaguchi	Coarse-grained model for protein-nucleotide interaction (139)
12:45 – 13:30	Florian Goth	Higher Order Auxiliary Field Quantum Monte Carlo Methods (157)
12:45 – 13:30	Wei Wu	Optical and magnetic signatures of topological edge states in a dimerised donor chain (177)
12:45 – 13:30	Lisa Matsukura	Simulation study of the function of the domain swapping in the HSP90 chaperone cycle (198)
12:45 – 13:30	Vu Sinh	Deep attention model for extracting material structure-property relationships (199)
12:45 – 13:30	Kazuya Shinjo	Effect of phase string on single-hole dynamics in the two-leg Hubbard ladder (207)
12:45 – 13:30	Takuma Yamashita	Four-body variational calculation of muonic molecules in an electron cloud (212)
12:45 – 13:30	Fu-Jiun Jiang	Quantum criticality at finite temperature for two-dimensional JQ_3 models on the square and the honeycomb lattices (249)

- 12:45 – **Ryota Morikawa** Simulation study of shape change of growing lipid bilayer vesicles using DPD method (251)
13:30
- 12:45 – **Helmia Jayinunnisya** Theoretical Investigation of Complex Aspirin and Hydroxypropyl- β -cyclodextrin in Solvent Phase (260)
13:30
- 12:45 – **Takaharu Otsuka** Alpha Clustering in Atomic Nuclei obtained by First Principles calculations and Characterization of the Hoyle state Reinforced by Statistical Learning technique (264)
13:30
- 12:45 – **Hidemi Nagao** Theoretical studies on association/dissociation process of plastocyanin in photosynthesis by a coarse-grained model (271)
13:30
- 12:45 – **Kakahara Yuito** Statistics of the hopping motion approaching the glass transition in the binary hard disk systems (279)
13:30
- 12:45 – **Masaki Ottawa** Interaction between PET tracer and the specific residues around the gate of the open form of Monoamine Oxidase B (MAO-B). (281)
13:30
- 12:45 – **Takahiro Koishi** Molecular dynamics simulation for large-scale water droplet systems using the tree method (282)
13:30
- 12:45 – **Yoh Noguchi** Molecular Dynamics Simulation of the Complex of PDE5 and Evodiamine (288)
13:30
- 12:45 – **Dian Fitrasari** Theoretical Studies of Dissociation Process of Plastocyanin by PaCS-MD Simulation (295)
13:30
- 12:45 – **Lilih Slti Solihat** Theoretical Study of Dynamics and Infra-Red Spectra of Myosins (310)
13:30
- 12:45 – **Esteban Velez** Construction of a neighbour linked list on a spherical surface (315)
13:30
- 12:45 – **Taichi Kosugi** Generic circuit for a linear combination of unitary operators: Green's functions and linear-response functions (318)
13:30

- 12:45 – **Jun Takahashi** Multicriticality of the deconfined quantum
13:30 critical point (371)
- 12:45 – **Kai-Hsin Wu** \mathbb{Z}_2 topological order and first-order quantum
13:30 phase transitions in systems with combinato-
rial gauge symmetr (372)
- 12:45 – **Pranay Patil** Unconventional $U(1)$ to \mathbb{Z}_q cross-over in quan-
13:30 tum and classical q-state clock (377)

Wednesday, 04 August 13:45–15:30 GMT+1: Lecture Hall 4

Parallel Session: Novel hardware and software 1

(Chairs: Massimo Bernaschi, Federico Rizzuti)

- 13:45 – **Joshua** Performance analysis and optimization of slab
14:15 **Romero** and pencil decompositions on modern GPU
(invited) systems
- 14:15 – **Mario Spera** A new high-performance N-body code to study
14:45 (invited) merging compact-object binaries
- 14:45 – **Itay Hen** Permutation Matrix Representation Quantum
15:15 (invited) Monte Carlo
- 15:15 – **Agustin Silva** Quantum routing approach for data networks:
15:30 a solution for the congestion problem

Wednesday, 04 August 13:45–15:30 GMT+1: Lecture Hall 3

Parallel Session: Lattice field theory 2

(Chairs: Constantia Alexandrou, Gert Aarts)

- 13:45 – **Kostas Orginos** Hadronic structure from first principles
14:15 (invited)
- 14:15 – **Takashi Abe** Ab initio description of nuclear structure in
14:30 no-core Monte Carlo shell model
- 14:30 – **Takuya Okuda** Digital quantum simulation for screening and
14:45 confinement in gauge theory with a topological
term

Wednesday, 04 August 13:45–15:30 GMT+1: Lecture Hall 2***Parallel Session: Materials and non-science 3****(Chairs: Luca Ghiringhelli)*

- 13:45 – **Stefano** To mix or not to mix? Addressing tangible
14:15 **Curtarolo** problems with entropy descriptors
(invited)
- 14:15 – **Noriko Akutsu** A Density-Matrix Renormalization-Group
14:30 Study for a Two-Dimensional Lattice-Gas on
the Ih-Ice Prism Surface
- 14:30 – **Akira Kusaba** First-principles study of Mg and O co-doping
14:45 mechanism in the growth surface during
GaN(0001) and AlN(0001) metalorganic va-
por phase epitaxy
- 14:45 – **Hitoshi** Effect of water atmosphere on low friction of
15:00 **Washizu** multi-layer graphene studied by molecular dy-
namics
- 15:00 – **Renata** The Phonon Quasiparticle Approach for An-
15:15 **Wentzcovitch** harmonic Properties of Solids

Wednesday, 04 August 13:45–15:30 GMT+1: Lecture Hall 1***Parallel Session: Statistical physics and complex systems 3****(Chairs: Lev Shchur, Francesco Parisen Toldin)*

- 13:45 – **Stefan** Finding the Theta temperature of a polymer
14:15 **Schnabel** with long-range interactions
(invited)
- 14:15 – **Hidemaro** Geometric allocation approach to accelerating
14:30 **Suwa** directed worm algorithm
- 14:30 – **Yuko Okamoto** Generalized-ensemble simulations of spin sys-
14:45 tems and biomolecular systems
- 14:45 – **Peter Werner** Extremely rare ultra-fast non-equilibrium pro-
15:00 cesses close to equilibrium

15:00 – **Giuseppe** Unlocking heterogeneous node activation in
15:15 **Torrisi** Boolean networks through dynamic programming

Wednesday, 04 August 16:00–17:45 GMT+1: Lecture Hall 4

Parallel Session: Computational physics education 1

(Chairs: Amy Graves, Larry Engelhardt)

16:00 – **Tim Atherton** Physicality, Modelling and Making in Computational Physics Courses
16:30 **(invited)**

16:30 – **Titus Beu** Molecular Dynamics made accessible
17:00 **(invited)**

17:00 – **Silke Henkes** Teaching computation for large student class sizes
17:30 **(invited)**

17:30 – **Joan Adler** Peter Borchers - Computational Physics
17:45 Teacher and Leader

Wednesday, 04 August 16:00–17:45 GMT+1: Lecture Hall 3

Parallel Session: Quantum many-body physics 3

(Chairs: Sylvain Capponi, Anders Sandvik)

16:00 – **Mario Motta** Towards the solution of the many-electron
16:30 **(invited)** problem: properties of the hydrogen chain

16:30 – **Takami** Numerical simulations of spectroscopic properties
16:45 **Tohyama** in two-dimensional Mott insulator

16:45 – **Maksim** Fermi Velocity renormalization in graphene
17:00 **Ulybyshev** from non-perturbative QMC calculations

17:00 – **Yuichi Otsuka** QMC study of the chiral Heisenberg Gross-
17:15 Neveu universality class

17:15 – **Xizhi Han** Neural Quantum States and Bootstrap in Matrix
17:30 Quantum Mechanics

17:30 – **Yusuke** Purifying Deep Boltzmann Machines for Thermal
17:45 **Nomura** Quantum States

Wednesday, 04 August 16:00–17:45 GMT+1: Lecture Hall 2***Parallel Session: Soft matter and biophysics 3****(Chairs: Juliane U. Klamser, Julia Yeomans)*

- | | | |
|------------------|----------------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| 16:00 –
16:15 | Matthew
Wilson | Comparison of Benchmark HP Lattice Proteins on Simple-Cubic and Face-Centered Cubic Lattices Using Replica-Exchange Wang-Landau Sampling |
| 16:15 –
16:30 | Shivani Gupta | Destabilization potential of phenolics on A β Fibril: Mechanistic insights from Molecular Dynamics Simulation |
| 16:30 –
16:45 | Hisashi
Okumura | Nonequilibrium molecular dynamics simulation to reveal a role of water molecules in laser-induced disruption of amyloid fibrils |
| 16:45 –
17:00 | Rudo Roemer | Flexibility and mobility of SARS-CoV-2-related protein structures |
| 17:00 –
17:15 | Duy Tran | Atomic mechanism of the complete association of intrinsically disordered peptide to protein |
| 17:15 –
17:30 | Elena Zubova | Modelling of the A-B transition in a short DNA molecule |
| 17:30 –
17:45 | Shaweta Garg | Single-channel dynamically disordered exclusion process with Langmuir kinetics |

Wednesday, 04 August 16:00–17:45 GMT+1: Lecture Hall 1***Parallel Session: Statistical physics and complex systems 4****(Chairs: Youjin Deng, Evgeni Burovski)*

- | | | |
|------------------|----------------------------|--------------------------------------------------------------------------------------|
| 16:00 –
16:15 | Gopika
Krishnan | Dynamics of transient cages in a 2D super-cooled liquid |
| 16:15 –
16:30 | Takayuki
Narumi | An agent-based modeling and simulation for the first stage of honeycomb construction |
| 16:30 –
16:45 | Dmitriy
Antonov | Mean-field interactions in evolutionary spatial games |

- 16:45 – **Huixin Zhang** Detecting early warning signals in higher-order
17:00 structures
- 17:00 – **Yannick Feld** Large-deviations of the SIR model
17:15
- 17:15 – **Toru Ohira** Pursuit and Evasion: Singles to Groups
17:30

Wednesday, 04 August 18:00–19:00 GMT+1: Poster Rooms 1-3
Poster Session 2

Thursday, 05 August 09:00–10:45 GMT+1: Lecture Hall 3

Parallel Session: Machine learning and algorithms 2

(Chairs: Gert Aarts)

- 09:00 – **Motoyuki** Self-Learning Hybrid Monte Carlo: A First-
09:15 **Shiga** Principles Method
- 09:15 – **Dominic Rose** Reinforcement learning for rare trajectory
09:30 sampling
- 09:30 – **Yusuke Tomita** Machine-learning study using improved corre-
09:45 lation configuration and application to the 2D
quantum XY model.
- 09:45 – **Saikat** Unsupervised Identification of Dynamical
10:00 **Chakraborty** Crossovers in Entangled Polymer Melt from
Conformational Fluctuations
- 10:00 – **Nobuyuki** Encoding solid-state electronic structures in
10:15 **Yoshioka** neural-network quantum states
- 10:15 – **Estelle Inack** Variational Neural Annealing
10:45 **(invited)**

Thursday, 05 August 09:00–10:45 GMT+1: Lecture Hall 4

Parallel Session: Materials and non-science 4

(Chairs: Luca Ghiringhelli)

- 09:00 – **Ryosuke** High temperature superconductivity in com-
09:15 **Akashi** pressed sulfur hydrides from first principles

- 09:15 – **Yuma Hizume** Effect of spin fluctuations on superconductivity in V and Nb: A first-principles study
09:30
- 09:30 – **Raja Sen** Analyzing the electron-phonon scattering rates and energy transfer rates of photo-excited carriers in semiconductors
09:45
- 09:45 – **Qinlin Wang** Unified time evolution technique for the electronic structure calculation
10:00
- 10:00 – **Fumihito Imoto** Order- N Orbital-Free Density-Functional Calculations with Machine Learning of Functional Derivatives for Semiconductors and Metals
10:15

Thursday, 05 August 09:00–10:45 GMT+1: Lecture Hall 1

Parallel Session: Soft matter and biophysics 4

(Chairs: Rudo Roemer, Julia Yeomans)

- 09:00 – **Jaehyeok Jin** Toward high-fidelity many-body mesoscopic models of fluids from bottom-up coarse-graining
09:30
(invited)
- 09:30 – **Takumi Sato** Effect of polymer chemical design on self-assembly of polymer-tethered nanoparticles in nanotubes
09:45
- 09:45 – **Kang Kim** Bridging the gap between molecular dynamics and hydrodynamics in nanoscale Brownian motions
10:00
- 10:00 – **Ten-Ming Wu** Optical Kerr Effect Spectra of Supercooled Water at Ambient Pressure: Contributions of Low-Density and High-Density Liquids
10:15
- 10:15 – **Youssef Ouldhnini** Atomistic insights into the structure and elasticity of densified 45S5 Bioactive Glass
10:30
- 10:30 – **Hayato Shiba** Effect of long-wavelength fluctuations on slow relaxation in a 2D glass-forming liquid
10:45

Thursday, 05 August 11:00–12:30 GMT+1: Audimax***Plenary Session 7******(Chairs: Susanne Horn, Martin Weigel)***

- 11:00 – **Ludovic** Equilibrium phase transitions and their univer-
11:45 **Berthier** sality class in models for glass-forming materi-
 als
- 11:45 – **Olga Shishkina** Scalings and structures in natural thermal con-
12:30 vection

Thursday, 05 August 13:30–15:30 GMT+1: Audimax***Plenary Session 8******(Chairs: Abhishek Kumar, Damien Foster)***

- 13:30 – **Steven** Lattice QCD Results from the Fermilab Lat-
14:15 **Gottlieb** tice and MILC Collaborations
- 14:15 – **Sergio Boixo** Beyond-classical quantum computing
15:00

List of Contributions

Burak Çivitcioglu	Machine Learning Methods applied to the 2D Ising Model
Gert Aarts	Lattice QCD at nonzero temperature and density
Takashi Abe	Ab initio description of nuclear structure in no-core Monte Carlo shell model
Ronojoy Adhikari	PyStokes: phoresis and Stokesian hydrodynamics in Python
Sagarika Adhikary	Collective Pattern Formation in a Binary Mixture of Self-Propelled Particles
Joan Adler	Peter Borchers - Computational Physics Teacher and Leader
Ryosuke Akashi	High temperature superconductivity in compressed sulfur hydrides from first principles
Nobuhiko Akino	Optical Properties of OLED Materials by TDDFT
Michail Akritidis	Geometrical clusters of the multi-replica Ising model
Noriko Akutsu	A Density-Matrix Renormalization-Group Study for a Two-Dimensional Lattice-Gas on the Ih-Ice Prism Surface
Dmitriy Antonov	Mean-field interactions in evolutionary spatial games
Togo Aoki	Molecular Dynamics Simulation on Vortex Dynamics in a Dirty Superconductor
Antonio Astillero	Parallel computation in GPU of the dynamic critical exponent of the three-dimensional Heisenberg model

Tim Atherton	Physicality, Modelling and Making in Computational Physics Courses
Dimitrios Bachtis	Quantum field theories, Markov random fields and machine learning
Hiroataka Banno	Diffusional characteristics of Newtonian Event-Chain Monte Carlo in hard disk systems
Lev Barash	A new method for calculating elements of matrix functions with application to the exponential of a transverse-field Ising model
Dwight Barkley	Universality and rare events in the subcritical route to turbulence
Djenabou Bayo	Machine Learning the 2D Percolation Transitions
Ludovic Berthier	Equilibrium phase transitions and their universality class in models for glass-forming materials
Titus Beu	Molecular Dynamics made accessible
Sergio Boixo	Beyond-classical quantum computing
James Boust	<i>Ab initio</i> theory of Nd ₂ Fe ₁₄ B-based hard magnetic materials
Evgenii Brikov	The experience of using of versions of binary correlation function approximations by proposed sets of functions for purposes of the structural quasicrystal analysis and model computations by means of variational principle of a functional of the equilibrium free energy of simple liquids
Evgeni Burovski	Ising model on an (interacting) SAW
Juan Carrasquilla	Neural autoregressive toolbox for many-body physics

Saikat Chakraborty	Unsupervised Identification of Dynamical Crossovers in Entangled Polymer Melt from Conformational Fluctuations
Sourav Chattopadhyay	Thermally driven dynamic phase transitions in site diluted Ising ferromagnet
Henrik Christiansen	Phase-ordering kinetics and persistence of the two-dimensional long-range Ising model at zero temperature
Philippe Corboz	Tensor network study of $\text{SrCu}_2(\text{BO}_3)_2$ under pressure
Sean Couch	Understanding Massive Stellar Death: Predictive Simulation of Core-collapse Supernovae
Gabor Csanyi	Machine learned force fields: status and challenges
Stefano Curtarolo	To mix or not to mix? Addressing tangible problems with entropy descriptors
Zoriana Danel	Dilute solution of ring and star polymers in confined geometries: theory and simulations
Samiran Das	Weakly relativistic effect in the formation of ion-acoustic solitary waves in dusty plasma
Christine Davies	Solving the quandary of the quark with High Performance Computing
Marco Dentz	Energy dissipated through Haines jumps in disordered media
Claudia Draxl	Excitations in solids: theoretical approaches, benchmarks, limitations, and perspectives towards exascale performance
Dao Duc Anh	Elucidating atomic-scale phenomena with transmission electron microscopy: a study of gold nanocontact

Paul Ebert	Population annealing with weighted averages: A case study for the Ising model
Ozan Ericok	On the topology and geometry of the configuration spaces of hard disks
Alfred Farris	Replica exchange Wang-Landau sampling of long HP lattice protein sequences
Yannick Feld	Large-deviations of the SIR model
Dian Fitrasari	Theoretical Studies of Dissociation Process of Plastocyanin by PaCS-MD Simulation
Masafumi Fukuma	Numerical sign problem and the tempered Lefschetz thimble method
Nikolaos Fytas	Universality aspects of the two-dimensional spin-1 Baxter-Wu model in a crystal field
Shaweta Garg	Single-channel dynamically disordered exclusion process with Langmuir kinetics
Denis Gessert	The Role of Resampling in Population Annealing
Florian Goth	Higher Order Auxiliary Field Quantum Monte Carlo Methods
Steven Gottlieb	Lattice QCD Results from the Fermilab Lattice and MILC Collaborations
Vera Guelpers	Lattice QCD calculations for Muon $g-2$
Emanuele Guidotti	An Explainable Probabilistic Classifier for Categorical Data Inspired to Quantum Physics
Thomas Guillet	Multi-dimensional, fully compressible, time-implicit simulations of hydrodynamical processes in stars
Emanuel Gull	Nevanlinna Analytic Continuation
Shivani Gupta	Destabilization potential of phenolics on $A\beta$ Fibril: Mechanistic insights from Molecular Dynamics Simulation

Minh Quyet Ha	Application of evidence theory to recommend solvent mixtures for chemical exfoliation of graphite
Xizhi Han	Neural Quantum States and Bootstrap in Matrix Quantum Mechanics
Gus Hart	Speeding up DFT with generalized regular k-point grids
Itay Hen	Permutation Matrix Representation Quantum Monte Carlo
Silke Henkes	Teaching computation for large student class sizes
Keiya Hirashima	Predicting the expansion of supernova shell for high-resolution galaxy simulations using deep learning
Yuma Hizume	Effect of spin fluctuations on superconductivity in V and Nb: A first-principles study
Andreas Honecker	Quantum Monte-Carlo simulations of highly frustrated magnets in a cluster basis
Susanne Horn	Tornado-Like Vortices in the Quasi-Cyclostrophic Regime of Coriolis-Centrifugal Convection
Fumihiko Imoto	Order- N Orbital-Free Density-Functional Calculations with Machine Learning of Functional Derivatives for Semiconductors and Metals
Estelle Inack	Variational Neural Annealing
Kunio Ishida	Dynamics of photoinduced entanglement generation between remote electron-phonon systems
Yoshiki Ishii	Molecular Modeling of Ionic Liquids and their Analogues via Self-Consistent Scheme with MD and DFT Methods

Nobuyasu Ito	Simulation of quantum computer on the Fugaku computer
Atsuthi Iwaki	Thermal Pure Quantum Matrix Product States
Wolfhard Janke	Aging in the Two-Dimensional Long-Range Ising Model with Power-Law Interactions
Helmia Jayyinnisya	Theoretical Investigation of Complex Aspirin and Hydroxypropyl- β -cyclodextrin in Solvent Phase
Fu-Jiun Jiang	Quantum criticality at finite temperature for two-dimensional JQ_3 models on the square and the honeycomb lattices
Jaehyeok Jin	Toward high-fidelity many-body mesoscopic models of fluids from bottom-up coarse-graining
Jeremy Jorgensen	Quadratic algorithm for computing the band energy and estimating its error
Tsuyoshi Kadokura	Orthogonal and antiparallel vortex tubes and energy cascades in quantum turbulence
Issaku Kanamori	General purpose lattice QCD code set Bridge++ 2.0 for high performance computing
Masaru Kato	Molecular + Field Dynamics Method for Vortex Dynamics in a Superconductor
Kazutomo Kawaguchi	Coarse-grained model for protein-nucleotide interaction
Naoki Kawashima	How to carry out the generic real-space renormalization group program
Kang Kim	Bridging the gap between molecular dynamics and hydrodynamics in nanoscale Brownian motions

Hyeon-Deuk Kim	Anomalous Properties of Condensed Hydrogen Systems under Extreme Thermodynamic Conditions Revealed by the Non-Empirical Ab Initio Molecular Dynamic Simulation Method
Kaito Kitaya	Molecular dynamics study on the nano-scale β -type Stirling engine
Juliane U. Klamser	Continuous-time limit of kinetic Monte Carlo for Active-Matter systems
Takahiro Koishi	Molecular dynamics simulation for large-scale water droplet systems using the tree method
Taichi Kosugi	Generic circuit for a linear combination of unitary operators: Green's functions and linear-response functions
Boris Kozinsky	Towards ex-machina computations of transport and transformations in complex materials
Gopika Krishnan	Dynamics of transient cages in a 2D supercooled liquid
Kazue Kudo	Compressed sensing using an Ising machine
Manoj Kumar	Critical properties of the three-dimensional three-state random-field Potts model
Akira Kusaba	First-principles study of Mg and O co-doping mechanism in the growth surface during GaN(0001) and AlN(0001) metalorganic vapor phase epitaxy
Piotr Kuterba	Molecular Dynamics simulations of ring polymers in a slit geometry of two parallel walls.
Justin Leontini	Gas transport in human airways during high-frequency ventilation

Uyen Lieu	Inverse Design of Two-dimensional Self-assembly of Patchy Particles
Valerio Lucarini	Dynamical landscape and multistability of a climate model
Biagio Lucini	Efficient computations of continuous action densities of states for lattice models
Argyro Mainou	Scaling of the Random-Field Ising Model in Two Dimensions
Suman Majumder	Knot are Generic Stable Phases in Semiflexible Polymers
Dipanjan Mandal	Phase transitions in a system of hard plates on the three dimensional cubic lattice
Edwin Mapasha	Li on a C-H divacancy in graphane
Ranna Masheyeva	Automated Complex for Investigation of the Dusty Plasma Properties
Martin Matas	Role of the M choice in Hf(M)SiBCN (M = Y, Ho, Ta, Mo) thin films: DFT, ab-initio molecular dynamics and experiment
Lisa Matsukura	Simulation study of the function of the domain swapping in the HSP90 chaperone cycle
Ryoji Matsumoto	Global Three-Dimensional Radiation Magneto-hydrodynamic Simulations of State Transitions in Black Hole Accretion Flows
Yoshihiro Matsumura	Microscopic insights into dynamic disorder in the conformational changes of the protein
Cristian Micheletti	Designing molecular knots
Ayori Mitsutake	Dynamical analysis for protein folding simulations using relaxation mode analysis

Hideaki Miura	Statistical properties of Hall MHD turbulence with a high magnetic Prandtl number
Yoshitaka Mizuhara	Phenomenological simulation on intermediate states in a type-I superconducting wire
Kengo Moribayashi	Application of plasma simulation and theory to heavy ion cancer therapy
Ryota Morikawa	Simulation study of shape change of growing lipid bilayer vesicles using DPD method
Mario Motta	Towards the solution of the many-electron problem: properties of the hydrogen chain
Lambert Muenster	Percolation Properties of Spin Glasses
Daigo Mugita	Efficiency of equilibration with three event-based algorithms in hard disk melting
Siddhartha Mukherjee	Active turbulence, a Lévy walk away from inertial
Hidemi Nagao	Theoretical studies on association/dissociation process of plastocyanin in photosynthesis by a coarse-grained model
Motokuni Nakajima	Molecular dynamics simulation for LIM2 domain mutants in FHL1 protein
Yoshifumi Nakamura	QCD software development and performance of Fugaku and ARM architectures
Prineha Narang	Computational Physics Approaches to Dynamics and Transport in Quantum Matter
Takayuki Narumi	An agent-based modeling and simulation for the first stage of honeycomb construction

DuongNguyen Nguyen	Active learning in discovery SmFe _{12-x-y} A _x B _y magnets A, B as Mo, Zn, Co, Cu, Ti, Al, Ga
Hiroshi Noguchi	Non-equilibrium dynamics of fluid membranes: traveling wave, Turing pattern, and membrane undulation
Yoh Noguchi	Molecular Dynamics Simulation of the Complex of PDE5 and Evodiamine
Yusuke Nomura	Purifying Deep Boltzmann Machines for Thermal Quantum States
Arsha Noushad	Study of velocity auto-correlation function of a confined Brownian particle
Toru Ohira	Pursuit and Evasion: Singles to Groups
Yuko Okamoto	Generalized-ensemble simulations of spin systems and biomolecular systems
Tsuyoshi Okubo	Tensor network approach to the magnetization of frustrated square lattice Heisenberg systems
Takuya Okuda	Digital quantum simulation for screening and confinement in gauge theory with a topological term
Hisashi Okumura	Nonequilibrium molecular dynamics simulation to reveal a role of water molecules in laser-induced disruption of amyloid fibrils
Hiroaki Onishi	Excitation and transport of bound magnon clusters in frustrated ferromagnetic chain
Kostas Orginos	Hadronic structure from first principles
Ludivine Oruba	Rotating convection in a penny shaped cylinder: from numerical models of idealized configurations to tropical cyclones
Koki Otaki	The formation of dark matter deficient galaxies through galaxy collisions

Yuichi Otsuka	QMC study of the chiral Heisenberg Gross-Neveu universality class
Takaharu Otsuka	Alpha Clustering in Atomic Nuclei obtained by First Principles calculations and Characterization of the Hoyle state Reinforced by Statistical Learning technique
Masaki Ottawa	Interaction between PET tracer and the specific residues around the gate of the open form of Monoamine Oxidase B (MAO-B).
Youssef Ouldhnini	Atomistic insights into the structure and elasticity of densified 45S5 Bioactive Glass
Francesco Parisen Toldin	Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class
Pranay Patil	Unconventional $U(1)$ to Z_q cross-over in quantum and classical q-state clock
Subhajit Paul	Effect of Vicsek-like Activity on the Dynamics of a Flexible Polymer
Sarun Phibanchon	The unstable analysis of soliton compression in Silicon photonic crystal
Annalisa Pillepich	Universe(s) in a box
Rico Pohle	Dynamics of spin-1 magnets from numerical simulations
Frank Pollmann	Exploring Topological Phases of Matter on Quantum Processors
Janett Prehl	Structural and dynamical properties of randomised mixed labyrinth fractals
Thomas Prellberg	Entropy of Dense Trails on the Square Lattice
Evan Rajbhandari	Optimal Design Under Uncertainty of a 3D Resistive Magnetohydrodynamic Generator with Ion-Slip

Geet Rakala	Fully-packed anisotropic hard-core plates on a cubic lattice.
Laura Ratcliff	Simulating Disordered Supramolecular Materials for Organic Electronics using Linear Scaling Density Functional Theory
Federico Rizzuti	3D hydrodynamic simulations of massive stars with the PROMPI code
Rudo Roemer	Flexibility and mobility of SARS-CoV-2-related protein structures
Martin Roetteler	Quantum resource estimation at scale
Joshua Romero	Performance analysis and optimization of slab and pencil decompositions on modern GPU systems
Dominic Rose	Reinforcement learning for rare trajectory sampling
Anthony Rouquier	Quasi-static magneto-hydrodynamic convection in a rotating cylinder
Shoichi Sakamoto	DFT-NEGF Study of Electron Transfer Property in Graphene Nanoribbon Double Barrier System
Leonardo Santos Lopes	Vicsek model with Malthusian Dynamics
Takumi Sato	Effect of polymer chemical design on self-assembly of polymer-tethered nanoparticles in nanotubes
Ryuhei Sato	Molecular Dynamic Study of the Relationship between Li-ion Migration and Disorder of Hydride Complexes in $\text{LiCB}_9\text{H}_{10}$
Andrew Saxe	Dynamics of learning in simple neural networks through the lens of statistical physics
Stefan Schnabel	Finding the Theta temperature of a polymer with long-range interactions

Nir Schreiber	Changeover phenomenon in randomly colored Potts models
Sijo Sebastian	Solitary waves in a multi-ion plasma
Raja Sen	Analyzing the electron-phonon scattering rates and energy transfer rates of photo-excited carriers in semiconductors
Erik Shalenov	The capture cross sections at the electron collisions with hydrogen atom in non Maxwellian dense semiclassical plasma
Hui Shao	Recent Development of the Stochastic Analytic Continuation Method
Lev Shchur	Acceptance rate is a thermodynamic function in local Monte Carlo algorithms
Hayato Shiba	Effect of long-wavelength fluctuations on slow relaxation in a 2D glass-forming liquid
Motoyuki Shiga	Self-Learning Hybrid Monte Carlo: A First-Principles Method
Hiroshi Shinaoka	Sparse sampling approach to efficient ab initio calculations at finite temperature
Kazuya Shinjo	Effect of phase string on single-hole dynamics in the two-leg Hubbard ladder
Jemma Shipton	Compatible finite element methods and parallel-in-time schemes for numerical weather prediction
Takashi Shiroto	A charge-momentum-energy-conserving alternative numerical method for the Vlasov–Maxwell system
Olga Shishkina	Scalings and structures in natural thermal convection
Agustin Silva	Quantum routing approach for data networks: a solution for the congestion problem

Vu Sinh	Deep attention model for extracting material structure-property relationships
Lilih SIti Solihat	Theoretical Study of Dynamics and Infra-Red Spectra of Myosins
Mario Spera	A new high-performance N-body code to study merging compact-object binaries
Miles Stoudenmire	Simulating Near-Term Quantum Computers with Approximate Tensor Network Algorithms
Tasrief Surungan	Phase diagram of the polyhedral spin models on square lattice with diluted bonds
Hidemaro Suwa	Geometric allocation approach to accelerating directed worm algorithm
Soichiro Suzuki	Plasma Propagation via Radiation Transfer in Millimeter-wave Discharge under Subcritical Condition
Daisuke Suzuki	Thermodynamic folding transition of a small protein molecule
Yusuke Suzumura	Molecular-Dynamics Simulation of Liquid Sulfur by Artificial Neural Network Potentials
Masayuki Takahashi	Coupling Simulation on Two-dimensional Axisymmetric Beaming Propulsion System
Jun Takahashi	Multicriticality of the deconfined quantum critical point
Mykhailo Tatochenko	Confinement effects on packings of disco-rectangles in slit pores
Dave Thirumalai	Sub-diffusive glassy dynamics to super-diffusion in an evolving cell colony
Synge Todo	Novel approaches for tensor renormalization group method - ATRG and BTRG

Takami Tohyama	Numerical simulations of spectroscopic properties in two-dimensional Mott insulator
Yusuke Tomita	Machine-learning study using improved correlation configuration and application to the 2D quantum XY model.
Mitsuyoshi Tomiya	Numerical Analysis of Electronic state of CNT/BNNT Heterojunction
Giuseppe Torrisi	Unlocking heterogeneous node activation in Boolean networks through dynamic programming
Duy Tran	Atomic mechanism of the complete association of intrinsically disordered peptide to protein
Maksim Ulybyshev	Fermi Velocity renormalization in graphene from non-perturbative QMC calculations
Alexandros Vasilopoulos	Crossover Phenomena in the 2D Random-Bond Blume-Capel Model
Esteban Velez	Construction of a neighbour linked list on a spherical surface
Dimitar Vlaykov	Convective non-locality: the impact of boundary layers on the convection dynamics in 2D stellar hydrodynamic simulations
Qinlin Wang	Unified time evolution technique for the electronic structure calculation
Lei Wang	Fermi Flow: Ab-initio study of fermions at finite temperature
Zhijun Wang	Topology and symmetry in materials
Hitoshi Washizu	Effect of water atmosphere on low friction of multi-layer graphene studied by molecular dynamics

Tomo-Hiko Watanabe	Kinetic simulation of multi-scale turbulence interactions and diffusion in magnetized plasma
Renata Wentzcovitch	The Phonon Quasiparticle Approach for Anharmonic Properties of Solids
Peter Werner	Extremely rare ultra-fast non-equilibrium processes close to equilibrium
Christopher White	How hard will it be to simulate many-body quantum dynamics?
Matthew Wilson	Comparison of Benchmark HP Lattice Proteins on Simple-Cubic and Face-Centered Cubic Lattices Using Replica-Exchange Wang-Landau Sampling
Emma Wood	Mesoscopic modelling of highly ordered mesophases of board-shaped polymers
Andy Woods	Dynamics Of Bubble And Particle Plumes
Ten-Ming Wu	Optical Kerr Effect Spectra of Supercooled Water at Ambient Pressure: Contributions of Low-Density and High-Density Liquids
Wei Wu	Optical and magnetic signatures of topological edge states in a dimerised donor chain
Kai-Hsin Wu	\mathbb{Z}_2 topological order and first-order quantum phase transitions in systems with combinatorial gauge symmetry
Takuma Yamashita	Four-body variational calculation of muonic molecules in an electron cloud
Saturnin Yoca Enzonga	Radiative-rate calculations of erbium-like ions Lu IV, Hf V and Ta VI of interest in fusion
Nobuyuki Yoshioka	Encoding solid-state electronic structures in neural-network quantum states

Kakihara Yuito	Statistics of the hopping motion approaching the glass transition in the binary hard disk systems
Huixin Zhang	Detecting early warning signals in higher-order structures
Zheng Zhou	Simulating Rokhsar-Kivelson quantum critical point in a realistic quantum Ising model
Elena Zubova	Modelling of the A-B transition in a short DNA molecule

Plenary Sessions

P1.1 – Universe(s) in a box**Annalisa Pillepich**

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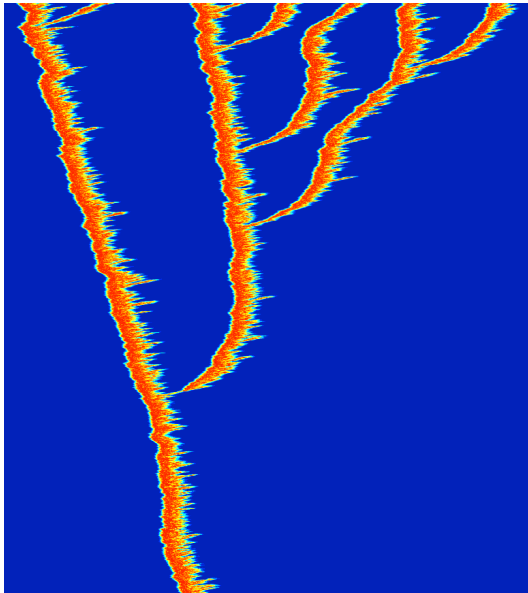
Contemporary cosmological hydrodynamical simulations are reaching unprecedented levels of sophistication and complexity. Numerical programs like IllustrisTNG (www.tng-project.org) are allowing us to model realistic populations of galaxies across an ever-wider range of masses, environments, evolutionary stages, and cosmic epochs. There we resolve and model the structural details of thousands of galaxies together with the large-scale cosmic web by solving the equations of gravity and magnetohydrodynamics and by including prescriptions for star formation, stellar evolution, metal enrichment, cooling and heating of the gas, galactic outflows and feedback from the supermassive black holes – all within the boundary conditions of our standard cosmological paradigm. In this talk, I will give an overview of our efforts to generate and effectively exploit the IllustrisTNG simulations, describe our strategies for dissemination, discuss what is explicitly and empirically solved in gravity+magnetohydrodynamics simulations for galaxy formation in a cosmological context, and what is required and what it means to “successfully” reproduce populations of galaxies that resemble the real ones. I will then showcase some of the astrophysical insights that these models are allowing us to uncover and quantify.

P2.1 – Universality and rare events in the subcritical route to turbulence

Dwight Barkley

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Recent years have witnessed a profound change in our understanding of the subcritical route to turbulence. In stark contrast to the classical Hopf-Landau picture where turbulence arises through an increase in the temporal complexity of fluid motion, the route to turbulence in subcritical shear flows occurs via spatio-temporal intermittency and falls in the class of non-equilibrium statistical phase transitions known as directed percolation. I will review important results in the field focusing on the spatio-temporal nature of the problem and how universality manifests itself. I will then describe recent work aimed at capturing the rare events dictating critical phenomena in turbulence flows.



Puff splitting in a theoretical model of transitional turbulence. Elementary patches of turbulence (red puffs) produce daughter patches via the process of puff splitting, ultimately leading to a percolation transition to sustained turbulence.

P2.2 – Machine learned force fields: status and challenges

Gabor Csanyi

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I will make the somewhat bold claim that over the past 10 years, a new computational task has been defined and solved for extended material systems: this is the analytic fitting of the Born-Oppenheimer potential energy surface as a function of nuclear coordinates under the assumption of medium-range interactions, out to 5-10 Å. The resulting potentials are reactive, many-body, reach accuracies of a few meV/atom, with costs that are on the order of 1-10 ms/atom. Important challenges remain: treatment of long range interactions in a nontrivial way, e.g. environment dependent multipoles, charge transfer, magnetism. Time is ripe for a “shakedown” of the details among various approaches (neural networks, kernels, polynomials), and more standard protocols of putting together the training data. Tradeoffs between system- (or even project-) specific fits vs. more general potentials will be ongoing. I am particularly concerned with the amount physics and chemistry that we impute into these approximations, and that they can be used to help “extrapolate” correctly into regions of configuration space far from those in the data set.

P3.1 – Dynamics Of Bubble And Particle Plumes

Andrew Woods

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In this presentation, I will describe a series of new experiments and supporting theoretical models to describe some of the dynamics of bubble and particle plumes, with application in a range of environmental and geophysical situations, including deep sea mining, volcanic eruption columns and gas plumes from subsea methane releases, as well as the role of bubble plumes in destratification of reservoirs.

The experiments and models will explore the mixing and transport of ambient fluid by these flows, and the importance of the slip speed of the bubbles or parti-

cles and of ambient currents on the motion of the flows.

P3.2 – Exploring Topological Phases of Matter on Quantum Processors

Frank Pollmann

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The interplay of quantum fluctuations and correlations in quantum many-body systems can lead to exciting phenomena: celebrated examples are the fractional quantum Hall effect and topological quantum spin liquids. Most strikingly, these systems support particle-like excitations that carry fractional quantum numbers and cannot be characterized by conventional symmetry breaking. Instead they are described by topological invariants, forming a new kind of topological order. Exploring the emergent physics in such systems is extremely difficult because of the exponential growth of complexity with system size.

Universal quantum computers are potentially an ideal setting for simulating such quantum many-body phenomena. Here we discuss two applications to the study of topologically ordered systems: First, we demonstrate how to represent ground states of Hamiltonians using shallow quantum circuits and observe a quantum phase transition between different symmetry-protected topological phases on a quantum device. For this we measure a non-local order parameter as topological invariant to characterize the phases. The simulation that we perform is easily scalable and is a practical demonstration of the utility of near-term quantum computers for the study of quantum phases of matter. Second, we show how to prepare the ground state of the toric code Hamiltonian, a paradigmatic example of a topological spin liquid, using an efficient quantum circuit on a superconducting quantum processor. We measure the topological entanglement entropy and simulate anyon interferometry to extract the braiding statistics of the emergent fractionalized excitations. Furthermore, we investigate key aspects of the surface code, including logical state injection and the decay of the non-local order parameter. These results demonstrate the potential for quantum processors to provide key insights into topological quantum matter and quantum error correction.

P4.1 – Solving the quandary of the quark with High Performance Computing

Christine Davies

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Christine Davies will discuss how the theory of the strong interaction, Quantum Chromodynamics (QCD), can be solved numerically using a method called lattice QCD. This is computationally very demanding and a key 'Grand Challenge' for High Performance Computing. It offers the possibility of accurate results from first principles for the properties of the bound states of quarks known as hadrons. Comparison with experimental results can then lead to stringent tests of our understanding of fundamental particle physics as well as searches for discrepancies that can point to new interactions at a deeper level. She will describe some of these calculations, the results that have been obtained and prospects for the future.

P4.2 – Sub-diffusive glassy dynamics to super-diffusion in an evolving cell colony

Dave Thirumalai

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Collective migration dominates many phenomena, from cell movement in living systems to abiotic self-propelling particles. By focusing on the early stages of tumor evolution, I hope to enunciate scenarios for collective movements in cell dynamics and highlight their implications in understanding similar behavior in abiotic soft glassy materials. Using simulations and theory I will show that tumor cells at the periphery move with higher velocity perpendicular to the tumor boundary, while motion of interior cells is slower and isotropic. The mean square displacement, of cells exhibits glassy behavior at times comparable to the cell cycle time, while exhibiting super-diffusive behavior at longer times. A sketch of the theory for these characteristics motion will be given. In the process we establish the universality of super-diffusion in a class of non-equilibrium systems. Our findings for the collective migration, which also suggests that tumor evolution occurs in a polarized manner, are in quantitative agreement with in vitro experiments.

Although set in the context of tumor invasion the findings should also hold in describing collective motion in growing cells and in active systems where creation and annihilation of particles play a role.

- [1] Abdul N Malmi-Kakkada, Xin Li, Himadri S. Samanta, Sumit Sinha, and D. Thirumalai, Phys. Rev. X 8: 021025 (2018).
- [2] H. S. Samanta and D. Thirumalai, Phys. Rev. E 99: 032401 (2019).
- [3] Abdul N Malmi-Kakkada, Xin Li, Sumit Sinha, and D. Thirumalai, biorxiv.org doi: <https://doi.org/10.1101/683250>

P5.1 – Topology and symmetry in materials

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Topological states and materials have been attracted many interests these years. Symmetry plays an important role to classify different topological states and properties. Many interesting materials have been predicted to be topological via first-principles calculations. First, I will review some typical topological states and symmetry protections. Then, I will talk about topological quantum chemistry (TQC) and band representations, which can be applied to diagnose topological materials. Lastly, I will introduce an open-source code - IRVSP - to compute the irreducible presentations of the electronic states in the DFT calculations. The application of band representations of TQC can be widely used in materials calculations.

P5.2 – Excitations in solids: theoretical approaches, benchmarks, limitations, and perspectives towards exascale performance

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Many-body perturbation theory is the state-of-the-art approach to describe charged and neutral excitations in crystalline materials. Likewise, time-dependent density functional theory (TDDFT) enables the study of excitations in molecules and solids either via time propagation or by computing their response to external perturbations in the linear regime. Such high-level approaches are, however, compute-intensive, often hampering either full convergence with respect to all computational parameters and/or their application to complex systems. This is in particular so, if highly accurate basis sets are employed. In this talk, we will discuss current limitations and present various algorithms to overcome some of the bottlenecks. An example concerns an iterative solver for diagonalizing huge sparse matrices that appear when treating low-dimensional systems in codes that apply periodic boundary conditions. Making use of this method, allows us to reach microHartree precision for the energies of atoms and molecules [1]. Building on this, we are extending this approach towards the time domain in TDDFT [2]. Moreover, we make use of a recently developed algorithm for substantially speeding up the solution of the Bethe-Salpeter equation [3] and demonstrate the successful implementation in **exciting** [4] by applications to complex systems. Finally, we will discuss how to bring high-level approaches to exascale as envisioned in the European Centre of Excellence NOMAD [5]. All this allows us to provide benchmark data and assess data quality by unsupervised learning [6].

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- [2] R. Rodrigues Pela and C. Draxl, *Electronic Structure* (2021); in print.
- [3] F. Henneke, L. Lin, C. Vorwerk, C. Draxl, R. Klein, and C. Yang, *Commun. Appl. Math. Comp. Sci.* 15, 89 (2020).
- [4] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, *J. Phys: Condens. Matter (Topical Review)* 26, 363202 (2014).
- [5] NoMAD Center of Excellence, <https://nomad-coe.eu>. NOMAD CoE receives funding from the European Union's Horizon 2020 research and innovation program under the grant agreement N° 951786.
- [6] M. Kuban, S. Rigamonti, and C. Draxl, preprint.

P6.1 – Dynamics of learning in simple neural networks through the lens of statistical physics

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Deep neural networks have transformed the practice of machine learning, yielding state-of-the-art performance in a wide range of tasks. For the most part, these empirical successes have outpaced our theoretical efforts to understand deep networks, which largely remain black boxes into which we have little insight. Approaches from statistical physics have shed light on the learning behavior of deep networks by considering a variety of simple solvable synthetic models. I will describe several lines of work in this vein, which explore how prior knowledge can shape subsequent learning in deep networks, yielding simple models of continual learning, curriculum learning, and transfer learning. These examples show how the learning algorithm, dataset structure, initialization, and network architecture interact to yield rich generalization dynamics. Finally I will describe how these same models, taken as hypotheses about learning dynamics in the brain, make testable predictions that can help establish or refute links between artificial deep networks and biological learning.

P6.2 – Computational Physics Approaches to Dynamics and Transport in Quantum Matter

Prineha Narang

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Quantum systems host spectacular nonequilibrium effects and unconventional transport phenomena, but many of these remain challenging to predict and consequently, technologically unexplored. My group's research, therefore, focuses on how quantum systems behave, particularly away from equilibrium, and how we can harness these effects. By creating predictive theoretical and computational approaches to study dynamics, decoherence and correlations in matter, our work will enable technologies that are inherently more powerful than their classical counterparts ranging from scalable quantum information processing to ultra-high effi-

ciency optoelectronic and energy conversion systems. Capturing these phenomena poses unique computational and theoretical challenges. In fact, the simultaneous contribution of processes that occur on many time and length-scales have eluded state-of-the-art computational physics and model Hamiltonian approaches alike, necessitating a new computational and theoretical lens. In this context, I will focus on our work in computational approaches to describe excited-states in quantum matter, including electron-electron and electron-phonon interactions, and predicting states introduced by various external drives. Light-mediated manipulation of quantum matter is particularly attractive, as it enables control at fundamental timescales and access to novel nonequilibrium states. This approach brings quantum optics, ultrafast dynamics, and condensed matter together to create unexpected and useful properties, including surprisingly long coherence times and propagation lengths. Simultaneously it necessitates new methods, as I will convey, and show examples of how our computational approaches enable new quantum probes of quantum matter. Next, I will discuss our methods in spatially-resolved non-equilibrium transport in quantum matter. By introducing GPU-accelerated computational large-scale transport frameworks that retain microscopic scattering, we are overcoming long-standing barriers in the field and taking transport to the exascale. Finally, I will share our vision for the future towards describing correlated matter, crossing the finite-extended system divide, and leveraging the power of both classical high-performance exascale computing and quantum computation paradigms in predicting new physical phenomena.

P7.1 – Equilibrium phase transitions and their universality class in models for glass-forming materials

Ludovic Berthier

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Computer simulations give unique insights into the microscopic behavior of amorphous materials. It became recently possible to generate equilibrium configurations of deeply supercooled liquids using a simple swap Monte Carlo algorithm for a broad variety of model glass-formers. This novel computational tool, which provides an equilibration speedup of more than 10 orders of magnitude, has allowed the exploration of thermodynamic properties and putative equilibrium phase transitions underlying the formation of glasses with unprecedented accuracy. I

will summarize these recent findings and provide a broad picture about the thermodynamic phase diagram describing the physics of liquids undergoing a glass transition.

P7.2 – Scalings and structures in natural thermal convection

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Turbulent thermal convection which occurs due to the temperature differences imposed at the boundaries of the domain is omnipresent in nature in technology. In this talk, we will consider three classical setups, namely, Rayleigh-Benard convection, vertical convection, and horizontal convection. For these systems, we will discuss the scaling relations of the global heat and momentum transport, the proper boundary layer equations, and the large-scale flow organization. We will show that in some cases, the scaling of the global heat transport and the temperature profiles can be predicted by solving the proper boundary-layer equations that include turbulent fluctuations and correct boundary conditions. Further, we will discuss the global flow structures in turbulent Rayleigh-Benard convection in slender and wide containers. We will see that the self-organized turbulent flow takes the form of several convection rolls on top of each other if the container is slender or in a form of convection rolls that are attached to each other in a horizontal direction if the container is wide. The shape of these rolls strongly influences the global heat transport in the system. Finally, we will explain the reasons why the size of the self-organized rolls is quite restricted.

P8.1 – Lattice QCD Results from the Fermilab Lattice and MILC Collaborations

Steven Gottlieb

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Quantum Chromodynamics (QCD) is the theory of nature's strong force responsible for binding quarks and anti-quarks into mesons and baryons, and protons and neutrons into atomic nuclei. Lattice QCD is a nonperturbative treatment of the theory that allows us to determine fundamental parameters of the Standard Model such as the quark masses and the Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix that describes decays due to the weak force. Precise calculations of Standard Model processes are essential for finding evidence for new physics in so-called Precision Frontier experiments. This talk will concentrate on recent results from the Fermilab Lattice and MILC collaborations, and may include performance information on new GPUs from NVIDIA and AMD.

P8.2 – Beyond-classical quantum computing

Sergio Boixo

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I'll review what is the current state of quantum computing with superconducting qubits. I'll explain several experiments from Google's Quantum AI group, including an article published in Nature in 2019 in which we carried out a computational task on an experimental quantum processor vastly outperforming current supercomputers. I will conclude with various projections on the expected advances in quantum computing in the next ten years.

Parallel Sessions

Astrophysics, gravitation, cosmology

AS1.1 (invited) – Understanding Massive Stellar Death: Predictive Simulation of Core-collapse Supernovae

Sean Couch

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Core-collapse supernovae are the luminous explosions that herald the death of massive stars. While core-collapse supernovae are observed on a daily basis in nature, the details of the mechanism that reverses stellar collapse and drives these explosions remain unclear. I will discuss the recent developments in the study of the supernova mechanism and progress toward a predictive theory of massive stellar death. In particular, I will discuss the important role turbulence is playing in the supernova mechanism and our efforts to develop more realistic initial conditions for supernova simulations with fully 3D massive stellar evolution calculations. Such realistic 3D initial conditions turn out to be favorable for successful explosions, in large part because they result in stronger turbulence behind the stalled supernova shock. I will also discuss the role of ubiquitous rotation and magnetic fields in altering the character of supernova explosions. As the realism of our supernova simulations improves, it is crucial to make connection with observational and experimental data. I will conclude with a discussion of the impacts of improved physics on observational features of supernovae, including on the gravitational wave emission from these stellar explosions.

AS1.3 (invited) – Multi-dimensional, fully compressible, time-implicit simulations of hydrodynamical processes in stars

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A. Le Saux¹, J. Pratt², T. Goffrey³**

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The life and evolution of stars are ruled by the dynamics of their structure and interior. Understanding stellar flows requires modelling complex dynamical processes, including the interplay of compressible turbulent convection, thermal diffusion, and magnetic fields. These mechanisms are to this day very challenging to simulate realistically, because they cover a wide span of time and length scales.

MUSIC is a time-implicit code for magnetohydrodynamics designed to study convection in stars in 2D and 3D. The code solves the fully-compressible equations of hydrodynamics and ideal MHD using an implicit LES approach, accounting for thermal conductivity and realistic opacities and equations of state. The implicit solver relies on a so-called Jacobian-Free-Newton-Krylov method to advance the simulation state forward in time with low memory requirements.

In this talk, I will present the MUSIC code and how it addresses some of the challenges of simulations of stellar interiors. I will also discuss some recent applications of MUSIC to the study of the penetration of turbulent convective flows into stably stratified layers, as well as to the properties of internal waves in stably stratified regions of stars.

AS1.5 – Predicting the expansion of supernova shell for high-resolution galaxy simulations using deep learning

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The formation and evolution of galaxies is a nonlinear phenomenon involving a complex combination of gravity, hydrodynamics, star formation, and supernova explosions, and has been studied using numerical simulations. In galaxy formation simulations, three types of particles are used: particles that interact only with gravity (dark matter particles and stellar particles) and particles that interact with hydrodynamics (Smoothed Particle Hydrodynamics particles; SPH particles). A typical galaxy contains about 100 billion stars. However, even the highest resolution simulations represent the galaxy with about 100 million particles, and the typical mass resolution is limited to about 1000 solar masses. This is because the current algorithms are limited in the degree of parallelism at which sufficient parallel efficiency can be achieved.

We are developing a high-resolution simulation of galaxy formation using more than 100 billion particles of stars, dark matter, and gas, and resolving them down to individual stars. We aim to increase the number of particles by a factor of 1000 and achieve the first ever direct comparison between simulations and observations. However, the increase in resolution requires the reproduction of small-scale phenomena (such as supernova explosions) for galaxies. Although the number of particles affected by a supernova explosion is only a small fraction of the total number of particles in the galaxy, these particles increase the number of operations required for time integration of all other particles by a factor of several hundred, making it impossible to run the simulation in a realistic time frame. This is the subject of this research and future high-resolution galaxy formation simulations, and I am developing algorithms for this part of the research. In order to reduce the number of computations, I aimed to separate the regions according to the length of the timescale. For this purpose, I developed a method to predict the distribution of gas particles whose timescale will be shortened in the future by using deep learning[1].

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AS1.6 – The formation of dark matter deficient galaxies through galaxy collisions

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In the standard galaxy formation model, cold dark matter (CDM) drives the hierarchical structure formation. However, recently it is suggested that the satellite galaxy NGC1052-DF2, a member of the elliptical galaxy NGC1052 group, has a very little dark matter component compared to the theoretical predictions[1]. 27 dark matter deficient galaxies (DMDGs) have been discovered, but it is difficult to explain these formation process in the CDM model.

We investigate the formation process through dark matter sub-halo (DMSH) collisions using an analytic model and three-dimensional numerical simulations. As a result, we derive critical collision-velocities for the bifurcation sequence of the formation of dark-matter-dominated galaxies and dark-matter-deficient galaxies. In the case of low-speed collisions, a merger of the two sub-halos produces dark-matter-dominated galaxies. However, the two dark matter halos slip through each other, but the gaseous mediums collide for the middle-speed encounter. The enhancement of the gas density induces a burst of star formation, and then a dwarf galaxy without a dark matter halo forms at the interface of the sub-halo collision. In the case of high-speed collisions, no galaxies form because shock-breakout of the gaseous medium ejects most of the gas from the system.

The result of N -body/SPH simulations of the head-on collision between DMSHs shows that the critical collision-velocity to form the dark-matter-deficient galaxies is 50-200 km s⁻¹ for the total mass of 10⁹ M_⊙. We will present our model and numerical experiments for various galaxy masses and collision speed in detail.

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AS1.7 – 3D hydrodynamic simulations of massive stars with the PROMPI code

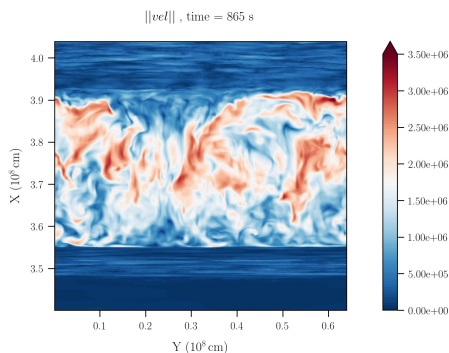
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When simulating the evolution of massive stars, many three-dimensional processes should be taken into account, e.g. convection, rotation, magnetic activity. However, it is not computationally possible to simulate the entire lifetime of a star while also following its fluid motion explicitly. 3D hydrodynamic simulations are used to study a short time range (minutes or hours).

PROMPI is a multi-dimensional hydrodynamics code developed specifically for simulations of stellar interiors. It was developed to perform on parallel computing platforms through domain decomposition. PROMPI has been successfully used over the years to simulate different burning stages of massive stars (carbon and oxygen in particular). In this talk, I will present PROMPI simulations of the neon burning phase in a massive star, focusing on the interplay between turbulence and nuclear reactions as well as discussing the impact that different resolutions and boosting factors of the nuclear rates have on the results.



Vertical cross-section of the velocity magnitude during a PROMPI simulation.
Colour map in cm/s.

Computational physics education

ED1.1 (invited) – Physicality, Modelling and Making in Computational Physics Courses**Tim Atherton**

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Computation is deeply interwoven with virtually every aspect of contemporary Physics research practice including design of experiments, creation of theory, simulations as well as collection, analysis and visualization of data. In contrast, computational activities in Physics classrooms have tended to focus on coding, problem-solving and simulation. To bridge this gap between pedagogy and practice, we have developed a series of making activities whereby students create physical artifacts from low-cost materials, collect quantitative data describing their motion, build models to predict their behavior and reconcile experiment and theory. Results from our first two trials in a group and project-based Computational Physics class will be presented, showing how this approach enables students to engage in disciplinary practice. An epistemic model of how computation produces knowledge is used both to create the design and analyze student work. Design and implementation advice for instructors interested in adopting similar techniques will be provided.

ED1.3 (invited) – Molecular Dynamics made accessible**Titus-Adrian Beu**

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Molecular Dynamics (MD) has matured into one of the most powerful and reliable computational tools in present-day research, not only having the ability to

explain in detail known behavior, but also to anticipate uncharted phenomenology. In spite of its wide-spread use, due the growing complexity of the models and methodologies amassed in state-of-the-art MD simulators, amplified by complications associated with preparation and post-analysis of the runs, employing and, moreover, developing MD software becomes increasingly intricate and risks to remain the apaanage of “initiates”.

In this contribution, we present a concept and a software repository for introducing MD at graduate/post-graduate level, based on unifying data structures and programming techniques in Python and C/C++. The main aim is to enable acquisition of specific coding abilities in parallel with operation skills of an established MD code.

Essentially, Python scripting is used for building the complex initial structures and post-analyzing the MD trajectories. The developed MD modules rely on the numerical and graphical libraries already published [1, 2]. On the other hand, C/C++ is used to build a suite of simple MD simulators mimicking the functionalities of an established MD code, in a sequence of gradually growing complexity, along with the introduction of new theoretical elements.

Fundamental aspects such as molecular models, force fields, time propagation, thermodynamic reservoirs, electrostatics in periodic systems, and acceleration techniques are given particular emphasis. The results of the simulation test runs are consistently compared with output from established MD codes to clarify the relevance of the various modeling aspects.

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ED1.5 (invited) – Teaching computation for large student class sizes

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Teaching computation to large groups of students is a challenge that is made harder by the COVID pandemic which necessitates that we also teach remotely. I will present our 2nd year course 'Mathematical Programming' in the School of Mathematics at the University of Bristol as a case study. Our course, which

is running for the 2nd time this year, has a headcount of 240, and is delivered through a combination of remote and in person teaching. This course is for computing novices and uses Python, together with Jupyter notebooks, to introduce the fundamentals of programming, algorithms and data analysis, and we deliver it through a combination of recorded lectures and small-group tutorials (both online and in person). Our teaching materials are lectures and tutorials in the form of Jupyter notebooks that are hosted on our LMS site and also on a JupyterHub server hosted by EDINA, a University of Edinburgh startup. We assess the course through a combination of autograded homeworks using the Nbgrader Jupyter plugin and hand-graded assessments. A significant fraction of the course consists of group work centred around a mini research project on a set of physical and mathematical topics, including planetary motion, random walks, and the Vicsek model of flocking.

ED1.7 – Peter Borchers - Computational Physics Teacher and Leader

Joan Adler

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Early computational physics courses that have been described in the archival literature include Peter Bocherd's [1] class taught since about 1984 in laboratory format. I have been teaching such a course since 1988 with a manuscript published only in 2014 [2]. Although developed independently these have loose similarities, such as hands-on experience in class. Peter used color graphical displays with BBC micros and had an orientation towards numerical analysis and programming. There are many, many more courses, both similar to the above as late undergraduate courses and more integrated or specialised. A comparison between several will be given in this presentation.

The Computational Physics community and the present author in particular owe the late Peter Borchers much appreciation for his leadership and encouragement of Computational Physics European and International Computational Physics collaboration in both C20 of IUPAP and the EPS-CPG group.

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FD1.1 (invited) – Tornado-Like Vortices in the Quasi-Cyclostrophic Regime of Coriolis-Centrifugal Convection

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Tornadoes are the most intense atmospheric vortices. They have been observed on all of Earth's continents (except for Antarctica) as well as on Mars. The most dangerous and most damaging tornadoes develop within the mesocyclone updrafts of supercell thunderstorms. However, the properties determining whether a mesocyclone becomes tornadic or remains non-tornadic are still largely unknown. In fact, less than 25% of all mesocyclones bear tornadoes.

Turbulent Coriolis-centrifugal convection (C^3) in a cylindrical domain constitutes an idealised model of tornadic storms, where the rotating cylinder represents the mesocyclone of a supercell thunderstorm [1]. Using a suite of direct numerical simulations, we show that the C^3 system can produce a similar richness of tornado morphologies as found in nature. We analysed the influence of centrifugal buoyancy and the bottom boundary conditions on the formation of tornado-like vortices (TLVs). TLVs are self-consistently generated, provided the flow is within the quasi-cyclostrophic regime, in which the dominant dynamical balance is between pressure gradient and centrifugal buoyancy forces. Our studies bring forth insights into natural supercell thunderstorm systems and present a possible explanation for why seemingly similar mesocyclones may or may not spawn tornadoes. It is not just the absolute dimensional value of the vertical angular velocity, but also the mesocyclone geometry and the temperature difference that requires consideration.

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FD1.3 – Solitary waves in a multi-ion plasma

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We have investigated the existence of solitary waves in a multi-ion plasma composed of lighter ions, electrons of both cometary and solar origin and heavier pair ions. Both the electrons are modelled by kappa distribution function. The reductive perturbation theory is used to derive the KdV equation. We have plotted the amplitude and width of the solitary waves with different physical parameters relevant to comet Halley. From the plots, it is seen that different physical parameters significantly affect the solitary waves.

FD1.4 – Plasma Propagation via Radiation Transfer in Millimeter-wave Discharge under Subcritical Condition

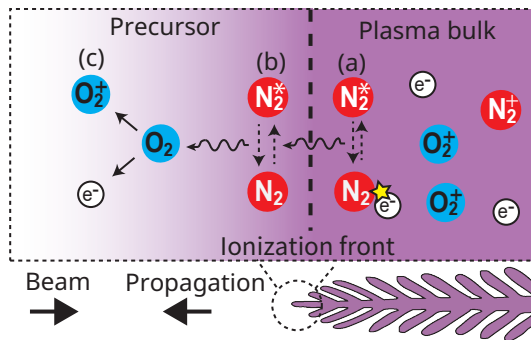
**Soichiro Suzuki, Chinami Kato, Masayuki Takahashi,
and Naofumi Ohnishi**

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Experiments and numerical calculations have been carried out to study discharge phenomena caused by a high-power millimeter-wave irradiation [1, 2, 3, 4, 5]. A millimeter-wave discharge has been discussed to apply beaming rocket propulsion “microwave rocket” that can dramatically reduce a transportation cost to outer space[2]. A discharge physics induced by the millimeter-wave can be classified into overcritical and subcritical conditions depending on the electric field intensity. Under the subcritical conditions, the discharge is caused by a neutral gas heating, not by an electron impact ionization[4]. In the subcritical millimeter-wave discharge experiments, a comb-shaped plasma has been observed, while propagating toward the beam source at a supersonic speed[1, 2]. However, numerical calculations performed by Takahashi *et al.* have only reproduced the structure and not

the propagation velocity. Furthermore, their model coupled with electromagnetic wave propagation, plasma fluid model, and compressible fluid model can not reproduce discharge if the incident electric-field intensity is below 1.4 MV/m [4]. Because the microwave rocket uses a millimeter-wave beam with the electric-field intensity in this range and a thrust performance depends on the propagation velocity, we developed a one-dimensional millimeter-wave discharge model that introduced detailed chemical reactions and radiation transport into Takahashi's model to reproduce discharge phenomena. We used zero-dimensional plasma chemical kinetics solver ZDPlasKin to evaluate the reaction rate, heating rate, and density of neutral particles. The present numerical model reproduced the discharge process in a lower electric-field intensity (above 0.2 MV/m), which had a quantitative agreement with the past experiments [1]. The radiative de-excitation of nitrogen in the plasma bulk region emits extreme ultraviolet (EUV) (process a in the figure below). The photoexcitation of nitrogen occurs if nitrogen absorbs EUV (process b). The photoionization of oxygen occurs in the precursor region if oxygen absorbs EUV and generates precursor electron (process c). The ionization front propagates toward the beam source because the precursor electron and diffusion electron heat and expand neutral gasses and the reduced electric-field increases.

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Schematics of a millimeter-wave plasma propagation mechanism. The right bottom figure is a comb-shaped discharge structure observed in Oda and Bogatov experiments. (a) The EUV emission by the radiative de-excitation. (b) The photoexcitation of nitrogen. (c) The photoionization of oxygen.

FD1.5 – Coupling Simulation on Two-dimensional Axisymmetric Beaming Propulsion System

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A beaming rocket system [1, 2] was proposed to reduce a launch cost from the earth to outer space by removing a fuel equipped on the vehicle. However, a beam divergence, plasma screening, and flight instability can disturb a beam-riding flight. In this study, an in-tube acceleration concept was applied to a microwave rocket system to avoid these three issues and improve a thrust performance. A two-dimensional axisymmetric simulator was developed by coupling a plasma transport with an electromagnetic wave propagation and neutral gas dynamics. A coupling simulator captured a beam propagation process in tube, which induced a strong focal point behind a thruster. A strong shock wave was generated from the focal point because an electron energy was transferred to a neutral gas energy. The thrust performance was finally evaluated by integrating surface pressure on the vehicle, which was higher than conventional beaming techniques.

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FD1.6 – Kinetic simulation of multi-scale turbulence interactions and diffusion in magnetized plasma

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Kinetic turbulence developing in multi-dimensional phase space plays a key role in transport of particle, momentum, and energy in fusion, space, and astrophysical plasmas with a mean magnetic field. Separation of characteristic scales in charged particle motions in non-uniform and non-stationary electromagnetic field induces a variety of instabilities and turbulence in the magnetized plasma. Gyrokinetic plasma simulations performed on a peta-scale (or beyond) parallel super computers enable us to attack a long-standing issue in research of plasma turbulence where microscale and mesoscale turbulences interact to each other over the scale-separation [1, 2].

Recently, we have carried out multi-scale plasma turbulence simulations, where the microscale turbulence driven by an electron temperature gradient stabilizes the mesoscale turbulence driven by cross-field drift motions of electrons trapped in an external magnetic field, leading to a coarse-grained turbulent diffusion. The anomalous electron heat transport driven by the mesoscale turbulence is thus reduced as a result of the cross-scale interaction of turbulence. The giant killing found in the magnetized plasma has a strong impact in fusion plasma confinement, as it implies that a steep electron temperature gradient benefits the heat confinement.

We have also been working on a theoretical modeling of the coarse-grained diffusion caused by the microscale turbulence and extension to cases with hydrogen isotopes for studying burning plasma physics.

Acknowledgments

This work was partially supported by MEXT as “Program for Promoting Researches on the Supercomputer Fugaku” (Exploration of burning plasma confinement physics).

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FD2.1 (invited) – Gas transport in human airways during high-frequency ventilation

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Medical ventilation has one aim - to provide oxygen and remove waste gases for a patient that cannot breathe for themselves. This simple aim can become very complex to achieve when a patient has damaged or delicate lungs, as the pressure and tissue distension induced by the ventilator can do further damage. One technique to avoid this that is used reasonably successfully in neonates is low-volume, or high frequency, ventilation (HFV). Here, only small volumes of gas are moved in and out of the airway each "breath", but it is done much faster than normal breathing with rates upwards of 10Hz. The volume moved each cycle is much less than the dead space of the airway - so how does oxygen get in and waste gases out? A lack of understanding of the gas transport mechanisms means HFV application is a hit-and-miss affair, and it has not found success in adults. Despite at least six mechanisms being proposed for the gas transport, there is little understanding on how these mechanisms can be exploited to optimise the ventilation process.

We have conducted direct numerical simulations of model geometries of various generations of the human airway (see figure 1), where a generation is defined as the division of one airway vessel into two at a bifurcating joint. Our results show that the reciprocating flow during ventilation generates longitudinal Dean vortices leaving the bifurcation, caused by a centrifugal instability of the flow passing through the curved path of the bifurcation. These Dean vortices are conditional, appearing in different locations at different times during the ventilation cycle. This conditional appearance leads to a strong streaming flow that appears adequate to provide ventilation. Further, these conditional Dean vortices lead to conditional turbulence. The appearance of turbulence is linked to the instantaneous flow rate - this is markedly different to model reciprocating flows in straight tubes where turbulence is linked to acceleration.

We propose that an understanding of these underlying vortices can lead to the development of ventilation strategies that deliberately strengthen them, and therefore improve ventilation for a wide cohort of patients.

FD2.3 – Global Three-Dimensional Radiation Magneto-hydrodynamic Simulations of State Transitions in Black Hole Accretion Flows

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We have developed a three-dimensional radiation magnetohydrodynamic code CANS+R to study the time variabilities of accretion flows around a gravitating object. The code adopts HLLD Riemann solver and fifth-order MP5 scheme to compute cell boundary values [1]. For radiation fields, moment equations of radiative transfer are solved. The initial state is a hot accretion flow formed by mass accretion from a dense, weakly magnetized torus. When the density of the accretion flow exceeds the upper limit for radiatively inefficient, hot accretion flow, the flow shrinks in the vertical direction by radiative cooling. The vertical contraction of the disk stops when the enhanced azimuthal magnetic field supports the disk. Hot accretion flow near the black hole and outer cool disk co-exist during this state. When the density of the disk increases further, the outer cool disk becomes optically thick for Thomson scattering. We found that radial oscillation is excited in the transition region when the radiation pressure becomes dominant [2]. This oscillation appears when the luminosity is around 1% of the Eddington luminosity. Numerical results can explain rapid time variabilities, quasi-periodic oscillations (QPOs), and spectral changes observed during hard-to-soft state transitions in black hole X-ray binaries and in active galactic nuclei.

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FD2.4 – Optimal Design Under Uncertainty of a 3D Resistive Magnetohydrodynamic Generator with Ion-Slip

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Magnetohydrodynamics (MHD) is the study of an electrically-conductive medium flowing through a magnetic field. By artificially generating a plasma and applying a magnetic field, an electric field and current arise, which can be extracted as a power source. Understanding this generation of power consists of solving stationary Maxwell's equations, coupled with the generalized Ohm's law. Coupling these two results in a non-linear system of partial differential equations. It is established that including the oft-neglected ion-slip parameter has a non-negligible impact on power generation. By allowing the hall parameter, and ion-slip parameter to be random variables, optimal design of the generator under uncertainty is considered. The control parameters utilized for this optimal design include the tapering length of the magnetic field at inlet/outlet of the generator, the channel-width to electrode-height ratio, the velocity profile, as well as the conductivity profile. Choice of the optimal parameter set will reflect the optimal expected power generation of the channel.

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FD2.5 – Quasi-static magneto-hydrodynamic convection in a rotating cylinder

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We present a numerical study on the topic of magnetoconvection in a cylinder under the quasi-static magneto-hydrodynamic approximation using a spectral-element solver. The aim of this work is to obtain a better understanding of the convection process in planetary cores, in particular the formation of anticyclonic polar inside the tangent cylinder. The secular variation of the Earth's magnetic field points to the existence of anticyclonic polar vortices in the Earth's core [2]. We consider the motion of an electrically conducting fluid in a closed cylinder with electrically insulated boundaries. An external homogeneous magnetic field \mathbf{B}_0 is imposed across the cylinder length. In this work is used the quasi-static approximation, such that the agglomerated magnetic field is indistinguishable from \mathbf{B}_0 . We also work under the Boussinesq approximation.

The governing equations are solved using the spectral-element code Nektar++. In this the computational domain is divided into elements where the variables are projected within a polynomial basis within each element. We will be conducting a linear analysis of the system in order to find steady states. Then branch tracing, using a Newton-Raphson solver, will be used to study the phase space and find potential bifurcation points as well as obtain nonlinear solutions of the problem in function of the magnetic field and convection strength and how they compare to experimental data. Another question we seek to answer is the importance of the wall-modes for strong magnetic fields.

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Geophysics and porous media

GP1.1 (invited) – Dynamical landscape and multistability of a climate model

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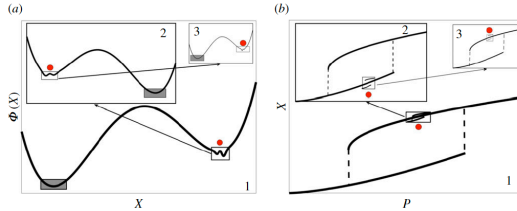
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We investigate the multistability properties of a hierarchy of climate models. We first show how to construct the Melancholia states, chaotic saddles included in the basin boundaries of the competing attractors [1], Drawing from the theory of quasi-potentials, we infer the relative likelihood of the identified metastable climate states when stochastic perturbations are included. We investigate the most likely transition trajectories as well as the expected transition times between them [2, 3]. In the case of the most complex model considered here, we complement classical numerical modelling with techniques from data science, and specifically manifold learning, in order to characterize the data landscape within a fully agnostic and unsupervised framework. We discover that that the topography of the dynamical landscape of the model becomes considerably more complex, as stronger macroscopic currents appear in the phase space, implying that the system is farther away from equilibrium conditions. We attribute this to the enhanced entropy production due to the presence of an active hydrological cycle. In a model configuration, our analysis reveals, apart from the well known warm and snowball Earth states, a third intermediate stable state. Finally, we propose conceptual framework for understanding the multiscale nature of the multistability of the climate system [4].

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Multiscale nature of the Earth's multistability: Quasi-potential $\Phi(X)$. (b) Corresponding hysteresis loops as a function of a parameter P .

GP1.3 (invited) – Rotating convection in a penny shaped cylinder: from numerical models of idealized configurations to tropical cyclones

Ludivine ORUBA

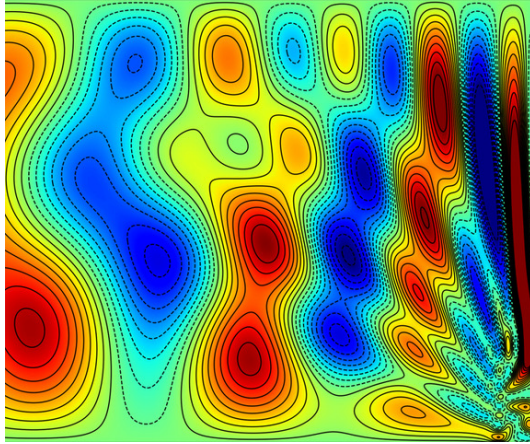
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We investigate atmospheric vortices using idealized mathematical models and direct numerical simulations. We establish connection both with geophysical observations and asymptotic developments. We consider rotating convection in an elongated cylindrical domain, which intends to model the troposphere. We examine the conditions under which the main vortex develops an eye at its core, which is reminiscent of that seen in a tropical cyclone; that is, a region where the poloidal flow reverses and the angular momentum is low. We first focus on the stationary flow and highlight the key role played by the viscous bottom boundary layer in the eye formation. We show that the eye results from a non-linear instability. In a mixed numerical/asymptotic approach, we then study the linear inertial wave activity which develops in the time dependent problem. These inertial waves are indeed reminiscent of oscillations which have been observed near the eye of actual tropical cyclones.

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GP1.5 (invited) – Compatible finite element methods and parallel-in-time schemes for numerical weather prediction

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I will describe Gusto, a dynamical core toolkit built on top of the Firedrake finite element library; present recent results from a range of test cases and outline our plans for future code development.

Gusto uses compatible finite element methods, a form of mixed finite element methods (meaning that different finite element spaces are used for different fields)

that allow the exact representation of the standard vector calculus identities $\text{div-curl}=0$ and $\text{curl-grad}=0$. The popularity of these methods for numerical weather prediction is due to the flexibility to run on non-orthogonal grid, thus avoiding the communication bottleneck at the poles, while retaining the necessary convergence and wave propagation properties required for accuracy.

Although the flexibility of the compatible finite element spatial discretisation improves the parallel scalability of the model it does not solve the parallel scalability problem inherent in spatial domain decomposition: we need to find a way to perform parallel calculations in the time domain. Exponential integrators, approximated by a near optimal rational expansion, offer a way to take large timesteps and form the basis for parallel timestepping schemes based on wave averaging. I will describe the progress we have made towards implementing these schemes in Gusto.

GP1.6 – Energy dissipated through Haines jumps in disordered media

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We study energy dissipation in quasistatic two-fluid displacements in disordered media, analytically, numerically and experimentally. We establish the energy balance for a recent model that successfully reproduces collective capillary instabilities (Haines jumps), hysteresis and memory of pressure-saturation trajectories [1]. Strikingly, we discover that energy dissipation can emerge from cooperative behavior mediated by lateral correlations between individually reversible capillary displacements. This contrasts the widely-used compartment (Everett) model which rely on the existence of a basic noninteracting hysteretic unit. We show how to compute the energy dissipated in individual Haines jumps between two consecutive equilibrium configurations (i) needs not to be proportional to the corresponding increase in saturation (avalanche size), (ii) spans many orders of magnitude, and (iii) can greatly exceed the work invested in driving the system between these two configurations. We study parametrically how the dissipation depends on system properties such as the microstructural heterogeneity and gravity (Bond number). Finally, we expose the connection between dissipation and

large-scale imbibition-drainage hysteresis. We show that the accumulated dissipation along a cyclic pressure-saturation trajectory coincides with the area enclosed by the cycle.

[1] Holtzman, R. et al., Nature Communications Physics, 3:222 (2020).

Novel hardware and software

HS1.1 (invited) – Performance analysis and optimization of slab and pencil decompositions on modern GPU systems

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Within various computational physics domains, one-dimensional (slab) and two-dimensional (pencil) spatial decompositions are commonly used to distribute data among parallel processes. For example, spectral computational fluid dynamics solvers often use such decompositions to compute three-dimensional fast fourier transforms (FFT) to compute derivatives. In these solvers, the distributed slab/pencil data must be transposed in order to collect complete input FFT data that is local to each process. It is well known that the communication of data between processes during these transposes accounts for the majority of the computational cost, especially on GPU systems where local FFT and packing operations can be accelerated. As such, it is imperative that users select appropriate decomposition layouts and communication libraries to maximize network performance; however, making an optimal selection is not a simple task. The task is made even more difficult on modern GPU systems due to complex multi-socket, multi-GPU node topologies with fast on-node peer-to-peer connections (e.g., NVIDIA NVLink) and lower bandwidth internode network connections.

In this talk, we will present an analysis of slab and pencil decomposition performance on several large GPU installations. We compare the performance across systems with very different node topologies and available network bandwidth to show how these characteristics impact decomposition selection for best performance. Additionally, we will compare the performance of several communication

libraries available on these systems, such as OpenMPI, SpectrumMPI, and the NVIDIA Collective Communication Library (NCCL).

HS1.3 (invited) – A new high-performance N-body code to study merging compact-object binaries

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On September 14, 2015, the two detectors of the Laser Interferometer Gravitational-wave Observatory (LIGO) reported the first detection of gravitational waves, a signal generated from the coalescence of two stellar-mass black holes. The discovery represented the beginning of an entirely new way to investigate the Universe. From the theoretical point of view, the formation and evolution of compact-object binaries are still very uncertain. One of the main issues is that most stars form in dense stellar environments, and numerical simulations of merging compact-object binaries in such crowded stellar systems are very challenging. In this work, I review the main numerical bottlenecks that hamper our knowledge on merging binaries in dense environments and I present a new GPU-accelerated N-body code, called ISTEDDAS, that can overcome most of the obstacles. Finally, I will present some potential applications of the ISTEDDAS code for the astrophysical interpretation of present and forthcoming gravitational-wave detections.

HS1.5 (invited) – Permutation Matrix Representation Quantum Monte Carlo

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We present a quantum Monte Carlo algorithm for the simulation of general quantum and classical many-body models within a single unifying framework. The

algorithm builds on a power series expansion of the quantum partition function in its off-diagonal terms and is both parameter-free and Trotter error-free. In our approach, the quantum dimension consists of products of elements of a permutation group. As such, it allows for the study of a very wide variety of models on an equal footing. To demonstrate the utility of our technique, we use it to clarify the emergence of the sign problem in the simulations of non-stoquastic physical models. We showcase the flexibility of our algorithm and the advantages it offers over existing state-of-the-art by simulating transverse-field Ising model Hamiltonians and comparing the performance of our technique against that of the stochastic series expansion algorithm. We also study a transverse-field Ising model augmented with randomly chosen two-body transverse-field interactions.

[1] J. Stat. Mech. (2020) 073105

HS1.7 – Quantum routing approach for data networks: a solution for the congestion problem

**Agustin Silva, Omar Gustavo Zabaleta,
Constancio Miguel Arizmendi**

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Because of the sustained growth of information and mobile users transmitting a great amount of data packages, modern network performances are being seriously affected by congestion problems. In this context, we propose a novel framework for solving the congestion problem on communication networks using a quantum game theory model, where network packages compete selfishly for the shortest route. The classic and quantum versions are simulated in order to compare performances. As it is shown, the outcome space increases when the network is extended from a classical to a quantum structure enabling more efficient solutions. Optimal outcomes are not possible classically because players are constrained by a trade-off between the routing and traveling times. On the other hand, it is possible to get rid of this trade-off by the use of quantum entanglement and quantum superposition, and users who play quantum can reach a Pareto optimal. That is, the best possible combination between routing time and traveling time can be reached. Because of its generality, this model can also be used both in local networks and more complex networks such as 5G or LTE-A. This leads to the opportunity of

developing full-stack protocols that may be capable of taking advantage of the quantum properties for optimizing communication systems.

Lattice field theory

LA1.1 (invited) – Lattice QCD at nonzero temperature and density

Gert Aarts

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I will review recent developments in the field of lattice QCD at nonzero temperature and density, describing in particular the transition from the hadron gas to the quark-gluon plasma.

LA1.3 (invited) – Lattice QCD calculations for Muon $g-2$

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One of the most promising quantities for the search of signatures of physics beyond the Standard Model of Particle Physics is the anomalous magnetic moment $g-2$ of the muon. A new experimental result released earlier this year has further increased the discrepancy between experimental result and the Standard Model prediction to 4.2 sigma. In this talk I will give an overview and discuss the status and recent developments of lattice calculations for muon $g-2$.

LA1.5 – General purpose lattice QCD code set Bridge++ 2.0 for high performance computing

**Yutaro Akahoshi¹, Sinya Aoki¹, Tatsumi Aoyama²,
Issaku Kanamori³, Kazuyuki Kanaya⁴, Hideo Matsuferu²,
Yusuke Namekawa¹, Hidekatsu Nemura⁵,
Yusuke Taniguchi⁴**

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Bridge++[1] is a general purpose code set for numerical simulation of lattice QCD, designed on the object-oriented programming and described in C++ language. The project goal is to develop a readable, extensible, and portable code set with sufficient high performance.

At the time of the first release in 2009, our major target platforms were parallel scalar systems. At present, recent supercomputers adopt a variety of architecture: multicore parallel machines with wide SIMD (Fugaku and Intel Xeon clusters), clusters with accelerator devices such as GPUs and PEZY-SC, and vector processors (NEC SX-Aurora). We have investigated how to tune our code for these architectures and integrate the optimized codes into the Bridge++ framework.

A typical bottleneck in lattice QCD simulation lies in solving the linear equations for the fermion operators that are large sparse matrices and to be solved frequently in numerical simulations. We classify the program components into data manipulations and algorithms. The former, including the performance-sensitive fermion matrix operators, are optimized for individual target platforms, while the latter are implemented as C++ templates. It allows to apply to a new architecture incrementally. One only needs to implement the required operators and instantiate the desired algorithms. General parts of the application such as the Hybrid Monte Carlo updates and the measurements of physical observables are handled in a similar way.

We have extended and refactored the Bridge++ code set, and are preparing for the release of this revision as version 2.0. The new version includes the optimized code of the fermion matrix solver targeting the SIMD architectures (Arm A64FX and Intel AVX-512), vector architecture (NEC SX-Aurora TSUBASA), and that for offloading to GPU devices.

In this presentation we describe the structure of Bridge++, with some emphasis on the implementation for the A64FX architecture and its performance

measured on the Fugaku supercomputer at R-CCS, as one of our latest results of development. We also introduce the performance results on other systems such as an Intel Xeon cluster, the NEC SX-Aurora TSUBASA at KEK, and the Cygnus GPU cluster with NVIDIA V100 at the University of Tsukuba.

[1] Bridge++ project: <https://bridge.kek.jp/Lattice-code/>

LA1.6 – Efficient computations of continuous action densities of states for lattice models

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David Lancaster⁴, Antonio Rago⁴**

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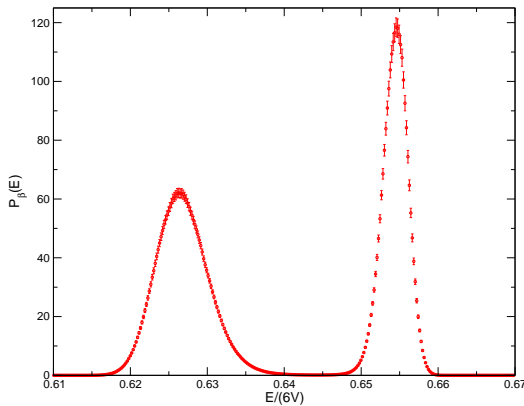
³Université Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

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Monte Carlo methods are widely used in Statistical Mechanics and Lattice Field Theory to compute values of physical quantities that are not accessible analytically. Over the years, very efficient Monte Carlo methods have been devised that enable us to obtain precise numerical evaluations of observables in various settings. Yet, there are relevant physics scenarios in which Monte Carlo methods are either inefficient or not applicable. In this talk, I will present an alternative strategy based on the computation of the density of states. The latter is obtained with the logarithmic linear relaxation (LLR) method [1], which reduces the problem to a set of stochastic root finding tasks over restricted energy intervals. The main advantage of this method (which is applicable to systems with a continuous spectrum) is exponential error reduction, which allows us to evaluate the density of states of a system over hundreds of thousands of orders of magnitude with a fixed level of relative accuracy [2]. After reviewing the algorithm, I will show an application in U(1) Lattice Gauge Theory that has enabled us to obtain the most accurate estimate of the critical coupling with modest computational resources (Fig. 1). Then, I will present an application to the decorrelation of the topological charge in SU(3) Lattice Gauge Theory near the continuum limit [3]. Finally, I will discuss the LLR method in the context of computations of partition functions [4] and apply it to studies of systems affected by a strong sign problem [5, 6].

- [1] K. Langfeld, B. Lucini and A. Rago, Phys. Rev. Lett. **109** (2012), 111601 doi:10.1103/PhysRevLett.109.111601 [arXiv:1204.3243 [hep-lat]].
- [2] K. Langfeld, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys. J. C **76** (2016) no.6, 306 doi:10.1140/epjc/s10052-016-4142-5 [arXiv:1509.08391 [hep-lat]].
- [3] G. Cossu, D. Lancastera, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys. J. C **81** (2021) no.4, 375 doi:10.1140/epjc/s10052-021-09161-1 [arXiv:2102.03630 [hep-lat]].
- [4] R. Pellegrini, B. Lucini, A. Rago and D. Vadicchino, PoS **LATTICE2016** (2017), 276 doi:10.22323/1.256.0276.
- [5] K. Langfeld and B. Lucini, Phys. Rev. D **90** (2014) no.9, 094502 doi:10.1103/PhysRevD.90.094502 [arXiv:1404.7187 [hep-lat]].
- [6] O. Francesconi, M. Holzmann, B. Lucini and A. Rago, Phys. Rev. D **101** (2020) no.1, 014504 doi:10.1103/PhysRevD.101.014504 [arXiv:1910.11026 [hep-lat]].



The action histogram at the critical value of the coupling in U(1) Lattice Gauge Theory on a 20^4 lattice, obtained with the LLR algorithm.

LA2.1 (invited) – Hadronic structure from first principles

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The internal structure of the nucleon is a central objective of the current experimental program in nuclear physics as it plays an important role both in our understanding of strong interactions as well in our quest for discovering new physics at high energy collider experiments. Lattice Quantum Chromodynamics (LQCD) provides a computational method for *ab initio* computations of hadronic structure. In this talk, I present the methodology as well as review recent results from lattice QCD calculations. Furthermore, I am discussing the future of such computations and their potential impact to phenomenology.

LA2.3 – Ab initio description of nuclear structure in no-core Monte Carlo shell model

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One of the challenges in nuclear theory is to describe nuclear structure from first principles. No-core Monte Carlo shell model (MCSM) [1] is such an *ab initio* method of full configuration interaction in nuclear many-body system, extending the original MCSM approach with an assumed inert core [2]. In this presentation, we introduce the no-core MCSM [3, 4] and show current status of this *ab initio* approach. Figure 1 summarizes the ground-state energy of light nuclei compared to the experimental values (AME2012 [5]). Computations are carried out on the

K computer [8] and the supercomputer Fugaku [9]. As seen in the comparison, we can obtain reasonable agreement between the results with Daejeon16 NN interaction [7] and experimental values up to around 20-body system of ^{20}Ne .

- [1] T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno and J. P. Vary, Phys. Rev. C **86** (2012) 054301.
- [2] T. Otsuka, M. Honma, T. Mizusaki, N. Shimizu and Y. Utsuno, Prog. Part. Nucl. Phys. **47** (2001) 319.
- [3] N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma and T. Otsuka, Prog. Theor. Exp. Phys. **01A205** (2012).
- [4] N. Shimizu, T. Abe, M. Honma, T. Otsuka, T. Togashi, Y. Tsunoda, Y. Utsuno and T. Yoshida, Phys. Scr. **92** (2017) 063001.
- [5] G. Audi, *et al.*, Chinese Physics C **36** (2012) 1603.
- [6] A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, Phys. Lett. **B644** (2007) 33.
- [7] A. M. Shirokov, I. J. Shin, Y. Kim, M. Sosonkina, P. Maris and J. P. Vary, Phys. Lett. **B761** (2016) 87.
- [8] The K computer, <https://www.riken.jp/en/collab/resources/kcomputer/>
- [9] The supercomputer Fugaku, <https://www.r-ccs.riken.jp/en/>

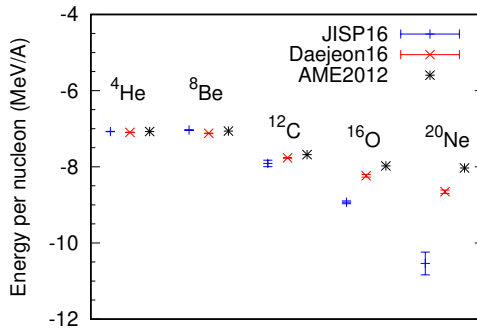


Fig. 1: Comparison of the no-core MCSM results of ground-state energy with experimental values (AME2012 [5]). The no-core MCSM employs two nonlocal NN interactions, JISP16 [6] and Daejeon16 [7]. The results are obtained by the extrapolation in harmonic-oscillator basis spaces ranging from 4 to 7 major shells.

LA2.4 – Digital quantum simulation for screening and confinement in gauge theory with a topological term

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In the conventional approach based on the Markov chain Monte Carlo algorithm, quantum field theories (QFTs) with topological terms are hard to simulate because of the so-called sign problem. A natural alternative is the application of quantum algorithms to the Hamiltonian formulation of QFTs. In this talk we describe our recent work [1] where we perform digital quantum simulation (on a classical simulator) to study screening and confinement in a QFT with a topological term, focusing on $(1+1)$ -dimensional quantum electrodynamics (Schwinger model) with a theta term. We compute the ground state energy in the presence of probe charges to estimate the potential between them, via adiabatic state preparation. We compare our simulation results and analytical predictions for a finite volume, finding good agreements. In particular our result in the massive case shows a linear behavior for non-integer charges and a non-linear behavior for integer charges, consistently with the expected confinement (screening) behavior for non-integer (integer) charges.

- [1] M. Honda, E. Itou, Y. Kikuchi, L. Nagano and T. Okuda, “Digital quantum simulation for screening and confinement in gauge theory with a topological term,” [arXiv:2105.03276 [hep-lat]].

Machine learning and algorithms

ML1.1 (invited) – Neural autoregressive toolbox for many-body physics

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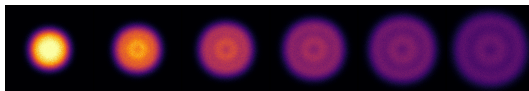
I will discuss our recent work on the use of autoregressive neural networks for many-body physics. In particular, I will discuss two approaches to represent quantum states using these models and their applications to the reconstruction of quantum states, the simulation of real-time dynamics as well as the approximation of ground states of many-body systems.

ML1.3 (invited) – Fermi Flow: Ab-initio study of fermions at finite temperature

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Fermi Flow is a variational free energy approach to thermal properties of interacting fermions in the continuum. The approach builds on classic works such as Feynman's backflow transformation and DeWitt's quantized point transformation. Crucially, one can leverage modern computing techniques for these physical transformations by exploiting their connection to recent advances in deep learning, such as equivariant normalizing flows and neural ordinary equations. I will discuss promising results of Fermi Flow applied to the uniform electron gas, a fundamental problem in condensed matter and warm dense matter research.



Flow of the electron density in a quantum dot.

ML1.5 – Quantum field theories, Markov random fields and machine learning

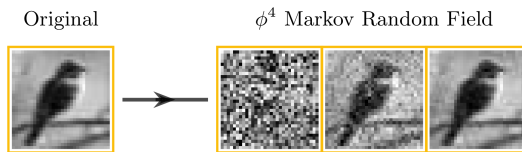
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The transition to Euclidean space and the discretization of quantum field theories on spatial or space-time lattices opens up the opportunity to investigate probabilistic machine learning from the perspective of quantum field theory. Here, we will discuss how discretized Euclidean field theories can be recast within the mathematical framework of Markov random fields which is a notable class of probabilistic graphical models with applications in a variety of research areas including machine learning. Specifically, we will demonstrate that the ϕ^4 scalar field theory on a square lattice satisfies the Hammersley-Clifford theorem, therefore recasting it as a Markov random field from which neural networks are additionally derived. We will then discuss applications pertinent to the minimization of an asymmetric distance between the probability distribution of the ϕ^4 machine learning algorithms and that of target probability distributions.

[1] D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. D **103** (2021) no.7, 074510.



Example reconstruction of an original image using the ϕ^4 quantum field-theoretic machine learning algorithm.

ML1.6 – An Explainable Probabilistic Classifier for Categorical Data Inspired to Quantum Physics

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We present Sparse Tensor Classifier (STC), a supervised classification algorithm for categorical data inspired by the notion of superposition of states in quantum physics. By regarding an observation as a superposition of features, we introduce the concept of wave-particle duality in machine learning and propose a generalized framework that unifies the classical and the quantum probability. We show that STC possesses a wide range of desirable properties not available in most other machine learning methods but it is at the same time exceptionally easy to comprehend and use. Empirical evaluation of STC on structured data and text classification demonstrates that our methodology achieves state-of-the-art performances compared to both standard classifiers and deep learning, at the additional benefit of requiring minimal data pre-processing and hyper-parameter tuning. Moreover, STC provides a native explanation of its predictions both for single instances and for each target label globally.

- [1] Emanuele Guidotti and Alfio Ferrara (2021), *An Explainable Probabilistic Classifier for Categorical Data Inspired to Quantum Physics*. <https://arxiv.org/abs/2105.13988>

ML1.7 – Order- N Orbital-Free Density-Functional Calculations with Machine Learning of Functional Derivatives for Semiconductors and Metals

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Orbital-free density functional theory (OFDFT) is expected to offer a scheme of electronic-structure calculation scaled with $\mathcal{O}(N)$ computation time for system size N , contrasted with $\mathcal{O}(N^3)$ in the conventional density functional theory (DFT), while exploration of its accurate algorithms is still in progress. The main challenge in OFDFT is to find an explicit form of the kinetic energy density functional (KEDF) $T[\rho]$ as a functional of electron density ρ . We here develop a novel scheme of the OFDFT calculations based on the machine-learning KEDF $T^{\text{ML}}[\rho]$ which is constructed to reproduce the kinetic-energy functional derivative (KEFD) $\delta T[\rho]/\delta\rho$ obtained by Kohn-Sham DFT calculations. The choice of the KEFD in the set of the training data is crucially important, because first, it appears directly in the Euler equation which one should solve and second, its better learning promotes more accurate reproduction of physical quantities expressed by the first derivative of the total energy. Using a neural network (NN) with the inputs s^2 and q and an output F^{NN} , we construct a NN KEDF as $T^{\text{ML}}[\rho] = \int \tau^{\text{TF}}(\mathbf{r}) F^{\text{NN}}(s^2, q; \{\mathbf{W}\}) d\mathbf{r}$, where τ^{TF} is the KEDF in the uniform density, $s = |\nabla\rho|/[2(3\pi^2)^{1/3}\rho^{4/3}]$, $q = \nabla^2\rho/[4(3\pi^2)^{2/3}\rho^{5/3}]$, \mathbf{r} is the spatial coordinate, and $\{\mathbf{W}\}$ is the set of NN parameters. Then we finally propose our NN KEDF, $\tilde{F}^{\text{NN}}(s^2, q) = X(q)F^{(0)}(s^2, q) + [1 - X(q)]F^{\text{NN}}(s^2, q)$, where $F^{(0)}$ and X are introduced to make KEDF satisfy known physical constraints: (a) $s \rightarrow 0$ limit in KEDF and linear response function as the expansion from the uniform density and (b) $s \rightarrow \infty$ limit in KEDF as the expansion from the dilute limit.

The accuracy and the transferability of our NN KEDF is achieved by our NN training system in which the KEFD at each real-space grid point for diamond is used for the training. We show that our OFDFT scheme reproduces the electron density obtained in the state-of-the-art DFT calculations and then provides accurate structural properties of 24 different systems, ranging from atoms, molecules, metals, semiconductors and an ionic material. The computational cost of the present OFDFT scheme indeed shows the $\mathcal{O}(N)$ scaling, as is evidenced by the

computations of the semiconductor SiC used in power electronics.

ML2.1 – Self-Learning Hybrid Monte Carlo: A First-Principles Method

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We introduce a method called self-learning hybrid Monte Carlo (SLHMC), which is a general method to make use of machine learning potentials to accelerate the statistical sampling of first-principles density-functional-theory (DFT) simulations [1]. The trajectories are generated on an approximate machine learning (ML) potential energy surface. The trajectories are then accepted or rejected by the Metropolis algorithm based on DFT energies. In this way, the statistical ensemble is sampled exactly at the DFT level for a given thermodynamic condition. Meanwhile, the ML potential is improved on the fly by training to enhance the sampling, whereby the training data set, which is sampled from the exact ensemble, is created automatically. Using the examples of α -quartz crystal SiO₂ and phonon-mediated unconventional superconductor YNi₂B₂C systems, we show that SLHMC with artificial neural networks (ANN) is capable of very efficient sampling, while at the same time enabling the optimization of the ANN potential to within meV/atom accuracy. The ANN potential thus obtained is transferable to ANN molecular dynamics simulations to explore dynamics as well as thermodynamics. This makes the SLHMC approach widely applicable for studies on materials in physics and chemistry.

- [1] Y. Nagai, M. Okumura, K. Kobayashi, and M. Shiga, Phys. Rev. B **102**, (2020) 041124(R).

ML2.2 – Reinforcement learning for rare trajectory sampling

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Very often when studying non-equilibrium systems one is interested in analysing dynamical behaviour that occurs with very low probability. These so-called rare events play a significant role in phenomena occurring throughout the sciences, ranging from large deviations in time-integrated statistics, to transition paths in chemical processes, up to a macroscopic level in climate models of natural disasters. The rarity of these events makes them inherently hard to observe and understand, necessitating the development of general techniques for their study. Here we develop such an approach by using a deep connection between trajectory sampling and reinforcement learning to develop efficient algorithms for the learning of an efficient sampling dynamics for rare trajectories. This provides access to not only probabilities and statistical information about the rare events studied, but an approximation to the stochastic dynamics by which it is likely to be observed. Applicable to both discrete [1] and continuous [2] time processes with any combination of jumps, drift and diffusion, we demonstrate the approach on a range of problems. These problems include: time-dependent dynamics generating finite-time rare trajectories, such as transition path problems from chemical physics, and time-homogenous dynamics used to study the statistics of time-integrated observables. The approach we take can be further applied to variable time problems such as first passage statistics, and Non-Markovian problems.

- [1] **D. C. Rose**, J. F. Mair and J. P. Garrahan, *New J. Phys.* 23 (2021) 013013
[2] A. Das, **D. C. Rose**, J. P. Garrahan and D. T. Limmer, ArXiv: 2105.04321 (2021)

ML2.3 – Machine-learning study using improved correlation configuration and application to the 2D quantum XY model.

Yusuke Tomita¹, Kenta Shiina², Yutaka Okabe²,
Hwee Kuan Lee³

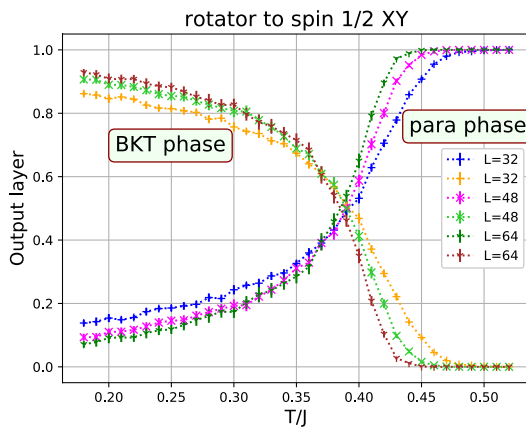
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Using the Fortuin-Kasteleyn representation, we improve the correlation configuration in the machine-learning study of the phase classification of spin models. The phases of classical spin models are classified using the improved estimators, and the method is also applied to the quantum Monte Carlo simulation using the loop algorithm. We analyze the Berezinskii-Kosterlitz-Thouless (BKT) transition of the spin-1/2 quantum XY model on the square lattice. The BKT phase and the paramagnetic phase of the quantum XY model are classified using the machine-learning approach. We show that the classification of phases of the quantum XY model can be performed by using the training data of the classical XY model.

- [1] Yusuke Tomita, Kenta Shiina, Yutaka Okabe, and Hwee Kuan Lee, Phys. Rev. E **102**, 021203(R) (2020).



The classification of the quantum XY model using the training data of the classical XY model (plane rotator). For the training data, the samples of T within the ranges $0.50 \leq T \leq 0.84$ and $0.96 \leq T \leq 1.30$ for the classical XY model are used.

ML2.4 – Unsupervised Identification of Dynamical Crossovers in Entangled Polymer Melt from Conformational Fluctuations

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In entangled linear polymer melt, motion of a typical chain is constrained in a "*tube*"-like region while equilibrium dynamics is dominated by "*reptation*", whereby kinks or structural defects propagate along the chain. We employ a data-driven approach to relate this conformational changes with the dynamics. To this end, conformational observables are used to form the higher dimensional feature space. The measurements of these observables are extracted from equilibrium molecular dynamics simulations of long semiflexible polymer chains in a melt. Unsupervised linear transformation techniques, principal component analysis, and time-lagged independent coordinate analysis (TICA) are employed to embed the data to a lower dimensional space. We show that few conformational attributes in lower dimensional space are able to discern different dynamic scaling regimes predicted by the Rouse and reptation theory. We analyze the TICA modes, and relate the amplitudes to signatures of deviation from Rouse behavior. The characteristic relaxation times of these modes show two step power-law decay with mode index. The latter matches with prediction of Rouse theory, and the former corresponds to the deviation from it. The crossover point yields the entanglement length. Values of various physical quantities calculated with this approach are consistent with standard routes of measurements.

ML2.5 – Encoding solid-state electronic structures in neural-network quantum states

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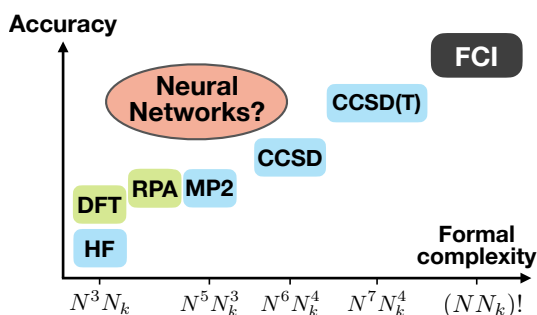
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Neural networks (NNs) are powerful tools to perform numerous machine learning tasks, ranging from image recognition and automated translation. Recent findings show that their high expressibility is also suited to represent quantum many-body states. The key feature of NNs is their dimension-free structure. In sharp contrast to tensor networks, such a property is expected to enable the variational state to capture complex correlations efficiently. In this talk, we demonstrate the power of the neural-network ansatz to investigate the essential properties of electronic structures in solid-state systems; the ground states and quasiparticle band structure. Our results show the capability of NNs to study complex electronic structures even in a situation where conventional methods, such as coupled-cluster theory, break down. The presentation is based on our paper [1].

- [1] N. Yoshioka, W. Mizukami, and F. Nori, accepted to Communications Physics, arXiv:2010.01358.



Schematic illustration of the relationship between the formal computational complexity and accuracy in various first-principles calculation methods for solid systems.

ML2.6 (invited) – Variational Neural Annealing

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Many combinatorial optimization problems relevant to computer science, computational biology and physics can be tackled with simulated annealing, which is a powerful framework for optimizing the properties of complex systems through the lens of statistical mechanics. However, simulated annealing and its quantum counterpart, simulated quantum annealing, are traditionally implemented via Markov chain Monte Carlo, often displaying slow convergence to optimal solutions for challenging optimization problems. Here we combine the variational principle in classical and quantum physics with recurrent neural networks, whose dynamics are naturally devoid of slow Markov chains to accurately emulate annealing in its classical and quantum formulations. We find that a variational implementation of classical annealing is not only superior to its quantum analog in terms of speed of convergence and accuracy of solutions but also outperforms traditional simulated annealing and simulated quantum annealing on average on several prototypical spin glass models as the annealing time is increased [1]. In addition, through the use of the sign-problem-free variational Monte Carlo method, our framework can emulate quantum annealing with non-stoquastic drivers at moderately large system sizes, thus providing a useful tool to benchmark the next generation of quantum annealing devices which implement non-stoquastic Hamiltonians.

- [1] Mohamed Hibat-Allah, Estelle M. Inack, Roeland Wiersema, Roger Melko, Juan Carrasquilla, arXiv:2101.10154

MS1.1 (invited) – Towards ex-machina computations of transport and transformations in complex materials

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Harnessing the accuracy of quantum mechanics to design complex materials requires a series of approximations to reach the desired length and time scales. I will describe our pursuit of the paradigm of “ex-machina” computations where data-driven approximations are automatically developed using machine learning algorithms and enable access to previously intractable systems. Non-parametric regression methods allow for learning of potential energy surfaces from expensive quantum calculations. To accelerate molecular dynamics calculations, we developed the Neural equivariant interatomic potential model (NequIP) based on tensor-valued symmetry-preserving layer architectures and used them to achieve state-of-the-art accuracy and training efficiency for simulating dynamics of molecules, liquids, heterogeneous catalysts, and ionic conductors [1]. In order to enable autonomous selection of the training set for reactive systems, we developed the FLARE adaptive closed-loop algorithm that constructs accurate and uncertainty-aware Bayesian force fields on-the-fly from a molecular dynamics simulation, using Gaussian process regression [2]. We demonstrate the performance of ML-accelerated MD simulations by studying 2D-to-3D transformations of layered quantum materials [3] and catalyst dynamics [4,5].

- [1] S. Batzner et al, Arxiv:2101.03164 (2021)
- [2] J. Vandermause, et al, NPJ Computational Materials, 6, 20 (2020)
- [3] Y. Xie et al, NPJ Computational Materials, 7, 40 (2021)
- [4] J. S. Lim, et al, JACS. 2020, 142, 37, 15907–15916 (2020)
- [5] J. Vandermause et al, arXiv:2106.01949 (2021)

MS1.3 – Optical Properties of OLED Materials by TDDFT

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Organic light emitting diodes (OLEDs) have been of great interest for display and lighting applications during decades and they have been utilized in smartphones and flat-panel displays. After the development of fluorescent materials, the phosphorescent materials have been introduced and have achieved high efficiency. However, phosphorescent materials require expensive heavy metal such as Ir and Pt. Recently, thermally activated delayed fluorescence (TADF) materials have been developed as a new class of light emitting material where triplet excitons are converted into singlet excitons without heavy metals in phosphorescent materials.[1] Theoretically, an internal quantum efficiency (IQE) of 100%, the same as for phosphorescent materials, can be expected.

In order to study the optical properties of materials, we have employed the time dependent density functional theory (TDDFT), which is one of the most prominent and widely used methods for calculating excited states of various molecules, and it is recognized as a powerful tool for studying their electronic transition. In our calculations, the real-time and real-space (RSRT) techniques are employed in solving time dependent Kohn-Sham equation by the finite difference approach [2] without using explicit bases such as plane waves and Gaussian basis. Within the frame work of this approach, we can solve for the wave functions on the grid with a fixed domain, which encompasses the physical system of interests.

In this study, we have focused on the spectrum of OLED materials. For their design, it is highly desirable to simulate the spectral profile, not only the peak wavelength of absorption and/or emission, but also its spectrum shape. RSRT-TDDFT is applied to analyze some typical organic materials to study their spectrum profiles. Although the research is in an early stage, current results show that this approach may be able to simulate the spectrum profile reasonably well.

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[2] N. Akino and Y.Zempo, *MRS Advances*, **1**(2016), 1773

MS1.4 – *Ab initio* theory of Nd₂Fe₁₄B-based hard magnetic materials

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Nd₂Fe₁₄B-based systems are the best high-performance permanent magnets currently available, with the magnetic hardness of parent Nd₂Fe₁₄B further enhanced by partial substitution of Nd by Tb or Dy. However, the high prices of heavy rare-earths have encouraged the ongoing search for alternative light rare-earth substitutions like Ce or La. The accurate description of magnetic anisotropy in rare-earth based hard magnets is therefore crucial; yet, it is also a notorious theoretical challenge as it involves strong Coulomb interactions, spin-orbit coupling and crystal field effects. In this work, we use a first-principles density functional theory + dynamical mean-field theory approach within a quasi-atomic approximation for the on-site electronic correlations of the 4*f* shell to evaluate crystal field effects and the contribution of Nd ions to the magnetic anisotropy in Nd₂Fe₁₄B, CeNdFe₁₄B and NdLaFe₁₄B. The magnetic properties (magnetic anisotropy, first-order magnetization process, spin reorientation transition) calculated with our *ab initio* method agree quantitatively with experiment in Nd₂Fe₁₄B. The study also reveals a higher magnetic anisotropy in CeNdFe₁₄B than in NdLaFe₁₄B. This suggests that the Nd magnetic anisotropy in Nd₂Fe₁₄B is strongly site dependent (the contribution from the *g* site is higher) which is an important result in the quest for new Nd replacements.

MS1.5 – Anomalous Properties of Condensed Hydrogen Systems under Extreme Thermodynamic Conditions Revealed by the Non-Empirical Ab Initio Molecular Dynamic Simulation Method

Hyeon-Deuk Kim

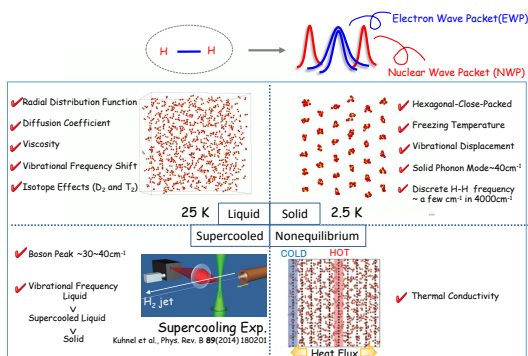
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We recently developed the non-empirical quantum molecular dynamics method called the nuclear and electron wave packet molecular dynamics (NEWPMD) method. The NEWPMD method describes floating and thawed Gaussian nuclear wave packets (NWP) via the time-dependent Hartree method, and electron wave packets (EWP) through the perfect-pairing valence bond theory that treats the Pauli exclusion energy. [1, 2]The non-empirical ab initio intramolecular and intermolecular interactions were explicitly derived with which the equations of motion (EOMs) for the NWP are time-evolved. The simple EOMs ensure a stable long-time solution of a time-dependent wave function even for condensed hydrogen systems. The NEWPMD method has successfully reproduced the various experimental observations as a result of computation without any empirical parameters such as (1) the radial distribution functions, diffusion coefficients, viscosity and shifts of the H-H vibrational frequency in the liquid hydrogens[1, 3, 4], (2) the stable hexagonal-close-packed lattice structure below the freezing temperature of 13.8 K, vibrational displacement and reasonable lattice phonon frequency in the solid hydrogens[5], (3) the discrete jump of the H-H vibrational frequency at the liquid-solid phase transition[5, 4], (4) the thermal conductivity of liquid hydrogens under a temperature gradient[6], (5) the isotope-dependent bond length and diffusion coefficient in the liquid deuterium[7], and (6) the decelerated diffusive dynamics at an optimal mixing rate for the H₂-D₂ mixture[8]. These successful agreements with the experimental results in the various phases and thermodynamic states demonstrate that the NEWPMD method reflects the real thermodynamic states of hydrogen systems at the same temperature and densities as the experimental values.

In this presentation, we will report our latest computational results on the two extreme thermodynamic states: (1) the decelerated liquid dynamics induced by component-dependent supercooling in hydrogen and deuterium quantum mixtures at low temperature, and (2) the distinct molecular dynamics dividing liquid like and gas-like supercritical hydrogens at higher temperature than the critical temperature (33K). In the former, we computationally found that the dynamics of

quantum H₂ and D₂ mixtures significantly slows down at a specific mixing ratio, which is directly connected to the experimentally observed anomalous slowdown of crystallization in the quantum mixtures at extremely low temperature. The latter proposes a new index to monitor the supercriticality and especially to identify distinct liquid-like and gas-like supercritical fluids which are distinguishable from normal liquid and normal gas. Both of the computationally predicted properties and obtained physical insights will help future experimental monitoring and searching the anomalous and unknown thermodynamic states.

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 [8] S. Yamaoka and K. Hyeon-Deuk, *J. Phys. Chem. Lett.* **11** (2020) 4186



Various experimental observations successfully reproduced by the NEWPMD method

MS1.6 – Role of the M choice in Hf(M)SiBCN (M = Y, Ho, Ta, Mo) thin films: DFT, ab-initio molecular dynamics and experiment

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Thin films based on light main group elements are attractive due to a unique combination of properties ranging from high hardness through optical transparency to high temperature stability and oxidation resistance (up to 1500 °C). The properties, in the first place electrical conductivity, can be further modulated by addition of early transition metals. Properties of amorphous Hf(M)SiBCN films are investigated by combining static DFT calculations with *ab-initio* molecular dynamics and their preparation using magnetron sputtering of composite B₄C–Hf–M–Si targets in Ar + N₂ reactive discharge gas [1]. First, we study the effect of the M choice and fraction on calculated mechanical properties and formation energy of binary MN and ternary Hf_xM_{1-x}N crystals. We discuss the dependence of formation energy on the crystal structure and on the distribution of Hf and M in the metal sublattice. The calculated mechanical properties of MN (rather than Hf_xM_{1-x}N) very well correlate with measured mechanical properties of a-HfMSiBCN. The driving force towards N incorporation, monotonically decreasing with increasing periodic table group number of M according to the calculated formation energy of MN, very well correlates with measured electrical conductivity and extinction coefficient of a-HfMSiBCN. Second, we use Car–Parrinello molecular dynamics to model the a-HfMSiBCN materials of experimental compositions and densities themselves. The calculated band gap, localisation of states around the Fermi level and bonding preferences of the M atoms (in particular their tendency to bind with N atoms) also correlate with the measured increasing metallicity with respect to the periodic table group number of M and confirm the possibility of predicting the trends in characteristics of a-HfMSiBCN using those of MN. Third, we identify optimum target compositions (B₄C covered by 15% Hf, 5% Ta and 15–20% Si) leading to hard (>20 GPa) a-HfMSiBCN films with relatively high conductivity at a given extinction coefficient. The results are important for the design of hard, conductive and/or transparent high-temperature coatings.

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MS2.1 (invited) – Simulating Disordered Supramolecular Materials for Organic Electronics using Linear Scaling Density Functional Theory

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Density-functional theory (DFT) is routinely used to simulate a wide variety of materials and properties, however, standard implementations of DFT are cubic scaling with the number of atoms, limiting calculations to a few hundred atoms. However, in recent years various linear scaling (LS) approaches have been developed, enabling simulations on tens of thousands of atoms. One key factor influencing the accuracy and cost of DFT is the basis set, where minimal, localized basis sets compete with extended, systematic basis sets. On the other hand, wavelets offer both locality and systematicity and are thus ideal for representing an adaptive local orbital basis which may be exploited for LS-DFT. One may also make further physically-motivated approximations, e.g. dividing a system into fragments or exploiting underlying repetition of local chemical environments, where each approximation may be controlled and quantified. This ability to treat large systems with controlled precision offers the possibility of new types of materials simulations. In this talk I will demonstrate the advantages of such an approach for large scale DFT calculations, as implemented in the wavelet-based BigDFT code. I will focus on the example of materials for organic LEDs, showing how this approach may be used to account for environmental and statistical effects on excited state calculations of disordered supramolecular materials.

MS2.3 – Speeding up DFT with generalized regular k-point grids

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Most DFT calculations use Monkhorst-Pack (MP) grids for the k-point integra-

tion. But for non-orthogonal lattice vectors, these grids often have lower symmetry than the electronic bands, which reduces efficiency. Our "generalized regular" (GR) grids guarantee the highest-possible symmetry reduction of the k-points and also optimize the uniformity of the grid. For high-throughput and machine learning applications, the use of GR grids increases efficiency by about 60

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MS2.4 – Quadratic algorithm for computing the band energy and estimating its error

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With increased adoption of the high-throughput approach to materials prediction comes a greater need to guarantee the accuracy of the data in databases of computationally simulated materials: surrogate models are trained on and are no more accurate than the data. The band energy calculation is the accuracy-limiting calculation for a material's formation enthalpy when computed using density functional theory (DFT) codes and the primary source of error in databases of DFT simulations. We present an algorithm that improves the efficiency and accuracy of the band energy calculation and gives a robust approximation of its error. This is one step towards DFT codes truly becoming black boxes where users may provide the desired error of the simulation, and the code intelligently selects all required algorithmic parameters.

MS2.5 – Inverse Design of Two-dimensional Self-assembly of Patchy Particles

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A challenging goal to materials chemistry and physics is to construct superstructures from a building block. The superstructures of complex periodic lattices (e.g. diamond structure) or aperiodic structures (e.g. quasicrystals) are basics for the generation of novel materials with special optical, mechanical and thermal properties. The structure of these novel materials can be self-assembled from a nano or colloidal building block. The building block is designed by its shape, anisotropic surface property, local cluster, and so on (Fig. 1A). One of the highlighting, promising building block to build up micro-crystals is colloidal patchy particles. Patchy particles (also referred to as Janus particles) are the particles with anisotropic surface patterns or patches on specific positions on the particle surface. The interaction of such particles is not only dependent on the distance, but also on their mutual orientations. Therefore, the patchy particles are capable of organising themselves into complex structures compared to the case of isotropic particles. The degrees of freedom of the patchy particle have direct impact on the possible outcome structures. If one tries the self-assembly of any possible particle design, it consumes exhausting time and cost due to uncountable design of the patchy particle.

This can be solved by applying inverse design, i.e., from a desired target structure, we seek for a type of patchy particle that can self-assemble into desired structures. From the target structure, a class of computational iteration techniques is used to tune the design of particle until it can self-assemble into given target. We have developed and applied our inversed design optimisation scheme to find what is the best design of patchy particles so that they can assemble into given target structures. In particular, among many candidate patchy particles, we are capable of determining the suitable patchy particle creating a square lattice, kagome lattice, dodecagonal quasicrystal (Fig. 1B-D).

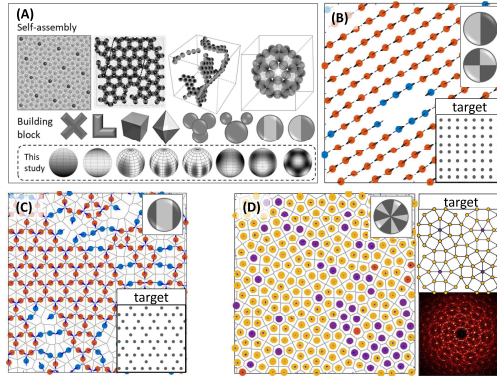


Fig. 1. (A) Illustration of the self-assembly, building blocks and the patterns on particles in this study by using spherical harmonics. (B,C,D) The generated structure from the optimisation scheme and the estimated patchiness in comparison with the target (inset). The target is square lattice (B), kagome lattice (C), and dodecagonal quasicrystal (D, with Fourier transform). The Voronoi tessellation is also embedded. The arrows on the particle are local orientational field. The particle colour is coded with the number of nearest neighbour N_{nb} as blue, orange, yellow, purple for $N_{nb} \leq 3$, $N_{nb} = 4, 5, 6$, respectively.

MS2.6 – Sparse sampling approach to efficient *ab initio* calculations at finite temperature

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Efficient *ab initio* calculations of correlated materials at finite temperature require compact representations of the Green's functions both in imaginary time and Matsubara frequency. In this talk, we introduce a general procedure which generates sparse sampling points in time and frequency from compact orthogonal basis rep-

representations [1], such as Chebyshev polynomials and intermediate representation (IR) basis functions [2]. These sampling points accurately resolve the information contained in the Green's function, and efficient transforms between different representations are formulated with minimal loss of information. As a demonstration, we apply the sparse sampling scheme to diagrammatic GW and GF^2 calculations of a hydrogen chain, of noble gas atoms and of a silicon crystal [2]. Furthermore, we review the application of the sparse sampling techniques to *ab initio* calculations of superconducting temperatures based on the Migdal-Eliashberg equation [3].

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MS3.1 (invited) – To mix or not to mix? Addressing tangible problems with entropy descriptors

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Disordered multicomponent systems occupying the mostly uncharted centers of phase diagrams, have been studied for the last two decades as innovative materials. By maximizing their entropy (mostly configurational) and stabilizing (near) equimolar mixtures, it has been possible to achieve robust systems with promising applications [1,2]. Still, effective computational discovery of useful materials remains challenged by the immense number of configurations. High-throughput approaches, analyzing large amount of data with a combination of thermodynamical and statistical means, can ease the task [3]. This presentation illustrates the ladder of disorder descriptors, including the ideal [2] and spectral scenarios [3], and the LTCV method for miscibility gaps [4]. Many legitimate scientific questions will also be answered with these entropy-descriptors, like why a high-entropy material forms? is it stable at low temperature? can we increase the melting point? What is the role of vibrations? [1] Oses et al., *Nature Reviews Materials* 5, 295 (2020); [2] Rost et al., *Nature Communications* 6, 8485 (2015); [3] Sarker et al., *Nature*

Communications 9, 4980 (2018); [4] Lederer et al., *Acta Mater.* 159, 364 (2018).

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MS3.3 – A Density-Matrix Renormalization-Group Study for a Two-Dimensional Lattice-Gas on the Ih-Ice Prism Surface

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The phase transition on a two-dimensional (2D) lattice-gas model of the Ih-Ice prism surface [1], which is the $(10\bar{1}0)$ surface on a Wurtzite crystal structure, is studied using the density-matrix renormalization-group (DMRG) method [2, 3, 4]. The phase transition temperature of the lattice gas provides a lower limit for the faceting (roughening) transition temperature [5]. Though the model is the 2D nearest-neighbor Ising model, it contains four sites in a unit cell on the prism surface for an Ih-Ice. Due to this complexity of the lattice structure, the DMRG method is required to obtain precise results. Comparing the phase transition temperature to the faceting transition temperature observed on a real ice crystal [6, 7], the effective surface energy and the temperature dependence of the coverage on each sub-lattice site in a unit cell are estimated approximately. The obtained surface energy is consistent with the one estimated by the recent molecular dynamical simulation [8].

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MS3.4 – First-principles study of Mg and O co-doping mechanism in the growth surface during GaN(0001) and AlN(0001) metalorganic vapor phase epitaxy

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Group III nitride semiconductors, GaN and AlN, are promising materials for next generation power devices and deep ultraviolet light emitting devices. The development of these semiconductors is based on the technology to make high-purity semiconductor crystals preventing unintentional impurity contamination and the technology to dope impurity for functionalization. To obtain p-type conductivity in nitride semiconductors, Mg doping has been extensively studied. In order to properly control the purity of the semiconductors, it is essential to understand the physics of unintentional impurity contamination in epitaxial growth. In this study, the effect of Mg doping on the unintentional oxygen (O) incorporation into GaN and AlN during metalorganic vapor phase epitaxial (MOVPE) growth, i.e., the possibility of Mg and O co-doping, was investigated by first-principles calculations. In particular, we focused on surface reconstruction in our modeling. This perspective is important in order to reflect realistic situations of the growth process in the analysis. This is because impurities are incorporated from the surface during the crystal growth process. The results show that the presence of Mg, which replaces group III atoms (Ga or Al) in the subsurface layer, energetically

promotes the unintentional oxygen incorporation. We also modeled the complex defects by focusing on the amount of hydrogen aggregated near the Mg impurity, because it has been reported that in MOVPE growth, unintentional H impurities are introduced to form complex defects with Mg. The presence of Mg + H complex defects in the subsurface layer was suggested to promote unintentional oxygen incorporation as well. Thus, the mechanism of unintentional oxygen incorporation promoted by magnesium doping and complex defect structures is discussed in terms of charge neutrality or electron counting model in the growth surface. The physics of unintentional O incorporation and complex defect formation with Mg acceptors during MOVPE of lightly doped GaN:Mg and AlN:Mg is revealed from a theoretical point of view.

MS3.5 – Effect of water atmosphere on low friction of multi-layer graphene studied by molecular dynamics

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The origin of low friction of solid layered materials is still not understood. Even for graphite, which shows very low friction in ambient air, is difficult to explain since we have to describe the mechanism by friction between transfer layer and solid graphite in commensurate condition. Thermal escape motion is the most reliable mechanism found by using coarse-grained simulation [1]. In this theory, the transfer layer finds a plain path on the potential surface by thermal fluctuation. This motion is also confirmed by all-atom molecular dynamics (MD) [2]. In the MD simulation, at room temperature, the thermal motion of graphene made instable structure and the thermal escape motion only exhibited in low temperature of 100 K. In this paper, low friction mechanism of layered graphene is analyzed by reactive molecular dynamics simulations with terminal groups and the water molecules in the ambient air. In the MD simulation, 8 layer graphene sheet is faced in commensurate condition with the slab graphene surface. The sliding of the top graphene sheet in constant velocity evolve the friction dynamics. At the hydrogen termination case and in vacuum and in low temperature of 50 K, the thermal escape motion [1, 2] is reproduced. In the hydroxyl group termination system in vacuum, the thermal escape motion is inhibited due to the functional groups. On

the other hand, the thermal escape motion is reproduced by surrounding these systems with a population of water molecules in room temperature. Thus, it is found for the first time that the low friction of graphite is greatly affected by the surrounding water molecules. The hydrophobic interaction stabilizes the sliding motion of transfer graphene layer.

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MS3.6 – The Phonon Quasiparticle Approach for Anharmonic Properties of Solids

Renata Wentzcovitch

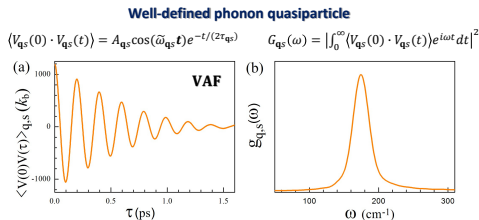
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In crystalline materials, anharmonicity is crucial in understanding several phonon-driven phenomena, e.g., high-temperature structure stabilization, phase transitions close to melting temperatures, thermal conductivity, etc. Anharmonicity can be characterized by the intrinsic, i.e., isochoric temperature (T) dependence of phonon frequencies. As such, the calculation of T-dependent phonon dispersions incorporating anharmonic effects is critical for predictive studies of thermodynamic and lattice transport properties.

In this talk, I will review the phonon quasiparticle approach [1], combining molecular dynamics (MD) simulations and lattice dynamics calculations to address phonon anharmonicity. The method invokes the concept of phonon quasiparticle characterized by two quantities, renormalized frequency and lifetime. These quantities can be extracted from the mode-projected velocity autocorrelation function sampled by MD simulations. In principle, anharmonic interactions are captured to infinite order in perturbation theory. Anharmonic phonon dispersions can be obtained by Fourier interpolation [1,2,3] of the renormalized frequencies, from which vibrational free energy [1,2,3], phase boundary [3], and thermodynamic properties [4] can be further computed. Quasiparticles' lifetime can also be used to calculate lattice thermal conductivity [5-7] using the linearized Boltzmann transport equation.

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MS4.1 – High temperature superconductivity in compressed sulfur hydrides from first principles

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The discovery of the superconducting phase discovered at 200 K in hydrogen sulfide [1] ignited intensive exploration of the superconductivity in extremely compressed hydrides. With the BCS theory for phonon-mediated superconductivity it has been predicted that the transition temperature is proportional to the phonon frequency mediating the Cooper pairs and therefore become high in light-element superconductors: the current discovery has proved this true. It is, however, difficult to observe the superconducting properties in the pressure cell and the experimental probes are limited. First-principles calculations give us insight: one can search stable crystal structures and calculate electronic, lattice dynamical and superconducting properties with an accuracy comparable to experiments.

We have conducted theoretical study of the superconducting phase in the compressed hydrogen sulfide using the first-principles calculation. Consistent explanation has been given with our study as to why it shows such a high transition temperature and its pressure dependence [2-4]. Especially we find intriguing mech-

anisms behind those observations, which may be common to other hydride superconductors: infinite sequence of metastable structures, anomalous peaking of the electronic density of states, etc. We introduce them in the presentation.

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MS4.2 – Effect of spin fluctuations on superconductivity in V and Nb: A first-principles study

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It is widely known that spin fluctuations can be the origin of electron pairing in unconventional superconductors. On the other hand, spin fluctuations also play an important role in conventional phonon-mediated superconductors. In nearly ferromagnetic metals, spin fluctuations induced by strong exchange interaction can lead to a significant suppression of singlet pairing and thus *s*-wave superconductivity. To investigate how spin fluctuations influence conventional superconductivity, Eliashberg theory has been extended to include the effect of spin fluctuations[1] and applied to some systems, e.g., V and Nb[2]. However, this treatment is rather empirical and fully non-empirical calculation of such effect has scarcely been performed so far.

In this study, we explored the interplay of spin fluctuations and superconductivity from first principles by using density functional theory for superconductors (SCDFT)[3] including the effect of spin-fluctuations[4]. We applied this method to the elemental transition metals V, Nb and calculated the effect of spin fluctuations on T_c [5]. We found that spin fluctuations compete with superconductivity

induced by the cooperation between phonons and plasmons. In particular, we have confirmed that the amount of reduction of T_c due to spin fluctuations reflects the degree of localization of valence states. Furthermore, we have shown that the inclusion of the spin-fluctuation effect enables us to reproduce the relation between T_c of V and Nb successfully, while it leads to the significant underestimation of T_c (Fig. 1). Finally, we have analyzed the exchange-correlation kernels, and it has been revealed that the mass renormalization of spin fluctuations is incomplete, which is different from that of phonons.

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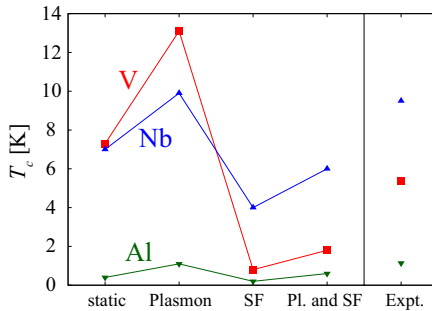


Fig. 1: Comparison of calculated T_c with and without the effect of plasmon and spin-fluctuation and experimental T_c in each material.

MS4.3 – Analyzing the electron-phonon scattering rates and energy transfer rates of photo-excited carriers in semiconductors

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In today's presentation, we will discuss the two physical quantities, namely, the total electron-phonon scattering rate and the rate of energy transfer from the energetic carriers to phonons. The two rates govern the ultrafast relaxation dynamics of photoexcited electrons in semiconductors, on the femtosecond and picosecond scale. While the total probability of all of the electron-phonon scattering processes (emission and absorption) determines the total electron-phonon scattering rate, the rate of energy transfer is mainly determined by the difference between phonon-emission and phonon-absorption rates, together with the effective frequencies of emitted and absorbed phonons. Considering the state-of-the-art density functional perturbation theory along with the efficient Wannier interpolation method [1,2], we have calculated both quantities for Si [3,4] and GaAs [5,6]. Our simulations have demonstrated, in agreement with the results of two-photon photoemission experiments, the striking difference in the temperature dependence of the two rates: while the total electron-phonon scattering rate rapidly grows with temperature as phonon populations increase, the energy transfer rate ascribed to electron-phonon interaction depends weakly on temperature and may even decrease with the increasing temperature [2,4]. Moreover, our analysis of the relative contributions of scattering channels involving optical and acoustical phonons to the two rates has shown that the main relaxation channels may differ for the total electron-phonon scattering rate and for the rate of energy transfer: while in silicon, the acoustical phonons contribute most to the total electron-phonon scattering rate at room temperature, the main contribution to the rate of energy transfer comes from the optical phonons.

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MS4.4 – Unified time evolution technique for the electronic structure calculation

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We have been studying the time-dependent technique, especially applied to the electronic structure calculation to obtain the optical properties estimated from the dipole moment by time evolution in real-space and real-time [1, 2]. This approach has a feature that, not only we can obtain a clear physical image, but the code is quite simple and significantly efficient. [3]. Despite of this simple calculation, we can obtain some information of the excited states. Prior to the time-dependent calculation, however, we have to prepare the ground state, obtained as the time-independent solution. To solve this inconvenience, we have introduced the imaginary-time evolution to obtain the ground state. The advantage of this technique is that the whole electronic calculation can be done in the same frame work of time evolution technique. We have applied this technique to some well-known systems and simple atoms, and elucidated the efficiency of this type calculation.

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QC1.1 (invited) – Quantum resource estimation at scale

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We use Microsoft's Quantum Development Kit for resource estimation of large scale quantum algorithms. We give an overview the programming language Q# and available libraries and discuss applications including Shor's algorithm applied to factoring and elliptic curves and Grover's algorithm applied to symmetric ciphers such as AES.

Based on joint work with Thomas Haener, Samuel Jaques, Michael Naehrig, Mathias Soeken, and Fernando Virdia.

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QC1.3 (invited) – How hard will it be to simulate many-body quantum dynamics?

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Simulating many-body quantum dynamics on classical computers is notoriously difficult: the exponential growth of Hilbert space dimension means that numerically exact simulations are exponentially costly, while approximate methods are often stymied by sign problems or entanglement growth. Error-corrected quantum computers promise fast (polynomial rather than exponential) simulations, but even they will be bottlenecked by certain operations: in many schemes so-called "Clifford" gates are fast, while non-Clifford gates are slow. "Magic" is a resource theory estimating the number of non-Clifford gates required to prepare a state.

I first give a qualitative overview of magic as a predictor of resource requirements. With that groundwork laid I consider the magic of the ground state of the \mathbb{Z}_3 Potts model, a generic interacting quantum field theory. In this state the magic is extensive, and near the phase transition it becomes nonlocal; this constrains tensor-network ansätze for the system. I then consider the magic of subsystems evolving under a thermalizing Hamiltonian; I argue that this magic rapidly peaks and subsides, suggesting that local approximations lead to efficient simulations of hydrodynamics.

QC1.5 (invited) – Simulating Near-Term Quantum Computers with Approximate Tensor Network Algorithms

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Quantum computing is currently generating great excitement and receiving large investments by major tech companies. One recent experiment by a group at Google performed a specific task that would definitely be impossible for a regular, classical

computer. But when taking into account the analog nature of Google's device, which incurs a small error at every step, is the real difficulty of the task unchanged?

Progress in simulations of quantum many-body systems have led to classical computing techniques with tradeoffs similar to Google's device. These techniques, based on tensor networks, can also run similar quantum circuits efficiently as long as they make a small error at each step too. So in this more realistic comparison, does the quantum computer still beat the classical one?

After introducing the details of Google's experiment and quantum circuits, and the classical tensor network techniques we used to simulate them, I will unpack some conclusions from the comparisons we carried out. We find that in some regimes, tensor network methods set a very high bar for quantum computer hardware to clear, and that this bar may have a "universal" value in a specific sense. While Google's results still edge out our best classical results for now, the closeness of the competition suggests that this race is just beginning.

QC1.7 – Simulation of quantum computer on the Fugaku computer

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Quantum information processing is simulated using the Fugaku computer. For k qubits, 2^k complex coefficients are stored and manipulated for the simulation, and efficient operations for these large memory space is a key of useful simulator. Previous 45 qubits simulation with double precision[1] used 0.5 EB on 65,536 nodes of the K computer using so-called the bit-swap algorithm[1,2]. The bit-swap algorithm assumes to use 2^n ($n = 0, 1, 2, \dots$) MPI processes and each MPI process handles 2^m ($m = 0, 1, 2, \dots$) coefficients, and therefore it works efficiently and elegantly on a massive parallel computer with 2^n nodes or processors.

In this talk, a modification of the bit-swap algorithm is proposed which works efficiently on a computer whose number of nodes is not 2^n number, and memory usage for coefficients on each node is not 2^m . This algorithm is implemented on the Fugaku computer[3] which has 158,976 nodes(processors) and each nodes has 32GB memory storage and original bit-swap algorithm will realize 47 qubits double-precision simulation using 131,072(= 2^{17}) nodes and 16GB on each node for coefficients, and the modified one will add one more, that is, 48 qubits using 158,976 nodes and 26.5GB on each node for coefficients.

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Quantum many-body physics

QP1.1 (invited) – How to carry out the generic real-space renormalization group program**Naoki Kawashima**ISSP, The University of Tokyo
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In lecture rooms, we often use some approximate real-space renormalization group (RG) prescription, such as the Migdal-Kadanoff method, as a heuristic example for explaining the RG idea. In doing so, however, our conscience keeps blaming us for not being able to offer the students a systematic way for improving it and finally, at least in principle, reach the exact estimates of various scaling properties. In my talk, I try to show a solution to this problem. Namely, we propose a way to carry out the canonical RG prescription in tensor space: write down the tensor RG equation, linearize it around a fixed-point tensor, and diagonalize the resulting linearized RG equation to obtain scaling dimensions, without resorting to the comparison with the conformal field theory. This approach is benchmarked in the context of the 2D Ising model.

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QP1.3 (invited) – Tensor network study of $\text{SrCu}_2(\text{BO}_3)_2$ under pressure**Philippe Corboz**Institute for Theoretical Physics and Delta Institute for Theoretical Physics,
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The frustrated quantum antiferromagnet $\text{SrCu}_2(\text{BO}_3)_2$ constitutes a realization of the paradigmatic Shastry-Sutherland model and exhibits a very rich phase diagram as a function of pressure and magnetic field. In this talk I report on re-

cent progress in the numerical study of this model using two-dimensional tensor network algorithms based on infinite projected entangled-pair states, which have recently been extended to finite temperature. We find a close agreement between the experimental and numerical data for the specific heat, revealing a sharp peak at pressures between 18-20 kbar [1]. We show that this feature corresponds to a finite-temperature critical point, analogous to the critical point of water, which terminates the first order line emanating from the discontinuous quantum phase transition between the dimer and plaquette phase at zero temperature. We numerically confirm that this critical point is compatible with the expected 2D Ising universality class.

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QP1.5 – Tensor network approach to the magnetization of frustrated square lattice Heisenberg systems

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In the frustrated spin systems, a lot of fundamental phenomena, including non-collinear magnetic orders, magnetization plateaus, and spin liquids, occur. Frustrated interactions often appear in geometrically frustrated situations, such as triangular, kagome, or pyrochlore lattices. However, when we consider further neighbor interactions or a combination of ferromagnetic and antiferromagnetic interactions in the nearest-neighbor interaction, frustrations can happen even in a standard square lattice. For example, several organic compounds contains both of ferromagnetic and antiferromagnetic interaction, and they can be considered as frustrated square lattice magnets [1, 2].

In this presentation, motivated by these compounds, we discuss the nature of $S = 1/2$ square lattice Heisenberg magnets with ferromagnetic and antiferromagnetic nearest-neighbor interactions. To investigate the magnetization process numerically, we employed the infinite tensor product state (iTPS) ansatz for the

ground state wave function. We show that in the model corresponding to the compound [1], a part of the spins reveals strong quantum spin fluctuation around the half of saturation magnetization, consistent with experimental observations [1]. The origin of such strong spin fluctuation is explained by a spin-singlet formed by spins connected through strong antiferromagnetic interaction. By varying the interaction strength, we show that such spin fluctuation is related to the 1/2 magnetization plateau stabilized in the vicinity of the model.

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QP1.6 – Novel approaches for tensor renormalization group method - ATRG and BTRG

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The Tensor Renormalization Group method (TRG) [1] has been widely used in recent years as a numerical method for strongly correlated many-body systems. TRG can be used to calculate physical quantities for large-scale classical and quantum systems efficiently. Researchers have developed various new methods such as the Second Renormalization Group [2], the Higher-Order Tensor Renormalization Group (HOTRG) [3], and the Loop TNR [4], to improve the accuracy near the phase transition point. However, these methods are computationally much more expensive than the original TRG. In addition, it was practically impossible to apply them to higher-dimensional systems.

To solve the problem, we have approached this problem from a different perspective. The Anisotropic Tensor Renormalization Group (ATRG) [5] can dramatically reduce the computational complexity in higher-dimensional systems by modifying the shape of the tensor that appears during the renormalization process. On the other hand, the Bond-weighted Tensor Renormalization Group (BTRG) [6]

extends the tensor network to a form in which tensors are placed not only on the vertices of the lattice but also on the edges connecting the vertices. As a result, we have increased the accuracy by orders of magnitude without increasing the computational complexity of conventional TRG. Furthermore, BTRG can have non-trivial fixed-point tensors at an optimal hyperparameter. This property indicates that BTRG performs the tensor contraction with high accuracy while keeping the scale-invariant structure of tensors.

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QP1.7 – Thermal Pure Quantum Matrix Product States

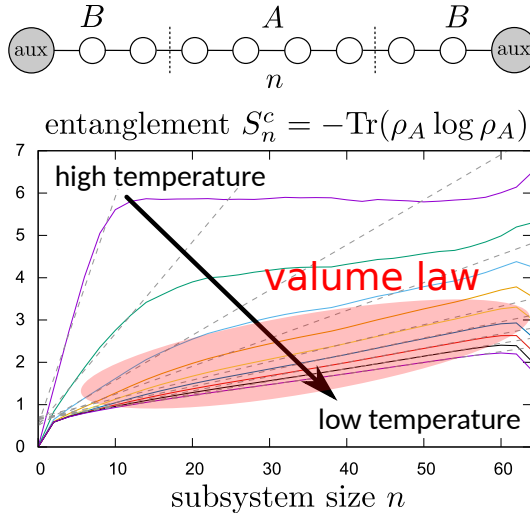
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Recent studies revealed that an equilibrium state can be represented as a *single thermal pure quantum (TPQ) state* instead of a conventional Gibbs ensemble [1]. Here, we explore a good matrix product state (MPS) representation of a TPQ state. The TPQ states having a volume-law entanglement was believed to be beyond the MPS description since the MPS's are known to have an area-law entanglement properly by construction. In order to overcome this difficulty, we attached auxiliaries to both edges of the MPS. Our TPQ-MPS shows a volume-law entanglement at low temperature when cutting out the subsystem from the center of the system. In addition, we succeeded for the first time in deriving the thermodynamic entropy numerically from the quantum entanglement, which is qualitatively different properties.

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The top image represents the auxiliary sites and the center subsystem. The bottom graph plots the subsystem size versus the entanglement entropy. The slope of the broken line corresponds to the thermodynamic entropy density.

QP2.1 (invited) – Recent Development of the Stochastic Analytic Continuation Method

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The measurement of real-frequency dynamic response functions is one of the outstanding challenges in regard to many numerical methods, such as QMC, lattice QCD, etc., with a general problem of given incomplete data of the imaginary time correlations, how to get the important dynamical features with the maximum fidelity. While the maximum entropy method is well established as a standard tool,

there is another competitive approach, the stochastic analytic continuation (SAC) method [1]. Our recent efforts on this method has made it more efficient, more systematic, and even capable to resolve features previously thought to be impossible to detect in the spectral functions [2,3]. I will discuss some of this progresses and show several cases where the SAC method has worked most successfully, including systems with possible fractionalized excitations.

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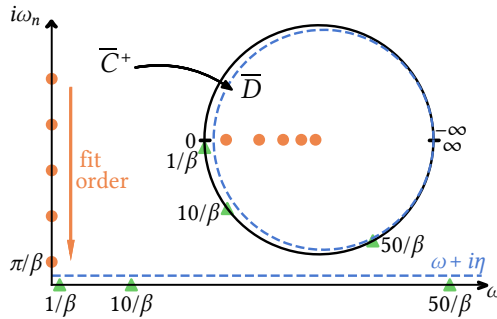
QP2.3 – Nevanlinna Analytic Continuation

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Simulations of finite temperature quantum systems provide imaginary frequency Green's functions that correspond one-to-one to experimentally measurable real-frequency spectral functions. However, due to the bad conditioning of the continuation transform from imaginary to real frequencies, established methods tend to either wash out spectral features at high frequencies or produce spectral functions with unphysical negative parts. Here, we show that explicitly respecting the analytic 'Nevanlinna' structure of the Green's function leads to intrinsically positive and normalized spectral functions, and we present a continued fraction expansion that yields all possible functions consistent with the analytic structure. Application to synthetic trial data shows that sharp, smooth, and multi-peak data is resolved accurately. Application to the band structure of silicon demonstrates that high energy features are resolved precisely. Continuations in a realistic correlated setup reveal additional features that were previously unresolved. By substantially increasing the resolution of real frequency calculations our work overcomes one of the main limitations of finite-temperature quantum simulations.

- [1] Phys. Rev. Lett. 126, 056402 (2021)



QP2.4 – Quantum Monte-Carlo simulations of highly frustrated magnets in a cluster basis

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Quantum Monte Carlo (QMC) simulations constitute nowadays one of the most powerful methods to study strongly correlated quantum systems, provided that no ‘sign problem’ arises. However, many systems of interest, including highly frustrated magnets suffer from the notorious sign problem in standard QMC simulations. Nevertheless, a possible sign problem depends on the simulation basis, and here we summarize how a suitable choice of cluster basis, combining specifically two (dimer basis) [1, 2, 3, 4, 5, 6, 7] or three spins (trimer basis) [8], can be used to eliminate or at least reduce the sign problem in highly frustrated magnets that were so far inaccessible to efficient QMC simulations. Applications of such cluster-based QMC methods include the thermodynamics of the two-dimensional Shastry-Sutherland model for $\text{SrCu}_2(\text{BO}_3)_2$ [5, 6, 7] as well as finite-temperature

critical behavior in bi- [4] and trilayer models [8].

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QP2.5 – Simulating Rokhsar-Kivelson quantum critical point in a realistic quantum Ising model

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Quantum dimer model (QDM) is an important model for understanding the low energy dynamics of valence bond systems. QDM hosts a peculiar point known as the “Rokhsar-Kivelson (RK) point”. RK points correspond to deconfined liquid states with remarkable physical properties but are extremely difficult to realize in experiments. We show that RK points can be simulated in some quantum spin systems that are realistic for experiments. Based on a generic proposal, we construct a particular spin model and present strong numerical evidence on the existence of RK point in the phase diagram through a quantum Monte Carlo study. We further employ the stochastic analytic continuation technique to simulate the quantum excitations of the spin model, from which we have identified not only excitations of the QDM, but also a new branch of excitations beyond QDM that has never been found before. We also discuss the experimental relevance of our

model in the context of cold atom and condensed matter systems.

QP2.6 – Numerical sign problem and the tempered Lefschetz thimble method

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The numerical sign problem is one of the major obstacles to the first-principles calculations for important physical systems, such as finite-density QCD, strongly-correlated electron systems and frustrated spin systems, as well as for the real-time dynamics of quantum systems. The tempered Lefschetz thimble method (TLTM) [1] was proposed as a versatile algorithm towards solving the numerical sign problem. There, the integration region is deformed into the complex space according to the antiholomorphic gradient flow equation, and the system is tempered using the flow time as a tempering parameter so as to solve both the sign and ergodicity problems simultaneously. In this talk, I explain the basics of the TLTM, and demonstrate the effectiveness and versatility of the algorithm by showing its successful applications to various models, such as the (0+1)-dimensional massive Thirring model [1], the Hubbard model away from half filling [2, 3], and the Stephanov model (a chiral random matrix model) [4]. I also would like to explain some of the recent improvements in the algorithm, which is expected to significantly reduce the numerical cost [3, 4].

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QP2.7 – A new method for calculating elements of matrix functions with application to the exponential of a transverse-field Ising model

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We introduce a method for calculating individual elements of matrix functions. Our technique makes use of a novel series expansion for the action of matrix functions on basis vectors that is memory efficient even for very large matrices. We showcase our approach by calculating the matrix elements of the exponential of a transverse-field Ising model, quantum transition amplitudes for large many-body Hamiltonians, and matrix inverses. We compare the performance of our method against the existing state-of-the-art demonstrating the advantages of the proposed approach.

QP3.1 (invited) – Towards the solution of the many-electron problem: properties of the hydrogen chain

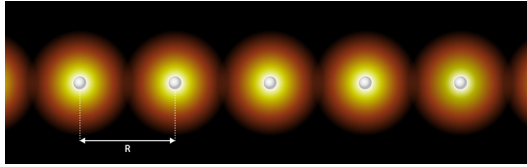
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Materials in which electrons strongly interact with one another exhibit a fascinating variety of structural, electronic and magnetic properties. Capturing the many underlying effects responsible for these properties is essential for understanding and predicting material behavior, but requires a reliable treatment of the many-electron Schrodinger equation. This contribution presents a computational study

[1,2] of the quantum-mechanical ground state of what is perhaps the simplest realistic model for a bulk material: an infinite chain of equally spaced hydrogen atoms. The combined use of state-of-the-art computational methods reveals a rich phase landscape, that sheds light on the variety of material properties. This computational study establishes the hydrogen chain as a key benchmark for further methodological developments and an important model for correlated electron systems. Its results can stimulate further efforts to characterize phase diagrams of low-dimensional materials.

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- [2] M. Motta et al (Simons collaboration on the many-electron problem) Phys. Rev. X 7, 031059 (2017)



A linear chain of hydrogen atoms, whose nuclei (protons) lie at equal distance R (colors indicate the electronic density. For large R , as seen in the figure, the system is essentially a collection of hydrogen atoms, and is insulating. As R is decreased, electronic wave functions begin to overlap, and an insulator-to-metal transition occurs. Figure adapted from D. Vollhardt, Physics 13, 142 (2020).

QP3.3 – Numerical simulations of spectroscopic properties in two-dimensional Mott insulator

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Mott insulators exhibit characteristic photoexcited states different from band insulators. However, our understanding of photoexcited states in two-dimensional

(2D) Mott insulators on square lattice is far from complete. This is due to theoretical difficulty in treating photoexcited carriers induced by photoirradiation, which are coupled with localized spins in the background. Clarifying the nature of photoexcited states is a typical many-body problem, where numerical simulations are useful. We first examine the spectral shape of the optical conductivity in the half-filled Hubbard model on square lattice by using time-resolved density-matrix renormalization group (tDMRG) [1]. At absorption edge, there is a shape peak resembling to an excitonic peak. The origin of the peak is attributed to magnetic one. The line shape of the calculated optical conductivity is similar to experimental data for cuprate Mott insulator such as Nd_2CuO_4 . We next investigate momentum-dependent transient spin dynamics in the half-filled Hubbard model on a square lattice by using time-dependent Lanczos-type exact diagonalization [2]. This work is motivated by the recent development of time-resolved resonant-inelastic x-ray scattering (trRIXS) in photoexcited antiferromagnetic Mott insulators. After turning off a pumping photon pulse, the intensity of a dynamical spin structure factor temporally oscillates with frequencies determined by the energy of two magnons in the antiferromagnetic Mott insulator. We find an antiphase behavior in the oscillations between two orthogonal momentum directions, parallel and perpendicular to the electric field of a pump pulse. The phase difference comes from the B_{1g} channel of the two-magnon excitation. Observing the antiphase oscillations will be a big challenge for trRIXS experiments.

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QP3.4 – Fermi Velocity renormalization in graphene from non-perturbative QMC calculations

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Application of Hybrid Monte Carlo (HMC) technique allowed us to perform the simulations of electronic properties of suspended graphene at as large as 102×102 lattices to directly observe the infrared renormalization of the Fermi Velocity for the first time in non-perturbative Quantum Monte Carlo (QMC) calculations [1]. We compared the results with experiment, and demonstrated the agreement in the specific case, when short-range electron-electron interactions are taken from cRPA approximation. Comparison of HMC data with perturbative calculations made within the Lattice Perturbation Theory (LPT) and in continuum QED demonstrates the importance of both lattice-scale physics and diagrammatic corrections beyond RPA level for the quantitative description of the Fermi Velocity renormalization. We also discuss the finite-temperature corrections, which appear to be of the opposite sign in perturbative series and in non-perturbative QMC signaling about possible breakdown of perturbation theory in strongly-correlated QED, which is the low-energy effective theory of electronic excitations in suspended graphene.

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QP3.5 – QMC study of the chiral Heisenberg Gross-Neveu universality class

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We investigate a quantum criticality of an antiferromagnetic phase transition in the Hubbard model on a square lattice with a d -wave pairing field by large-scale auxiliary-field quantum Monte Carlo simulations. Since the d -wave pairing field induces Dirac cones in the non-interacting single-particle spectrum, the quantum criticality should correspond to the chiral Heisenberg universality class in terms of the Gross-Neveu theory, which is the same as those expected in the Hubbard model on the honeycomb lattice, despite the unit cells being different (e.g., they contain one and two sites, respectively). We show that both the two phase transitions, expected to occur on the square and on the honeycomb lattices, indeed have the same quantum criticality. We also argue that details of the models, i.e., the

way of counting the total number of fermion components N and the anisotropy of the Dirac cones, do not change the critical exponents. The present estimates of the exponents for the $N = 8$ chiral Heisenberg universality class are $\nu = 1.05(5)$, $\eta_\phi = 0.75(4)$, and $\eta_\psi = 0.23(4)$ [1], which are compared with the previous numerical estimations [2, 3].

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QP3.6 – Neural Quantum States and Bootstrap in Matrix Quantum Mechanics

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Matrix quantum mechanics are a class of models with emergent spatial dimensions. As quantum mechanical theories, they provide a clean framework for understanding microscopic aspects of holography. However, as interacting many-body systems, exact solutions are often unavailable.

Starting with reviewing previously solved cases, we develop two complementary numerical methods for solving low-energy states in these theories. One method is a variational quantum Monte Carlo with neural networks as variational wavefunction ansatz. The variational energies are close to exact results in both bosonic and supersymmetric models, and the emergent locality is captured by an entanglement measure that we propose.

The other method is of bootstrap nature and directly works in the large N limit. Bootstrap algorithm gives rigorous and non-perturbative constraints of matrix observables at strong couplings.

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QP3.7 – Purifying Deep Boltzmann Machines for Thermal Quantum States

Yusuke Nomura

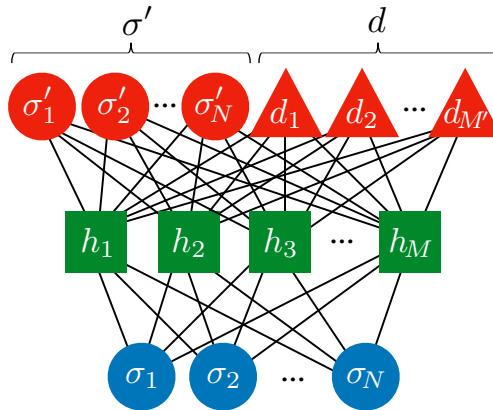
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Capturing both thermal and quantum fluctuations in finite-temperature quantum many-body systems is a great challenge in physics. Here, we present two novel approaches to encode many-body physics in thermal equilibrium into deep neural networks [1]. Both methods commonly represent purified finite-temperature states using a highly expressive neural-network wave function, exemplifying the idea of purification. In the first method, we find a completely deterministic way to construct deep Boltzmann machines representing the purified Gibbs state exactly. This certifies the outstanding flexibility of the ansatz, which can realize quantum-to-classical mapping [2]. The second method employs stochastic sampling to optimize the network parameters such that the temperature evolution is well approximated within the versatile expressibility of deep Boltzmann machines. These methods offer a compact representation of a many-body density matrix, suppressing the computational cost to scale only polynomially with respect to the system size. We perform numerical simulations for transverse-field Ising models and frustrated Heisenberg models and demonstrate that our methods are useful in investigating the finite-temperature properties of strongly-correlated quantum many-body systems, even when the frustration is present.

This work is done in collaboration with Nobuyuki Yoshioka (equal contribution) and Franco Nori.

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Deep Boltzmann machine for representing finite-temperature purified states.

Soft matter and biophysics

SM1.1 (invited) – PyStokes: phoresis and Stokesian hydrodynamics in Python

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This contribution introduces PyStokes, an open-source Python library for studying phoretic and hydrodynamic interactions between spherical particles, when these interactions are described, respectively, by the Laplace and Stokes equations. It uses a grid-free solution method, combining the integral representation of Laplace and Stokes equations, spectral expansion, and Galerkin discretization, to compute phoretic and hydrodynamic interactions between spheres with slip boundary conditions on their surfaces. The library also computes suspension scale quantities, such as rheological response, energy dissipation and fluid flow. The computational cost is quadratic in the number of particles and upto $1e5$ particles have been accommodated on multicore computers. The library has been used to model suspensions of microorganisms, synthetic autophoretic particles and self-propelling droplets. It

is freely available on GitHub at <https://github.com/rajeshrinet/pystokes/>.

SM1.3 – Continuous-time limit of kinetic Monte Carlo for Active-Matter systems

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The physics of active matter is determined by the non-equilibrium dynamics of the constituent particles. While constructing a non-equilibrium Monte Carlo (MC) dynamics for active matter is straightforward, the question remains to what extent this discrete-time dynamics faithfully captures real-world/continuous-time active systems. We focus on a kinetic MC version for the simplest kind of active matter: persistently moving, non-polar, interacting particles. On the multi-particle level, the MC dynamics captures not only Motility-induced phase separation[1, 2] but also features a non-equilibrium extension of the celebrated two-dimensional melting[2]. We show[3], however, that the continuous-time limit of existing MC dynamics[1, 2] is ill-defined, leading to the vanishing of trademark behaviours of active matter such as the motility-induced phase separation, ratchet effects, as well as to a diverging mechanical pressure. We show[3] how mixing passive/uncorrelated moves with active/time-correlated ones regularises this behaviour, leading to a well-defined continuous-time limit. We propose new active kinetic MC algorithms whose continuous-time limits are the Langevin descriptions of the work-horse active-matter models, namely Active-Ornstein Uhlenbeck, Active Brownian, and Run-and-Tumbles particles.

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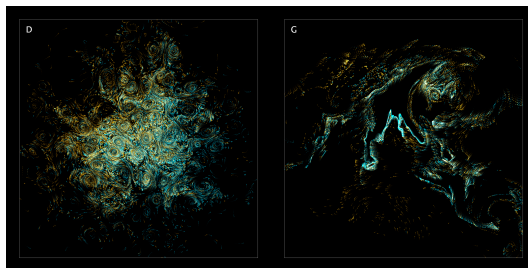
SM1.4 – Active turbulence, a Lévy walk away from inertial

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Active suspensions, like bacterial swarms, can self-organize into complex dynamical states like active turbulence – flows that are vortical, chaotic and multi-scale, hence reminiscent of inertial turbulence. Intriguingly, some experiments suggest that microorganisms in such suspensions can exhibit specialized movement patterns like Lévy walks that are means of efficient foraging and survival and lead to anomalous diffusion. However, detecting this anomalous behaviour has so far remained theoretically elusive. This is a key aspect, since in inertial turbulence particles are limited to inefficient classical diffusion. Using a hydrodynamic model of “active fluids”, we now show how anomalous super-diffusive and associated Lévy walks can masquerade as a crossover from ballistic to diffusive scaling in measurements of mean-squared-displacements. We trace the origins of this anomalous behaviour to hitherto undetected oscillatory “streaks” in the bacterial flow. Thus, while laying the theoretical framework for how activity drives living systems to defy bounds on inanimate matter, our work allows us to underline the essential differences between active and inertial turbulence.



Change in the characteristics of diffusion, for a “puff” of particles from (left) mildly active suspensions right (right) highly active suspensions.

SM1.5 – Collective Pattern Formation in a Binary Mixture of Self-Propelled Particles

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Self-organised collective patterns of active or self-propelled particles (SPPs) are observed in different length scales such as cells, bacterial swarms, army ants, flocking birds, even in pedestrian flow etc. [1]. Phase separation strategies in a mixture of SPPs with different properties are important to study in various branches of science. Different variants of the Vicsek model (VM) [2] are studied, mostly with the same particle velocities. However, in natural systems, two types the velocities can exist, for example, in a bacterial population, fast-moving (active) and slow (dormant) species or in daily traffic, some slow pedestrian and some speedy vehicle etc. In this work, a system with a binary mixture of polar SPPs is proposed with VM rules, where two types of particles have two different velocities.

In a two-dimensional square box of linear size L with periodic boundary conditions, N number of point-like particles are considered here. Two species with different velocities are present in the same proportion as $N/2$. The particles interact locally and align their directions of motion with that of their neighbours in the presence of some external noise, the same as the VM. The radius of the neighbourhood region is set to $R = 1$. Time is incremented as $t = t + \Delta t$, where $\Delta t = 1$ is the time between two successive updates. A particle i at the position \vec{r}_{xi} has a velocity \vec{v}_{xi} and moves with the velocity magnitude as per their type in the direction θ_{xi} . Where x represents the particle type as f for fast and s for slow. At the time t , the velocity of the i th particle is determined by evaluating the direction.

$$\theta_{xi}(t + \Delta t) = \langle \theta(t) \rangle_R + \Delta \theta \quad (1)$$

where $\langle \theta(t) \rangle_R$ denotes the average orientation over the particles within the radius R around the i th particle and $\Delta \theta$ is a random orientation chosen with a uniform probability from the interval $[-\eta\pi, +\eta\pi]$. Knowing the velocity $\vec{v}_{xi}(t)$ at every time step, the position of the i th particle \vec{r}_{xi} is updated as

$$\vec{r}_{xi}(t + \Delta t) = \vec{r}_{xi}(t) + \vec{v}_{xi}(t)\Delta t \quad (2)$$

Fast and slow SPPs have different velocity magnitude as v_f and v_s respectively. A system of size $L = 128$ and 256 is considered with a fixed density $\rho = N/L^2 = 0.5$ for the Monte Carlo simulation. The velocities are considered as $v_s = 0.01$ and $v_f = 100v_s$.

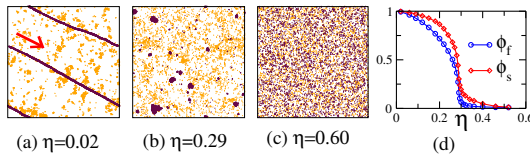
At different values of angular noise η , different phase-separated collective patterns are observed, which is shown in the figure. Orange and maroon colour represent fast and slow SPPs, respectively. At a small angular noise, in the figure. (a) with $\eta = 0.02$, a dense continuous lane pattern of slow SPPs has been observed with small dense clusters of fast SPPs. Here, the SPPs move in the same direction (red arrow) along the lane. At an intermediate angular noise, in the figure. (b) with $\eta = 0.29$, the lane is broken, and dense clump structures of slow SPPs appear in the system with less dense clusters of fast SPPs. However, at high angular noise, in the figure. (c) with $\eta = 0.60$, a homogeneously mixed phase of the two types of SPPs is observed. This type of pattern formation does not appear in the VM where all the SPPs have the same velocity.

As the angular noise strength, η is tuned from 0 to 1, the system undergoes a transition from an orientationally ordered state to a disordered state. The order-parameter is defined as

$$\phi_x = \frac{1}{N_x} \left| \sum_{j=1}^{N_x} \frac{\mathbf{v}_j}{|\mathbf{v}_j|} \right| \quad (3)$$

The order-parameter of the fast SPPs (ϕ_f) and the slow SPPs (ϕ_s) are plotted against the angular noise η in the figure. (d). Phase transition is observed for both types at $\eta_c = 0.29$ in this system. It is also observed that the polar order of slow particles is greater than the fast type for a given value of η . Generally, in the VM, polar order is relatively less with low particle velocity, whereas high velocity can retain the order up to a large η . In the VM, the phase transition is discontinuous for high velocity with a negative Binder cumulant at the transition. Whereas it has a positive dip at the transition in this model with a binary mixture of SPPs.

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Morphologies at different angular noise: (a) $\eta = 0.02$, (b) $\eta = 0.29$ and (c) $\eta = 0.60$ with system size $L = 128$. Orange and maroon colour represents the fast and slow SPPs respectively. (d) Plot of ϕ_f and ϕ_s against η with system size $L = 256$.

SM1.6 – Effect of Vicsek-like Activity on the Dynamics of a Flexible Polymer

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Wolfhard Janke¹

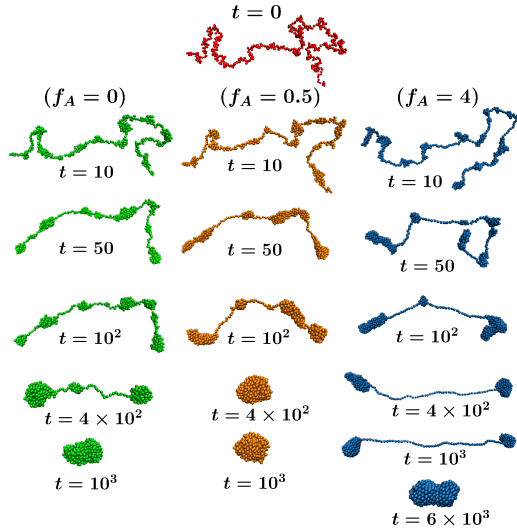
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The dynamics of many biological filaments can be understood within the framework of active polymer models. We construct a flexible bead-spring model with attractive Lennard-Jones interactions in which the activity among the beads is introduced via a Vicsek-like alignment rule. Due to the additional activity, the beads will try to align their velocities towards a particular direction with time. Following a quench from the high-temperature coil phase to a low-temperature state, we study its kinetics via molecular dynamics (MD) simulations using Langevin thermostat. For the passive polymer, we confirm the earlier observation from Monte Carlo studies that the low-temperature equilibrium state is a compact globule. Our results for active beads reveal that the typical final steady state is also of globular form. The nonequilibrium pathway, however, changes due to the effect of activity. In this work, we focus on the nonequilibrium coarsening kinetics and the associated scaling laws for the collapse time and growth of clusters. Interestingly we observe nonmonotonic behavior in coarsening with the variation of the strength of activity. In the final steady state, we study the motion of the polymer globule which changes from super-diffusive to ballistic behavior with increasing activity compared to a diffusive motion for the passive case.

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Conformations at different times during the collapse of a flexible polymer for the passive ($f_A = 0$) as well as active cases (non-zero values of f_A).

SM1.7 – Vicsek model with Malthusian Dynamics

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Active matter is the branch of physics that studies systems in which individuals are self-propelled, that is, they do not depend on an external agent to move. Some examples are a birds flocks and schools of fish. In the last few years much attention has been paid to this subject.

The Vicsek model [1] was the first and the simplest model to explain the collective movement and formation of herds using the phase transition perspective. This model received a lot of attention and has been shown to exhibit symmetry breaking, developing long-range order, even with only short-range interactions [3].

While the Vicsek model has been extensively studied over the years [5], a theoretical analysis has shown that it would be of interest to relax the conservation of the number of individuals [4]. In addition to its theoretical interest, there are

experiments in which the number of individuals is not conserved, including colonies of bacteria and other systems in which individuals are created and destroyed as they move.

In this work we study a system with Malthusian population dynamics (that is, the probability of a particle dying is proportional to the density in the vicinity of the particle) using computational methods, seeking to understand how the system's stationary density interacts with noise intensity, such as formation of groups interferes with the number of living individuals, as the implementation of noise interferes with the properties of the system. In addition, we seek to classify the phase transition and say whether the system exhibits banding.

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SM2.1 (invited) – Designing molecular knots

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The self-assembly of objects with a set of desired properties is a major goal of material science and physics. A particularly challenging problem is that of self-assembling structures with a target topology. Here we show by computer simulation that one may design the geometry of string-like rigid patchy templates to promote their efficient and reproducible self-assembly into a selected repertoire of non-planar closed folds including several knots. In particular, by controlling the template geometry, we can direct the assembly process so as to strongly favour the formation of constructs tied in trefoil or pentafoil, or even of more exotic knot types. A systematic survey reveals that these "privileged", addressable topologies are rare, as they account for only a minute fraction of the simplest knot types. This knot discovery strategy has recently allowed for predicting complex target topologies [1,2,3], some of which have been realized experimentally [4,5].

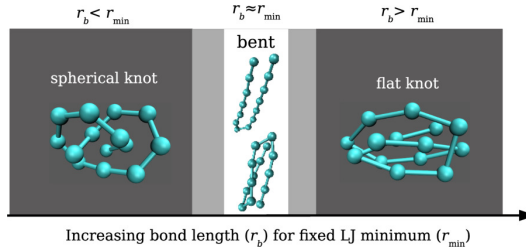
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SM2.3 – Knot are Generic Stable Phases in Semiflexible Polymers

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While investigations of knots in polymers have lured scientists for decades, the existence of phases characterized by a stable knot of specific type has attracted attention only recently. In this work, we treat two popular models that encompass the complete spectrum of real polymers (flexible to stiff) via extensive replica exchange Monte Carlo simulations, and show that the existence of stable knots in the phase diagram depends only on the ratio r_b/r_{\min} , where r_b is the equilibrium bond length and r_{\min} is the distance for the strongest nonbonded contacts in an attractive Lennard-Jones (LJ) potential. Our results provide evidence that irrespective of the specific model, bead-stick or bead-spring, if the ratio r_b/r_{\min} is outside a small window around unity then one always encounters for semiflexible polymers stable knotted phases at low temperatures.



SM2.4 – Non-equilibrium dynamics of fluid membranes: traveling wave, Turing pattern, and membrane undulation

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Biomembranes experience out-of-equilibrium conditions in living cells. We present (1) the coupling of reaction-diffusion dynamics with membrane deformation and (2) the undulation of a fluid membrane pushed by filament growth. (1) The mechanochemical feedback of curvature-inducing proteins changes stable patterns relative to those that occur on a non-deformable curved surface [1]. Budding and multi-spindle shapes are also induced by Turing patterns. The speed of traveling waves is positively or negatively correlated with the local membrane curvature depending on the spontaneous curvature and bending rigidity [2]. In addition, self-oscillation of the vesicle shape occurs, associated with the reaction-diffusion waves. (2) Their undulation spectra are different from those in thermal equilibrium [3]. When the tension is constrained, the low-wave-number modes are suppressed or enhanced at small or large growth step sizes, respectively, for high membrane surface tensions. In contrast, they are always suppressed for the tensionless membrane, wherein the wave-number range of the suppression depends on the step size. When the membrane area is constrained, in addition to these features, a specific mode is excited for zero and low surface tensions.

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[3] H. Noguchi and O. Pierre-Louis, *Sci. Rep.* 11, 7985 (2021).

SM2.5 – Mesoscopic modelling of highly ordered mesophases of board-shaped polymers

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Many industrially-relevant polymers, such as soluble semiconductors, are composed of molecules with board-like (sandic) shapes. These materials can have various different morphologies, ranging from amorphous to crystalline via a family of sandic liquid crystalline mesophases. [1] Developing efficient models for studying these sandic mesophases is important in view of potential technological applications, and for understanding the fundamental physics of liquid crystals.

Here we develop a generic model which enables the simulation of a highly ordered Σ_r sandic mesophase [1] using a Monte Carlo technique. Polymer chains are described by a hindered-rotation model, where interaction centres represent entire monomers, including side chains. Phenomenological ‘soft’ anisotropic nonbonded potentials are then used to reproduce the generic symmetries of molecular order in the Σ_r mesophase. [2]

Our analysis confirms that we have successfully simulated a Σ_r mesophase which is robust across a broad range of parameters. This mesophase comprises highly regular lamellae, with strong orientational and positional Smectic A order and an approximate 2D lattice of monomers within each lamella, and a tilted Smectic C order between lamellae (Figure 1). We have performed a detailed comparison between calculated X-ray scattering patterns and experimental data, in order to investigate structural similarities between the simulated and real systems. [1,3]

- [1] M. Ebert *et al.*, *Liquid Crystals* **7** (1990) 63.
- [2] C. Greco *et al.*, *Macromolecules* **52** (2019) 968.
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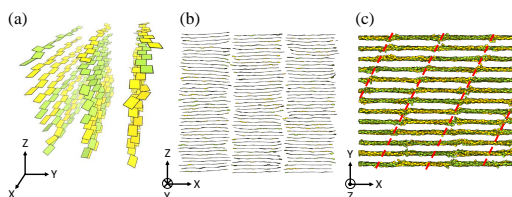


Figure 1. Snapshots of simulated Σ_r sandic mesophases, showing (a) general

lamellar structure, (b) orientational and positional Smectic A order within lamellae, and (c) tilted Smectic C order between lamellae.

SM2.6 – Dilute solution of ring and star polymers in confined geometries: theory and simulations

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The calculations of the dimensionless layer monomer density profiles for a dilute solution of phantom ideal ring polymer chains and star polymers with $f=4$ arms in a Θ -solvent confined in a slit geometry of two parallel walls with two repulsive surfaces and with one repulsive and the other one inert surface as well as in a solution of big colloidal particles with different adsorbing or repelling properties in respect to polymers were performed. The density-force relation for the above mentioned cases was analyzed and the universal amplitude ratio B was obtained. Taking into account the small sphere expansion allowed to obtain the monomer density profiles for a dilute solution of phantom ideal ring polymers immersed in a solution of small spherical particles, or nano-particles of finite size which are much smaller than the polymer size and other characteristic mesoscopic length of the system. The molecular dynamic simulations of a dilute solution of linear ($N=300$), ring ($N=300$ and 360) and star-shaped polymers with four arms with number of monomers $N=4 \times 300+1$ were performed. The interaction of the neighboring monomers was modeled by the finite extensible nonlinear elastic (FENE) and the Weeks-Chandler-Andersen (WSA) potentials for the attractive and repulsive part, respectively. The long-range interactions between monomers along the chain took into account via the 12-6 Lennard-Jones potential and the interaction of the monomers with the walls was modeled by the 9-3 Lennard-Jones potential with a variable cut-off. The obtained analytical and numerical results for ring and star polymers are compared with the results for linear polymer chains in confined geometries.

SM3.1 – Comparison of Benchmark HP Lattice Proteins on Simple-Cubic and Face-Centered Cubic Lattices Using Replica-Exchange Wang-Landau Sampling

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The hydrophobic-polar (HP) lattice protein model [1] is a coarse-grained model for simulating protein folding. While quite simple, the model is nevertheless extremely challenging to study, and has been historically examined on simple-cubic (SC) lattices. We implement a powerful, unbiased set of Monte Carlo trial moves on the face-centered cubic (FCC) lattice and use the replica-exchange Wang-Landau (REWL) algorithm [2] to determine the ground state and full density of states for a set of biologically-motivated benchmark HP sequences on the FCC lattice. This approach allows us to examine the density of states for the full range of energies of the sequences more successfully than previous simulations on the SC lattice. From estimates for the density of states, thermodynamics are calculated and examined for a range of temperatures over which folding processes occur. A direct comparison is made with published results [3] for the same sequences on the SC lattice, and we will describe the similarities and differences in the behaviors on the two different lattices.

[1] K. F. Lau and K. A. Dill, *Macromolecules* **22**, (1989) 3986.

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SM3.2 – Destabilization potential of phenolics on $A\beta$ Fibril: Mechanistic insights from Molecular Dynamics Simulation

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The clinical signature of Alzheimer's disease (AD) is the deposition of aggregated $A\beta$ fibrils that are neurotoxic to the brain. It is the major form of dementia affecting older people worldwide, impeding their normal sustenance. Finding and testing various natural compounds to target and disrupt stable $A\beta$ fibrils seems to be a promising and attractive therapeutic approach. The four phenolic compounds from plant sources were taken into consideration for the present work, which initially screened by Docking. The ellagic acid (REF) came out to be the best binder of $A\beta$ oligomer from docking studies. Further, to test the destabilization effect of REF on $A\beta$ oligomer, MD simulation was conducted. The simulation outcome obtained henceforth clearly indicates a drift of terminal chains from the $A\beta$ oligomer, leading to the disorganization of the characteristically organized cross β structure of $A\beta$ fibrils. Increased value of RMSD, Rg, RMSF, and SASA are indicative of destabilization of the $A\beta$ fibril in the presence of REF. The disruption of salt bridges and a notable decline in the number of hydrogen bonds and β -sheet content explain the conformational changes in the $A\beta$ fibril structure, ceasing their neurotoxicity. The MM-PBSA results revealed the binding of REF to chain A of the $A\beta$ oligomer. The destabilization potential of ellagic acid, as explained by the MD simulation study, establishes it as a promising drug to cure AD. The molecular level details about the destabilization mechanism of ellagic acid encourage intensive mining of other natural compounds as well for therapeutic intervention for AD.

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Destabilization potential of phenolics on $A\beta$ Fibril

SM3.3 – Nonequilibrium molecular dynamics simulation to reveal a role of water molecules in laser-induced disruption of amyloid fibrils

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Water plays a crucial role in the formation and destruction of biomolecular structures. The mechanism for destroying biomolecular structures was thought to be an active breaking of hydrogen bonds by water molecules. However, using nonequilibrium molecular dynamics simulations, in which an amyloid- β amyloid fibril was destroyed via infrared free-electron laser (IR-FEL) irradiation, we discovered a new mechanism, in which water molecules disrupt protein aggregates [1]. The intermolecular hydrogen bonds formed by C=O and N-H in the fibril are broken at each pulse of laser irradiation. These bonds spontaneously re-form after the irradiation in many cases. However, when a water molecule happens to enter the gap between C=O and N-H, it inhibits the re-formation of the hydrogen bonds. Such sites become defects in the regularly aligned hydrogen bonds, from which all hydrogen bonds in the intermolecular β -sheet are broken as the fraying spreads. This role of water molecules is entirely different from other known mechanisms. This new mechanism can explain the recent experiments showing that the amyloid fibrils are not destroyed by laser irradiation under dry conditions. Additionally, we found that helix structures form more after the amyloid disruption; this is because the resonance frequency is different in a helix structure. Our findings provide a theoretical basis for the application of IR-FEL to the future treatment of amyloidosis.

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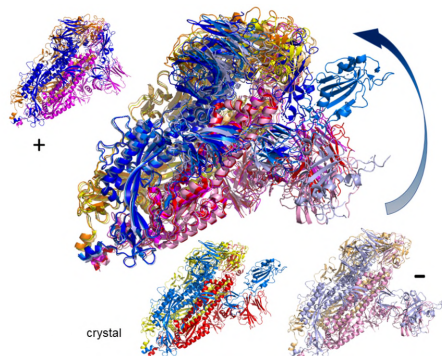
SM3.4 – Flexibility and mobility of SARS-CoV-2-related protein structures

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The worldwide CoVid-19 pandemic has led to an unprecedented push across the whole of the scientific community to develop a potent antiviral drug and vaccine as soon as possible. Existing academic, governmental and industrial institutions and companies have engaged in large-scale screening of existing drugs, in vitro, in vivo and in silico. Here, we are using in silico modelling of possible SARS-CoV-2 drug targets, as deposited on the Protein Databank (PDB), and ascertain their dynamics, flexibility and rigidity. For example, for the SARS-CoV-2 spike protein—using its complete homo-trimer configuration with 2905 residues—our method identifies a large-scale opening and closing of the S1 subunit through movement of the S^B domain. We compute the full structural information of this process, allowing for docking studies with possible drug structures. In a dedicated database, we present similarly detailed results for the further, nearly 300, thus far resolved SARS-CoV-2-related protein structures in the PDB.

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Possible motion along mode m_7 at $E_{\text{cut}} = 2$ kcal/mol in the *open* spike ecto domain (6vyb) in side view. The secondary protein structure is highlighted by the chosen "cartoon" representation. Colors yellow, blue and red denote chains A, B, and C, respectively, while color combinations light orange/orange,

pink/purple and light blue/dark blue show the extreme structural positions for the movements along the normal mode m_7 at $E_{\text{cut}} = 2$ kcal/mol. The smaller protein structures show the initial (crystal) structure as well as the extremes (+, -) along the possible motion directions for m_7 in the same colors as in the superimposed structure.

SM3.5 – Atomic mechanism of the complete association of intrinsically disordered peptide to protein

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In this work, we provide the complete picture of the atomic mechanism of the association of intrinsically disordered peptide to the protein surface by using Parallel Cascade Selection Molecular Dynamics simulations[1]. We show that the found binding mechanism is not well-fitted with either conformational selection or induced fitting. The association process includes three stage, first conformational selection to go to the partially-bound state of the complex, after that, induced fitting and dehydration of the binding interface. The work is published on Journal of Chemical Theory and Computation [1].

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SM3.6 – Modelling of the A-B transition in a short DNA molecule

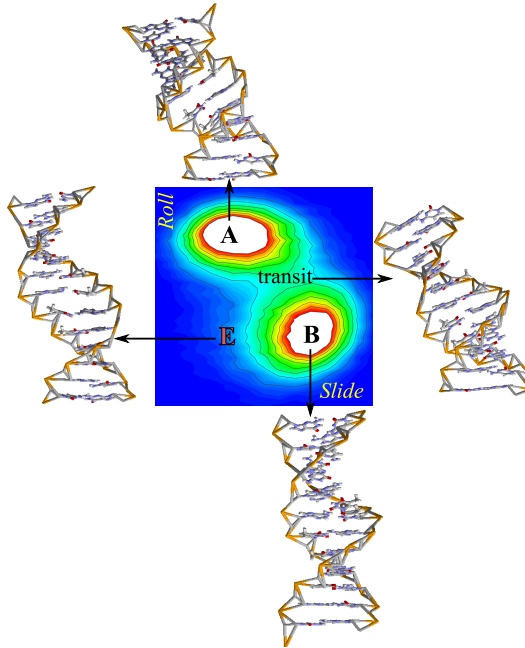
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In DNA-protein complexes, the DNA molecule takes the A form mostly when bound to polymerases or endonucleases. Some DNA sequences in crystals and in complexes with proteins exist in the forms intermediate between the B- and A-DNA (like E-DNA). It was implied that the B to A transition for any DNA molecule should go through E-DNA also in kinetics. In the present work [1], we simulated the kinetics of the B-A transition in a B-philic DNA oligomer in the framework of the "sugar" coarse-grained model [2] that reproduces ribose flexibility, preserves sequence specificity, employs implicit water and explicit ions. In the described system, the B to A conformational transformation proved to correspond to a first-order phase transition. The molecule behaves like a small cluster in the region of such a transition, jumping between the A and B forms in a wide range of available volumes [3]. The E-DNA has not been observed in the transition between the B and A forms. So, the existence of the intermediate DNA forms requires specific conditions shifting the common balance of interactions: certain nucleotide sequence in specific solution or/and the interaction with some proteins.

The work was supported by the Program of Fundamental Researches of the Russian Academy of Sciences (project no. 0082-2014-0013, state registration no. AAAA544 A17-117042510268-5). The calculations were carried out in the Joint Supercomputer Center of the Russian Academy of Sciences.

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- [2] N.A. Kovaleva, I.P. Koroleva, M.A. Mazo, E.A. Zubova J. Mol. Model. 23 (2017), 66.
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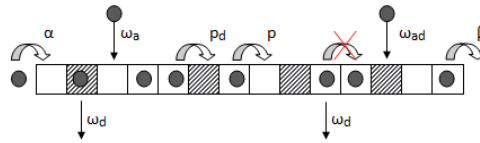
SM3.7 – Single-channel dynamically disordered exclusion process with Langmuir kinetics

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Intracellular transport is an essential process for cellular functions and is driven by molecular motors that carry cargoes along cytoskeletal filaments. The molecular motors, driven by ATP hydrolysis, come across roadblocks that slow down the transportation process. The transcription of the genetic information stored in DNA is carried out by a molecular motor called RNA polymerase (RNAP). The RNAP synthesizes RNA transcript to create messenger RNA (mRNA) which is composed of a sequence of codons. The mRNA is decoded in ribosome to form an amino acid chain. During translation, transfer RNAs (tRNAs) carry amino acids to mRNA to form protein. The DNA binding proteins serve as a bottleneck which may cause a jam on the microtubule track. The slow transport of

cargoes within the cell due to jamming may result in neurodegenerative diseases like Alzheimer's. The free diffusing motor proteins can attach to the microtubule filament and can also detach from the filament to the cytoplasm. The process can be modeled using discrete lattice gas model TASEP (Totally asymmetric simple exclusion process) with dynamic disorder and bulk particle attachment and detachment in a single-channel system (shown in figure). The particles representing motor proteins in a cell are distributed randomly obeying the hard-core exclusion principle. The unconstrained defect dynamics are considered in which a defect can bind or unbind dynamically to any site irrespective of the particle occupancy. The continuum mean-field equations are derived and solved numerically to obtain steady-state phase diagrams and density profiles. The effects of various parameters namely particle attachment rate, defect binding and unbinding rates, and binding constant have been investigated. Importantly, the appearance of shock in the steady-state has been observed. The shock dynamics have been examined thoroughly and the defect strength is found to have a significant effect on the shock position. The mean-field solutions are validated using extensive Monte Carlo simulations.



Schematic diagram of a single-channel TASEP with dynamic disorder and Langmuir kinetics. α and β are the entrance and exit rates with hopping rate $p_d < p$, w_a ($> w_{ad}$) and w_d are particle attachment and detachment rates respectively. The dynamic defect is represented as a shaded site. Crossed arrows shows forbidden transitions.

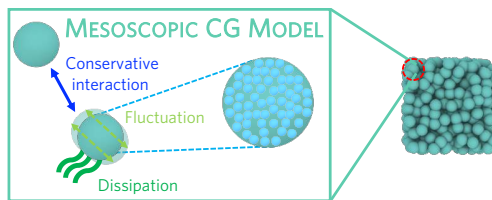
SM4.1 (invited) – Toward high-fidelity many-body mesoscopic models of fluids from bottom-up coarse-graining

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In the field of multiscale modeling of condensed matter, the complex organization and transport phenomena require a mesoscopic description beyond the molecular scale. These models are often substantiated from mesoscale (fluid mechanics) and macroscale physics (statistical field theory), but their underlying microscopic foundation is not yet well-defined. In this talk, I will deliver a systematic connection between the mesoscopic model and microscopic nature by developing a new bottom-up coarse-graining method. The explicit many-body conservative interactions are determined by combining the many-body dissipative particle dynamics and classical density functional theory. Witnessed from molecular coarse-graining models, other design principles for conservative interactions are pursued in order to faithfully recapitulate the mesoscopic structure of fluid. Furthermore, dissipative and fluctuation forces are obtained by the proposed novel parameterization algorithm. This algorithm consists of pairwise decomposable friction kernels under both non-Markovian and Markovian limits, where the dynamic features at the reduced resolution are finely recapitulated. The construction of many-body dissipative particle dynamic models of fluids that can account for microscopic nature allows for the design of bottom-up-driven mesoscopic models and naturally bridges microscopic and mesoscopic physics. This novel approach opens up a new rigorous design principle for constructing high-fidelity bottom-up multiscale models for soft condensed matter.

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Mesosopic coarse-grained model for fluids with underlying interactions that govern the static and dynamic correlations

SM4.3 – Effect of polymer chemical design on self-assembly of polymer-tethered nanoparticles in nanotubes

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Self-assembly of nanoparticles (NPs) has attracted a great deal of attention due to the high degree of freedom in structure and the variety of functionalities that can be generated [1,2]. These studies have shown that there is a clear relationship between self-assembly, physical properties, and functionality. In other words, as the morphology of the aggregates changes due to thermodynamic conditions and the surrounding environment, the physical properties such as optical response and mechanical strength also change. Therefore, understanding and controlling the self-assembly of NPs is a very important issue in the field of medical materials and material chemistry.

A common way to control the form of self-assembly of NPs is to design colloidal particles with anisotropic shapes and chemical interactions. Among them, the study of polymer tethered NPs, which connect an array of polymers to the surface of a functional polymer, has attracted much attention [3,4]. This is because PTNPs also have diverse self-assembled structures depending on various types of polymers. For example, the polydispersity of the shape in addition to the mobility of the nanoparticle surface has been shown to form dodecagonal quasicrystal[5].

In addition, due to the recent development of synthesis technology, it was reported that Janus gold NPs decorated on the opposite side of NPs can be synthesized using different polymer chains by using polymer single-crystal solid-phase graft polymerization and graft polymerization methods [6]. In addition, we showed that it is possible to control the properties of the material by grafting different polymers onto the NPs. The structures formed from these NPs are very diverse and difficult to classify. By confining the NPs in NTs, we reduced the number of self-assembled structures formed by contracting the spatial degrees of freedom, and simulated the effect of interaction on the structure formation. NP models with three types of surfaces, hydrophobic, hydrophilic, and Janus-type (amphiphilic), were created to investigate the morphologies that emerge by changing the radius of the NTs. The results showed that focusing on the arrangement of NPs, the three types of ordered structures were formed regardless of the type of polymer[7]. In this study, we focused on the properties of the polymers and investigated their influence on the formation of ordered structures. In particular, we explore whether the direction of Janus polymer grafted onto NPs affects the formation of self-assembled structures, and investigate the possibility of structural control.

The purpose of this study is to investigate the effect of polymer chemistry and graft order on the structure by creating a simple quasi-one-dimensional system and performing simulations with only the graft polymer as a parameter.

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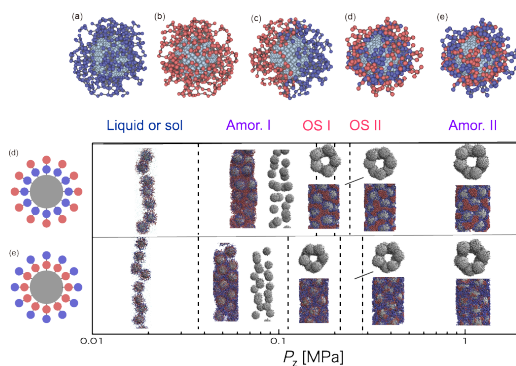


Fig. 1 Polymer-tethered NP model: (a) Hydrophilic, (b) Hydrophobic, (c) Janus surfaces, (d) diblock (HI-HO), (e) diblock (HO-HI). Eighty seven polymer chains are uniformly tethered to the surface of NP. Schematic phase diagram of three different polymer tether NP solutions confined in NT at $L = 3.5$.

SM4.4 – Bridging the gap between molecular dynamics and hydrodynamics in nanoscale Brownian motions

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Through molecular dynamics simulations, we examined hydrodynamic behavior of the Brownian motion of fullerene particles based on molecular interactions. The solvation free energy and velocity autocorrelation function (VACF) were calculated by using the Lennard–Jones (LJ) and Weeks–Chandler–Andersen (WCA) potentials for the solute–solvent and solvent–solvent interactions and by changing the size of the fullerene particles. We also measured the diffusion constant of the fullerene particles and the shear viscosity of the host fluid, and then the hydrodynamic radius a_{HD} was quantified from the Stokes–Einstein relation. The a_{HD} value exceeds that of the gyration radius of the fullerene when the solvation free energy exhibits largely negative values using the LJ potential. In contrast, a_{HD} becomes comparable to the size of bare fullerene, when the solvation free energy is positive using the WCA potential. Furthermore, the VACF of the fullerene particles is directly comparable with the analytical expressions utilizing the Navier–Stokes equations both in incompressible and compressible forms. Hydrodynamic long-time tail $t^{-3/2}$ is demonstrated for timescales longer than the kinematic time of the momentum diffusion over the particles’ size. However, the VACF in shorter timescales deviates from the hydrodynamic description, particularly for smaller fullerene particles and for the LJ potential. This occurs even though the compressible effect is considered when characterizing the decay of VACF around the sound-propagation timescale over the particles’ size. These results indicate that the nanoscale Brownian motion is influenced by the solvation structure around the solute particles originating from the molecular interaction.

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SM4.5 – Optical Kerr Effect Spectra of Supercooled Water at Ambient Pressure: Contributions of Low-Density and High-Density Liquids

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In this paper, we used the instantaneous-normal-mode (INM) analysis to dissect the optical Kerr effect (OKE) spectra of liquid and supercooled water at ambient pressure [1], where the spectra were obtained by molecular dynamics (MD) simulations [2]. Our studies focused on the contributions of low-density liquid (LDL) and high-density liquid (HDL), which local structures are characterized with tetrahedral order and disorder, respectively. Water configurations were generated by MD simulations with TIP4P/2005 force fields, and molecules were classified into LDL and HDL according to the microscopic structural descriptor [3]. The OKE spectra were calculated with a collective polarizability model involving the intrinsic polarizabilities of individual molecules and the dipole-induced-dipole (DID) interactions between molecules. By considering water as a mixture of LDL and HDL, the OKE spectra in the linearized INM theory is a sum of three contributions, resulted from each of the two partial liquids and a cross correlation associated with both of them. In the INM approximation, the formula of the OKE spectrum is similar as that for the static structure factor of a binary mixture. Two separation schemes on the collective polarizability model, where they are complementary to each other, were utilized to scrutinize the OKE spectra of supercooled water, and the results provide an insight into molecular mechanism causing the bands in the OKE spectra and their relations to the local structures of LDL and HDL. Our results indicate that the intermolecular stretching band in the OKE spectrum of supercooled water is mainly caused by the DID mechanism and dominated by LDL. This observation is consistent with experimental results measured by the time-resolved OKE spectroscopy [4].

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SM4.6 – Atomistic insights into the structure and elasticity of densified 45S5 Bioactive Glass

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Bioactive glasses have applications in restorative bone medicine, in view of their bioactivity, these materials are able to react with the body environment. 45S5 bioactive glass from Soda-lime phosphosilicate glasses represent a model system which started to take off commercially. Regardless of their importance as bioactive materials, the relationship between the structure features, density, and cooling process has not been studied in detail. In this investigation, we used molecular dynamics simulations to study the elastic and structural properties of densified 45S5 bioactive glass through a range of densities. A systematic analysis of the structure-density relationship was performed, correlating the change in the bioactive glass properties with the structural change to perform its mechanical properties while preserving their bioactive behavior. The findings show a repolymerization in the glass network structure, by increased network connectivity and a tetrahedral to octahedral polyhedral transition. We were able to tailor the elastic properties while keeping the bioactivity of the glass. The results presented here will provide some guidance to develop bioactive glasses with enhanced mechanical properties.

SM4.7 – Effect of long-wavelength fluctuations on slow relaxation in a 2D glass-forming liquid

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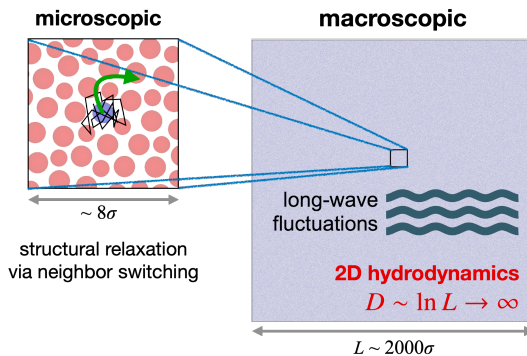
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When a liquid is cooled rapidly to form a glass, its structural relaxation becomes retarded, producing a drastic increase in viscosity. This slowdown is usually attributed to change in microscopic structural processes, and long-wavelength modes had never been considered to be relevant. In this contribution, we will show that strong long-wavelength fluctuations exist in a 2D glass-forming liquid, by means of large-scale molecular simulations of a binary mixture of millions of particles [1,2]. Its velocity autocorrelation exhibits a t^{-1} long-time tail, which covers up the microscopic structural changeover associated with the glassy slowdown. This long-time tail persists toward the glass transition to cause logarithmic divergence of transport coefficients, and hence qualitative nature of Stokes-Einstein violation is altered [2], suggesting that the 2D glass transition may be fundamentally affected by the long-wavelength fluctuations.

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Glassy relaxation in two dimensions is a superposition of microscopic structural

changes and diffusive relaxation of hydrodynamic fluctuations, which lead to logarithmic divergence of diffusivity D as a function of the box length L .

Statistical physics and complex systems

SP1.1 – Acceptance rate is a thermodynamic function in local Monte Carlo algorithms

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We study the properties of Markov chain Monte Carlo simulations of classical spin models with local updates [1]. We derive analytic expressions for the mean value of the acceptance rate of single-spin-flip algorithms for the one-dimensional Ising model. We find that for the Metropolis algorithm, the average acceptance rate is a linear function of energy. We further provide numerical results for the energy dependence of the average acceptance rate for the three- and four-state Potts model and the XY model in one and two spatial dimensions. In all cases, the acceptance rate is an almost linear function of the energy in the critical region. The variance of the acceptance rate is studied as a function of the specific heat. While the specific heat develops a singularity in the vicinity of a phase transition, the variance of the acceptance rate stays finite. The analytical result for the acceptance rate in the one-dimensional Ising model can be viewed as a complement to the Glauber dynamics. It is just the frequency of the spin flips discussed implicitly in [2].

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SP1.2 – Changeover phenomenon in randomly colored Potts models

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A hybrid Potts model where a random concentration p of the spins assume q_0 colors (Potts states) and a random concentration $1 - p$ of the spins assume $q > q_0$ colors is introduced. It is known that when the system is homogeneous, with an integer spin number q_0 or q , it undergoes a second or a first order transition, respectively. It is argued that there is a concentration p^* such that the transition nature of the model is changed at p^* . This idea is demonstrated analytically and by simulations for two different types of interaction: the usual square lattice nearest neighboring and the mean field all-to-all interaction. Exact expressions for the second order critical line in concentration-temperature parameter space of the mean field model together with some other related critical properties, are derived.

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SP1.3 – Phase diagram of the polyhedral spin models on square lattice with diluted bonds

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The study of phase transition is an important subject in condensed matter physics as some materials are more versatile when they are at certain phase. The low temperature ferromagnetic phase of magnetic material is a firm example of these. Passing by the Curie temperature, the paramagnetic phase of magnetic materials will change to a ferromagnetic phase. There are three main variables controlling a magnetic phase transition, namely the symmetry of spins, coupling interaction and the lattice structure. It is known that the discreteness can create low temper-

ature magnetic order, exemplified by the existence of a true- long range order for the 2D 6-state clock model at lower temperature [1, 2] In this talk we present our study of the ferromagnetic polyhedral spins model on square lattice with bond dilution. Polyhedral spins are the discrete counterpart of the continuous Heisenberg spin model. Two polyhedral spin models, i.e., the icosahedron and dodecahedron model are discussed. As previously reported, the non-diluted (pure) ferromagnetic case of these models exhibits finite temperature phase transition [3]. We use Monte Carlo simulation with a newly introduced algorithm, two-size PCC algorithm [4]; and probe whether the existing phase transitions are significantly affected by the bond dilution. We simulate the models with various bond concentrations and calculate their corresponding critical temperatures. The phase diagram of the models are presented as a plot of the obtained critical temperatures with respect to their corresponding bond concentrations.

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SP1.4 – Entropy of Dense Trails on the Square Lattice

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We estimate the entropy of self-avoiding trails on the square lattice in the dense limit, where a single trail passes through all edges of the lattice, as a function of the density of crossings.

For this, the largest eigenvalues of transfer matrices of size up to 6.547×10^8 was obtained, utilising 76GB memory.

SP1.5 – Ising model on an (interacting) SAW

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We study a lattice model of a magnetic elastomer, where Ising spins are located on the sites of a lattice self-avoiding walk. We consider the regime where both conformations and magnetic degrees of freedom are dynamic, thus the Ising model is defined on a dynamic lattice, and conformations generate an annealed disorder. We perform Monte Carlo simulations across the theta-point and find the joint ferromagnet-to-paramagnet and globule-coil transition.

SP1.6 – Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class

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We study the boundary critical behavior of the three-dimensional Heisenberg universality class, in the presence of a bidimensional surface. By means of high-precision Monte Carlo simulations of an improved lattice model, where leading bulk scaling corrections are suppressed, we prove the existence of a special phase transition, with unusual exponents, and of an extraordinary phase with logarithmically decaying correlations. These findings contrast with naïve arguments on the bulk-surface phase diagram, and allow us to explain some recent puzzling results on the boundary critical behavior of quantum spin models.

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SP1.7 – Replica exchange Wang-Landau sampling of long HP lattice protein sequences

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Despite the apparent simplicity of the HP lattice protein model [1], the vast, complex free-energy landscapes of HP sequences have captured the attention of researchers across many disciplines. As obtaining the ground state of an HP model is an extremely challenging, NP-complete problem [2], this model has emerged as an algorithmic testbed, wherein various numerical methods have been applied (with varying levels of success) to search for ground state energies and study the thermodynamics of different sequences. In this work, we use replica exchange Wang-Landau sampling [3] to study two “long” HP sequences (209 and 248 monomers) previously investigated [4] using PERM and replica exchange Monte Carlo. We find lower ground state energies for both sequences than previously reported, and, for the first time, extract specific heat curves for these sequences [5]. We compare these specific heat curves, qualitatively, to those reported in the literature for shorter HP model sequences [6]. These long sequences can now serve as benchmarks for new algorithms and new implementations of existing algorithms.

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SP2.1 – Fully-packed anisotropic hard-core plates on a cubic lattice.

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We consider fully-packed anisotropic 2×2 *hard-core* plates on a cubic lattice. Plates are assigned fugacities depending on their orientation. We study this system using local updates and a non-local cluster algorithm. We find that in the isotropic limit i.e., when all fugacities are equal the system is in a sublattice ordered phase. As we increase the fugacity of plates along one orientation, the system breaks translation invariance along the other two orientations and goes into a columnar order. On the other hand if we decrease the fugacity of plates along one orientation, the system breaks translation invariance along that orientation and goes into a layered phase where alternative bilayers are favorably populated by plates. In the layered phase we find that the plates are power-law correlated.

SP2.2 – Phase transitions in a system of hard plates on the three dimensional cubic lattice

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We study different phases and phase transitions in the system of $2 \times 2 \times 1$ hard plates on the three dimensional cubic lattice. Three types of plates are possible depending on whether they lie in xy , yz or zx planes. We show, using grand canonical Monte Carlo simulations, that the system undergoes two density driven phase transitions with increasing the density of plates: first from a disordered to a layered and second from the layered to a sublattice phase. In the layered phase, the system breaks up into weakly interacting slabs of thickness two along one of the three directions. Additionally the symmetry between the three types of plates is broken as two types of plates have higher density compared to the third type. In the sublattice phase, one of the eight sublattices is preferentially occupied by the plates. We also show that the disordered to layered transition is continuous and consistent with the $O(3)$ universality class perturbed by cubic anisotropy, while

the layered to sublattice transition is discontinuous.

SP2.3 – On the topology and geometry of the configuration spaces of hard disks

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Simple fluids are often modeled as a system of hard disks. Mechanically-balanced configurations, aka the critical points, in the hard disk configuration spaces are involved in estimating the configurational entropy, and could provide new insights about the origins of phase transitions in more general systems. Since the configuration spaces generally contain indistinguishable configurations related by the physical symmetries, they are usually quotiented by the action of these symmetries. In this work, two different quotient maps respecting the desired physical symmetries are proposed, and how these maps transform the original configuration space are examined. The original and the quotiented configuration spaces are represented as metric spaces, and are explicitly triangulated as α -complexes for a small number of disks on a square and hexagonal torus. A study of the topological and geometric properties reveals that the number of the critical points depends in unexpected ways on the application of physical symmetries, and the diameter (as measured by the diffusion distance) of the quotient spaces remains similar.

SP2.4 – Phase-ordering kinetics and persistence of the two-dimensional long-range Ising model at zero temperature

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We investigate the phase-ordering kinetics of the $d = 2$ dimensional long-range Ising model with power-law decaying interactions $\propto 1/r^{d+\sigma}$. Recently, we have numerically confirmed that the characteristic length $\ell(t)$ after a quench to $0 < T < T_c$ grows like a power law $\ell(t) \sim t^\alpha$ in accordance with a long-standing prediction by Bray and Rutenberg, i.e., with $\alpha = 1/2$ for $\sigma > 1$ and $\alpha = 1/(1 + \sigma)$ for $\sigma < 1$ [1]. This means, for quenches to finite T the growth is σ dependent. We now perform a quench to $T = 0$ [2], for which we observe that the growth exponent $\alpha \approx 3/4$ is independent of σ and different from $\alpha = 1/2$ as one would expect for the nearest-neighbor model. Additionally, we investigate the persistence of the local order parameter and provide estimates for the persistence exponent θ and the fractal dimension d_f of the persistent lattice. In the limit of large σ only the fractal dimension d_f of the nearest-neighbor Ising model is recovered, while θ differs significantly. This we understand from the unexpected value for α and a conjectured relation between these exponents, which we confirm numerically for the long-range model.

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SP2.5 – Aging in the Two-Dimensional Long-Range Ising Model with Power-Law Interactions

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The current understanding of aging phenomena is mainly confined to systems with short-ranged interactions. Little is known about the aging of long-ranged systems. Here we present first results of Monte Carlo simulations for the aging in the phase-ordering kinetics of the $d = 2$ dimensional Ising model with power-law long-range

interactions $\propto r^{-d+\sigma}$ [1]. The dynamical scaling of the two-time spin-spin autocorrelator is shown to be well described by simple aging for all interaction ranges studied. The autocorrelation exponents are consistent with $\lambda = 1.25$ in the effectively short-range regime with $\sigma > 1$, while for stronger long-range interactions with $\sigma < 1$ the data are consistent with $\lambda = d/2 = 1$. For very long-ranged interactions, strong finite-size effects are observed. We discuss whether such finite-size effects could be misinterpreted phenomenologically as sub-aging.

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SP2.6 – Thermally driven dynamic phase transitions in site diluted Ising ferromagnet

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Nonequilibrium phase transition in bistable systems is far less understood in comparison to its equilibrium counterpart. An external time-varying field can drive the system between two metastable phases of a bistable system. There are two competing timescales in a system undergoing a nonequilibrium phase transition, namely, the average metastable lifetime $\langle\tau\rangle$ of the system and the time period of the external field. Usually, the system response has some delay while following the field that causes hysteresis, a characteristic feature of a nonequilibrium dynamical system [1, 2]. The Ising ferromagnet is a bistable system below the critical temperature (T_c) of ferromagnet to paramagnet transition and has two symmetry broken ordered phases. An external oscillating field can push the system to either of the equivalent ordered phases, and the other ordered phase remains metastable. There exists a critical period P_c , at which the half period ($P_{1/2}$) of the field becomes comparable with $\langle\tau\rangle$, the Ising ferromagnet undergoes a dynamic phase transition (DPT) from asymmetric phase (with asymmetric hysteresis loops) to symmetric phase (hysteresis loops become symmetric) for the first time. If the period of the oscillating field is small ($P < P_c$), the system will remain in one of the metastable wells over a full period. Whereas for a higher period ($P > P_c$), the system will move from one free energy well to the other and vice versa in half period of the external field [3].

A real magnetic material can have several kinds of disorders. We often encounter physical disorder where a few magnetic ions or spins are physically missing at random or replaced by non-magnetic elements in the regular magnetic material. As the system morphology and the interactions among the spins get affected in disordered magnets, it is expected that such a diluted magnetic system will show distinctive critical properties and phase transition in comparison to a pure magnetic substance.

The ferromagnet to the paramagnet phase transition is well studied on a diluted Ising spin system [4, 5]. It will be interesting to know how nonequilibrium dynamic phase transition dynamics are affected by the underlying diluted lattice morphology, far less studied [6]. The main aim of this study is to know how the disorder influences the critical behaviour of the system and its universality class. According to Harris criterion [7], if the specific heat critical exponent α of a pure system is positive, the values of the critical exponents change with the introduction of weak disorder in the system, and consequently disorder changes the universality class. On the other hand, there will be no change in the values of the critical exponents with the increase in disorder in the system if $\alpha < 0$ for the corresponding pure system. The site diluted 2d equilibrium Ising model is particularly interesting as it corresponds to a marginal case, as $\alpha = 0$ for the pure 2d Ising model. This work discusses extensive Monte Carlo study results to describe nonequilibrium phase transitions on the 2d diluted Ising model under an external sinusoidal field varying the system's temperature below respective $T_c(q)$. The dynamic transition temperature is found to depend on dilution. The phase transitions, critical exponents, and nature of hysteresis loops are determined from a detailed finite-size study on several system sizes and dilution concentrations. The DPT in the 2d diluted Ising model under external sinusoidal field seems to follow the weak scaling hypothesis [8].

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SP2.7 – Parallel computation in GPU of the dynamic critical exponent of the three-dimensional Heisenberg model

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The study of the dynamics in and out of equilibrium in a critical phase is of paramount importance since it permits one to extract the critical exponents of the system, hence, to characterize its universality class. In the last decades a great amount of work, analytical, numerical, and experimental, has been devoted to study these issues. One of the most studied systems has been the three-dimensional (isotropic) classical Heisenberg model. The main goal of our study is to improve the value of z using numerical simulations by studying the dependence of the integrated correlation time in the equilibrium regime and the behavior of the correlation length, susceptibility, and energy with the simulation time in the out-of-equilibrium region. In this way, we can compare the performance of equilibrium and out-of-equilibrium methods in the computation of the dynamic critical exponent [1]. In the equilibrium part we compute the integrated correlation time, avoiding some of the problems which appear in the computation of the exponential one (e.g. assume that the autocorrelation function is a single exponential function [2, 3, 4]).

In the last two decades, the correlation length has played an important role in both out-of-equilibrium numerical simulations and experiments in spin glasses. Due to this, powerful numerical techniques have been developed to compute this observable with high accuracy, which has allowed a precise determination of the dynamic critical exponent just at the critical point as well as inside the critical spin glass phase. We apply these techniques to the three-dimensional (nondisordered) Heisenberg model. In addition to the computation of the dynamic critical exponent, we have checked the consistency of previous and very accurate determinations of the static critical exponents (ν and η) in the out-of-equilibrium regime. We have also measured the dynamic critical exponent from the decay of the energy at criticality. This decay has also been studied in the past in finite dimensional spin glass and recently has played a central role together with the behavior of the correlation length in the analysis of the Mpemba effect, a striking memory effect.

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SP3.1 (invited) – Finding the Theta temperature of a polymer with long-range interactions

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Recently [1] we adapted a Monte Carlo method for generating self-avoiding walks on lattice geometries which employs a binary-tree data-structure [2] for polymers with continuous degrees of freedom. Data suggests that the time per Monte Carlo move scales logarithmically with polymer length. We generalized the method to Lennard-Jones polymers with untruncated monomer-monomer interaction. To this end we proposed a variant of the Metropolis algorithm which in combination with the tree data-structure preserves logarithmic scaling. Here, we determine the Theta-temperature for Lennard-Jones polymers using two different approaches and present the results for chains with up to 16384 repeat units.

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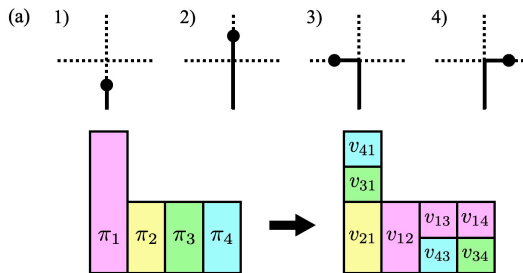
SP3.3 – Geometric allocation approach to accelerating directed worm algorithm

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The worm algorithm is a versatile technique in the Markov chain Monte Carlo method for both classical and quantum systems. The algorithm substantially alleviates critical slowing down and reduces the dynamic critical exponents of various systems. We have proposed a directed worm algorithm that significantly improves computational efficiency. We use the geometric allocation approach to optimize the worm scattering process: worm backscattering is averted, and forward scattering is favored. Our approach successfully enhances the diffusivity of the worm head (kink). We have demonstrated the performance improvement for the Ising model at the critical temperature by measurement of exponential autocorrelation times and asymptotic variances. Our worm algorithm is approximately 25 times as efficient as the conventional worm algorithm for the simple cubic lattice model and, surprisingly, more efficient than the Wolff cluster algorithm. We have estimated the dynamic critical exponent of the simple cubic lattice Ising model to be $z \approx 0.27$ in the worm update. Our approach can be applied to a wide range of physical systems, such as the $|\phi|^4$ model, the Potts model, the $O(n)$ loop model, frustrated spin systems, and lattice QCD.

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Geometric allocation for the directed worm transition probability in the square lattice Ising model. The weight of each state is denoted by π_i ($i = 1, 2, 3, 4$), and the allocated stochastic flow from i to j is denoted by v_{ij} . In our approach, the rejection (backscattering) probability is reduced to zero, and the forward scattering probability is maximized.

SP3.4 – Generalized-ensemble simulations of spin systems and biomolecular systems

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Conventional Monte Carlo and molecular dynamics simulations are greatly hampered by the broken-ergodicity problem, where the simulations tend to get trapped in some of astronomically large number of local-minimum energy states. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms which are based on non-Boltzmann weight factors (for reviews, see, e.g., Refs. [1,2] and for our recent algorithm developments and their applications, see, e.g., Refs. [3-8]). With these algorithms we can explore a wide range of the conformational space. In this talk, I will present the latest results of our applications of generalized-ensemble simulations to spin systems and biomolecular systems.

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SP3.5 – Extremely rare ultra-fast non-equilibrium processes close to equilibrium

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Typical fast non-equilibrium trajectories, e.g. induced by varying an external parameter, are very different from the corresponding equilibrium infinitely-slow processes. Nevertheless, there are connections between equilibrium and non-equilibrium behaviors, e.g. the theorems of Jarzynski and Crooks, which relate the distribution $P(W)$ of non-equilibrium work to the free energy differences ΔF . Still, when systems grows beyond very small sizes, the processes which contribute to the determination of ΔW are very rare, i.e. $P(W)$ is extremely small, like 10^{-40} . Whether those relevant but rare trajectories, which exhibit these work values, show a higher degree of similarity to equilibrium, i.e. with respect to the visited microscopical configurations, is studied here. Thus, we want to know whether the similarity goes beyond exhibiting "suitable" work values.

For this purpose, RNA secondary structures under influence of a varying external force are advantageous, since these exhibit complex behavior, like showing the influence of quenched disorder realizations and also having a complex free energy landscape. One further benefit of RNA is that there are already experiments yielding work distributions performed on physical realizations of the model. Moreover, by an extension of the sampling algorithm of Higgs, it is possible to perfectly sample configurations efficiently in true equilibrium, which enables easy comparison between equilibrium and non-equilibrium folding and unfolding trajectories. Fast non-equilibrium processes are simulated by means of Monte-Carlo sampling, starting from equilibrium configurations, while measuring the performed work. Using a sophisticated large-deviation algorithm, which is based on the utilization of random numbers in the simulation, work distributions are resolved with high precision for a medium-size (length $L = 100$) RNA hairpin structure down to probabilities as small as 10^{-46} .

Through exact free-energy calculations, the theorems of Crooks and Jarzynski are verified with high precision down to very small probabilities. To investigate the similarity of equilibrium and non-equilibrium processes, their respective dynamics are compared by means of force-extension curves $n(f)$ and overlap profiles $\sigma(f)$ of secondary structure configurations during unfolding and refolding, conditioned to various values of the measured work W . Results indicate that indeed extreme low-probability trajectories with $W \approx \Delta F$ are most and actually quite similar to the equilibrium trajectories. This means, one is able to observe sequences of snapshots of dynamically and very quickly generated configurations that are very similar to sequences of configurations from corresponding equilibrium processes by

sampling in the extreme tails of the work distributions.

SP3.6 – Unlocking heterogeneous node activation in Boolean networks through dynamic programming

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We consider the dynamics of node activation in networks of Boolean linear threshold units with fully asymmetric connectivity in the presence of noise, for which the dynamic cavity method provides the most efficient way to evaluate probabilities of dynamic trajectories. However, the complexity of the cavity approach grows exponentially with the in-degrees of nodes, which creates a de-facto barrier for the successful analysis of systems with fat-tailed in-degree distributions. We present a dynamic programming algorithm that overcomes this barrier by reducing the computational complexity in the in-degrees from exponential to quadratic, whenever couplings are chosen randomly from (or can be approximated in terms of) a discrete set of equidistant values. As a case study, we analyse the dynamics of a random Boolean network with a fat-tailed degree distribution and fully asymmetric binary $\pm J$ couplings, and we use the power of the algorithm to unlock the noise dependent heterogeneity of stationary node activation patterns in such a system.

SP4.1 – Dynamics of transient cages in a 2D supercooled liquid

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Supercooled state of a liquid is characterized by extremely slow and spatially heterogeneous dynamics attributed to caging of particles by their neighbours [1, 2, 3]. Here, the dynamics of cages in a model 2D supercooled liquid is studied by an-

alyzing single-particle trajectories. I will discuss the temperature dependence of cage times [4] and cage sizes and the observed correlation between cage sizes and cage survival time. We find that, at higher temperatures, bigger cages survive for longer. However, this behaviour changes at low enough temperatures, where smaller cages stay for the longest time. We study the particle dynamics within the cages by analyzing the frequencies with which particles move inside the cages. We show that although cage-time and cage-size fluctuations are sensitive to the temperature, the frequencies are not affected in a significant way.

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SP4.2 – An agent-based modeling and simulation for the first stage of honeycomb construction

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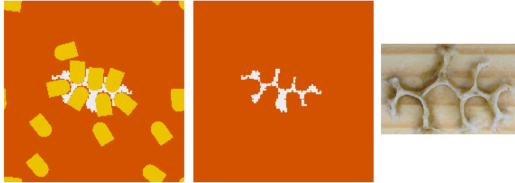
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Honeybees construct their nests that consist of well-arranged hexagonal cylinders. In the first stage of honeycomb construction, they build a linear sequence of tripod structures that form the basis of honeycomb. However, it is unknown how honeybees produce that initial pattern. Herein, to understand the mechanisms of honeycomb construction, we propose an agent-based model, the attachment-excavation model [1], in which worker honeybees are classified into attachers and excavators. We then conduct two-dimensional simulations that show how the initial pattern emerges.

The simulation results show that a tripod pattern emerges due to competition between the attachers and excavators. As time advances, the isotropic wax growth causes the tripods to connect planarly. We then employ anisotropic wax growth to obtain a linear sequence of constructed tripods, as shown in the bottom

figure. It suggests that anisotropic growth is a significant contributor to the first stage of honeycomb construction. We conclude that the first stage of honeycomb construction can be understood in terms of self-organization, i.e., the formation of tripod structures (dissipative structure) and their one-dimensional connections (self-assembly), to achieve complexity during the first stage of honeycomb construction.

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Honeycomb construction in the attachment-excavation model (left and center) and an observed initial structure of the honeycomb (right). The left panel shows wax (white) with agents (yellow), but the center does without agents.

SP4.3 – Mean-field interactions in evolutionary spatial games

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We introduce a mean-field term to an evolutionary spatial game model. Namely, we consider the game of Nowak and May, based on the Prisoner's dilemma, and augment the game rules by a self-consistent mean-field term. This way, an agent operates based on local information from its neighbors and non-local information via the mean-field coupling. We simulate the model and construct the steady-state phase diagram, which shows significant new features due to the mean-field term. The main effects are observed for stationary steady states, which are parametrically close to chaotic states: the mean-field coupling drives such stationary states into spatial chaos. Mean-field games demonstrate continuous change between steady-states contrary to the original Nowak and May game discontinuous

changes.

SP4.4 – Detecting early warning signals in higher-order structures

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Foreseeing critical transitions is a fundamental target in ecology, which has propelled great research interest in early warning signals based on the detection of changes before one system collapses. These advances, however, are restricted to pairwise interactions and little attention has been paid to the higher-order structures. Detecting early warning signals will be difficult if the target system is constantly perturbed by big noise, making the critical point is far from the original bifurcation point and thus hard to detect the critical point by early warning signals. In this paper, we develop a criterion to lease the effect of big noise on higher-order structures using the transformed higher-dimensional data. We demonstrate the effectiveness of our method on detecting early warning signals in real ecological systems with higher-order structures.

SP4.5 – Large-deviations of the SIR model

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Not only due to the current COVID-19 pandemic, research in disease spreading is a well studied topic in interdisciplinary science.

Here we investigate the standard *susceptible-infected-recovered* (SIR) model on small-world networks with given initial conditions. We are particularly interested in the phase where an outbreak (per time unit) is very unlikely, while the model is still close to the epidemic transition. This regime is of particular interest, because for even lower infection rates, basically no outbreak will ever occur, thus the disease is like not existing. On the other hand, beyond the epidemic transition, a

disease will have occurred already a long time ago and typically almost all people are immune, i.e., such a virus will actually not be regarded as a threat. Thus, the regime of rare outbreaks is most interesting. We are able to investigate this regime by using special large-deviation techniques. We study the probability density functions of the cumulative number C of infections and the maximum M of the number of currently infected people down to very small probabilities like 10^{-2000} . We also measure correlations with other measurable quantities to identify reasons for the occurrence of outbreaks.

SP4.6 – Pursuit and Evasion: Singles to Groups

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"Chases and Escapes" is a traditional mathematical problem. The act of balancing a stick on human fingertips represents an experimental paradigm of typical one-to-one chase and escape. Recently, we have proposed a simple extended model where one group chasing another group, called a "Group Chase and Escape". This extension connects the traditional problem with current interests in collective motions of animals, insects, cars, etc. I will present our basic model and its rather complex behaviors. Each chaser approaches its nearest escapee while each escapee steps away from its nearest chaser. Although there are no communications within each group, aggregate formations are observed. How these behaviors appear as a function of parameters, such as densities will be discussed. Also, we consider different expansions of this basic model. First, we introduced a fluctuation. Players now make errors in taking their step directions with some probability. It turns out that some level of fluctuations works better for more effective catching. Secondly, we introduce a delay in the reaction of chasers in catching a target. Distance-dependent reaction delay can cause quite complex behaviors. We also report the effect of a probabilistic conversion of the caught targets into chasers.

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Poster Presentations

Poster 1 (No. 17) – Elucidating atomic-scale phenomena with transmission electron microscopy: a study of gold nanocontact

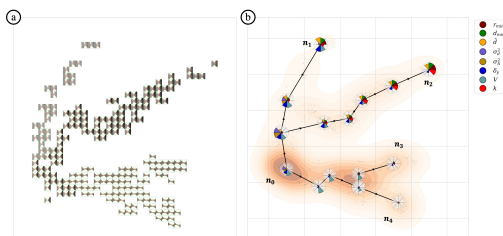
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The mechanical and electrical properties of nanomaterials are extremely important since the emergence of sensors composed of metals and/or semiconductor nanowires [1]. The integration of nano-physical properties measurements into a transmission electron microscope (TEM) promotes the study of gold nanocontacts (Au NCs) and accelerates the fabrication process of novel nanomaterials. In the previous study, we have developed a TEM holder incorporating a crystal oscillator that can measure mechanical response with high sensitivity, allowing observations of changes in Au NC geometry along with the measured spring constant and conductance [2, 3]. In this study, we focus on comprehending the physical phenomena of Au NC's properties at the atomic scale. Initially, five experiments are prepared to obtain time series sequences of three properties: 2D geometrical shape, spring constant, and electrical conductance of different Au NCs. All the properties are recorded by a TEM equipped with force sensors. To preprocess the TEM data, we segment the Au NC regions from non-contact regions using a U-net based deep learning model [4]. As a result, the model achieves a high precision segmentation which outperforms conventional density-based segmentation approaches. The geometry of the segmented Au NC region is modelled with thirteen geometrical features. After that, we project all the experiments on an embedding space that integrates both geometrical information and the recorded physical properties [5]. In addition to representing different prototypes of Au NC geometrical shape, the embedding space unveils the most correlated features with the Au NCs spring constant. Furthermore, exploiting the embedding space, we generate virtual experiments to simulate the ideal process of Au NC formation and investigate the

coherent correlations between the geometrical features and the spring constant.

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Map of the embedding space representing Au NC geometry. The map is illustrated by: (a) recorded TEM snapshots in five experiments; and (b) representative snapshots as nodes with corresponding values of geometrical features (the black lines indicate links between nodes in vicinity while the arrows indicate increasing trend of spring constant over those nodes).

Poster 1 (No. 18) – Molecular-Dynamics Simulation of Liquid Sulfur by Artificial Neural Network Potentials

Yusuke Suzumura, Shuji Munejiri

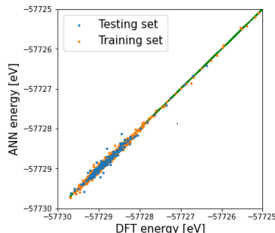
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Liquid sulfur near the melting point is a molecular liquid consisting of eight-membered-ring molecule S_8 . When the temperature and pressure are increased,

it becomes a complex liquid consisting of various molecular species. We have investigated the static structure of liquid sulfur for a wide range of density and temperature using first-principles molecular-dynamics simulations [1]. We also want to study the dynamic structure, but it requires a long simulation times, which is not easy to carry out. In recent years, in order to solve the problem of the computational complexity of first-principles molecular-dynamics, machine learning molecular-dynamics has been used as a means to perform highly accurate simulations while reducing the computational complexity [2]. The first purpose of this study is to create an Artificial Neural Network(ANN) potential using the atomic configurations, energy and forces of liquid sulfur as training data obtained by first-principles molecular-dynamics. The second purpose is to investigate the dynamic structure of liquid sulfur near the melting point. We ran first-principles molecular-dynamics simulations using 64 sulfur atoms to obtain the training data. The resulting configurations and energies were used to create the ANN potential. As shown in the figure below, we were able to predict the energy. However, we were not able to predict the force, so we are currently training the ANN potential by adding force data.

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Energy of first-principles molecular-dynamics and Artificial Neural Network potential

Poster 1 (No. 24) – Confinement effects on packings of disco-rectangles in slit pores

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The behavior of two-dimensional hard particles confined in a slit pore between two parallel walls was analyzed using simulation approach. The packing's were produced using the random sequential adsorption (RSA) model with continuous positional and orientational degrees of freedom. The aspect ratio (length-to-width ratio) of the particles was varied within the range $\varepsilon \in [1, 20]$ and distance between walls was varied within the range $L_y/d \in [1, \infty]$ (Fig. 1). The kinetics of RSA process and parameters of deposits in jamming state (packing fraction, φ , order parameter, S , and long-range (percolation) connectivity distances along the channel, δ_x , and in perpendicular direction, δ_y , were studied numerically. The values of ε and L_y/d significantly affected the structure of the packings and the percolation connectivity. Particularly, the observed complicated dependencies of the jamming coverage $\varphi(\varepsilon)$ or $\varphi(L_y/d)$ were explained by the interplay of the different geometrical factors related with confinement, orientation degrees of freedom and excluded volume effects.

We acknowledge funding from the National research foundation of Ukraine, Grant No. 2020.02/0138 (M.O.T., N.V.V.), National Academy of Sciences of Ukraine, Project Nos. 7/9/3-f-4-1230-2021 (N.I.L.)

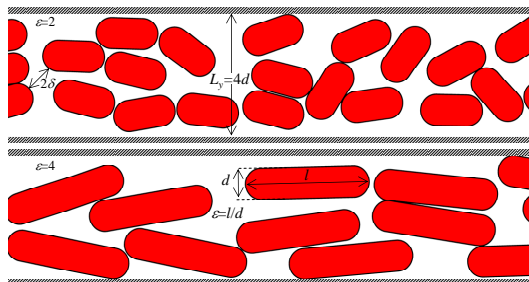


Fig. 1. Examples of RSA packings in the jamming state for disco-rectangles with aspect ratios $\varepsilon = 2$ and $\varepsilon = 4$ for distance between walls $L_y/d = 4$. Here, 2δ is a minimum distance between two particles.

Poster 1 (No. 49) – Study of velocity auto-correlation function of a confined Brownian particle

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Motivated by the simple models of molecular motor obeying a linear force-velocity relation, we have studied the stochastic dynamics of a Brownian particle in the presence of a linear velocity dependent force, $f_s(1 - \frac{v}{v_0})$ where f_s is a constant. The position and velocity auto correlation functions in different situations of the dynamics are calculated exactly. We observed that the velocity auto correlation function shows an exponentially decaying behaviour with time and saturates to a constant value in the time asymptotic limit, for a fixed f_s . It attains saturation faster with increase in the f_s value. When the particle is confined in a harmonic well, the spectral density exhibits a symmetric behaviour and the corresponding velocity auto correlation function shows a damped oscillatory behaviour before decaying to zero in the long time limit. With viscous coefficient, a non-systematic variation of the velocity auto correlation function is observed. Further, in the presence of a sinusoidal driving force, the correlation in velocities increases with increase in the amplitude of driving in the transient regime.

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Poster 1 (No. 58) – The capture cross sections at the electron collisions with hydrogen atom in non Maxwellian dense semiclassical plasma

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Semiclassical plasma is a dense high-temperature plasma that appears inside giant planets, white dwarfs, in experiments on the compression of warm plasma. It has become the object of intensive experimental and theoretical research [1-2]. In this case, the extreme values of densities and energies lead to a significant deviation of the particle velocity distribution function from the equilibrium Maxwellian distribution. Spacecraft measurements have shown that deviations from the Maxwellian particle distribution are often found in the solar wind, in the plasma of planetary magnetospheres, and in some other astrophysical objects due to the presence of high-energy particles [2-4]. In many situations, the distribution has a “suprathermal” power-law tail at high energies. They were built several possible distributions corresponding to the empirical data. Among them, the family of κ (kappa) - distributions stands out, since they model well the "suprathermal" power-law tail and has found interesting applications in both space and laboratory plasmas.

To date, the κ - distribution is widely used to analyze a large number of different phenomena in plasma. For example, in Ref. [5], this distribution was applied to the study of the Landau damping phenomenon for ion-acoustic waves in cosmic plasma. And in Ref. [6], dust-acoustic solitons in dusty plasma with κ - distributed ions were investigated.

One of the elementary processes in plasma is the electron capture process. In this work the electron capture processes by the hydrogen atom was investigated. The motion of the electron in the field of the the motionless atom was considered on the basis of the solving of the equation of motion. The interaction potential between the electron and the hydrogen atom was presented in works [7-10]. This effective potential, taking into account dynamic screening, quantum mechanical effect of diffraction and kappa distribution effect, has finite values at the distances close to zero.

In this work the electron capture radius, which was determined by equating the kinetic energy of impacting electron and the interaction energy between the electron and the hydrogen atom, was presented [11]. The trajectories of the electron in the field of the atom was simulated. Obtained results of the electron capture by the atom without and with kappa distributions were compared. Using the electron

capture probability, the electron capture cross section was calculated.

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Poster 1 (No. 84) – A charge-momentum-energy-conserving alternative numerical method for the Vlasov–Maxwell system

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Particle-in-cell (PIC) method has been widely used especially in communities of plasma physics, astrophysics, and beam acceleration. The law of charge-momentum-energy conservation is one of the most important principles in kinetic plasmas, and violation of the conservation results in numerical instabilities. This is the reason why many computational works have been carried out to develop conservative schemes. Although conservative finite-difference scheme for Vlasov–Maxwell system is relatively easy to be composed [1], fully-conservative PIC method has not been reported yet despite continuous effort [2].

The reason why conservative PIC method cannot be realized is inconsistency of

the spatial variables; the spatial variables are assumed to be dependent variables in the equation of motion although these are independent variables in the Maxwell's equations. To overcome this issue, we propose an alternative methodology in which a hybrid representation of Vlasov and Klimontovich equations is employed as follows:

$$\frac{\partial f_j}{\partial t} + (\mathbf{v}_j \cdot \nabla) f_j = 0, \quad (4)$$

$$m_j \frac{d\mathbf{v}_j}{dt} = \mathbf{F}_j, \quad (5)$$

where $f_j = f_j(t, \mathbf{x})$, $\mathbf{v}_j = \mathbf{v}_j(t)$, $\mathbf{F}_j = \mathbf{F}_j(t)$, and m_j are the shape function, velocity, electromagnetic force, and mass of the j -th superparticle, respectively. These equations are analytically derived from the Vlasov equation if the distribution function is expressed as follows:

$$f(t, \mathbf{x}, \mathbf{v}) = \sum_j f_j(t, \mathbf{x}) \delta(\mathbf{v} - \mathbf{v}_j). \quad (6)$$

Numerical experiments of two-stream and Weibel instabilities show that the conservation laws are exactly preserved if the finite-difference schemes are selected appropriately.

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Poster 1 (No. 105) – Compressed sensing using an Ising machine

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Compressed sensing is a technique to solve sparse signal reconstruction problems. The problem considered here is to reconstruct an N -dimensional source signal vector x from an M -dimensional vector y and a design matrix A . The matrix A is an $M \times N$ matrix and represents measurement. Under the assumption that the number of nonzero components of x is sufficiently small, the problem is formulated as

$$x = \arg \min_x \|y - Ax\|_2^2 \quad \text{subject to } \|x\|_0 \leq K.$$

Here, $\|x\|_k$ is the L_k norm, and $K (< M)$ is a positive integer. Solving the problem requires an exhaustive search for the appropriate combination of nonzero components of x .

We propose an algorithm of compressed sensing using an Ising machine as an approach to this problem. Ising machines are special-purpose computers for solving combinatorial optimization problems. They usually accept the Ising model or quadratic unconstrained binary optimization (QUBO) formulation. In other words, Ising machines use only Ising or binary variables, not continuous ones. To solve the problem considered, we replace x with $z \circ c$, where z and c are real and binary variables, respectively, and \circ denotes the Hadamard product. The proposed algorithm consists of iterative two-fold optimization. After an Ising machine returns optimal c for a given z , a conventional (classical) computer calculates z for the obtained values of c . Although the computational cost of this algorithm is not low, it is a promising approach to compressed sensing. We discuss the advantages and disadvantages of the algorithm.

Poster 1 (No. 124) – Molecular + Field Dynamics Method for Vortex Dynamics in a Superconductor

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There are four levels of simulation methods for vortices in a superconductor under an external field. Most microscopic method uses the Bogoliubov-de Gennes equations, or Gor'kov equations, which treat electrons. The second method uses phenomenological Ginzburg-Landau equations, which treat a macroscopic wave function. The third one uses the molecular dynamics method, which treats vortices as particles. Final method solves the macroscopic Maxwell equations and vortices are averaged out to macroscopic magnetic induction.

In order to investigate ten thousands of individual vortices, the molecular method is useful. However, in the molecular dynamics method, we must calculate vortex-vortex interaction, which is the Lorentz force from the current around the vortex, for every vortex pair. It costs much when we consider many vortices. In order to reduce the computation costs, we introduce a current field, which includes

currents from all of the vortices. We treat the current field with the finite element method. So, we solve following equations.

$$\eta \frac{\partial \mathbf{r}_i}{\partial t} = \mathbf{f}_i^{imp} + \mathbf{f}_i^f + \mathbf{f}_i^C,$$

where \mathbf{f}_i^{imp} and \mathbf{f}_i^f are a pinning force from impurities and a thermal fluctuation force, respectively. $\mathbf{f}_i^C(\mathbf{r}_i) = \mathbf{J}(\mathbf{r}_i) \times \frac{\Phi_0}{c} \hat{\mathbf{z}}$ is the Lorentz force from the current $\mathbf{J}(\mathbf{r}_i)$. The current around a vortex is given by $\frac{\Phi_0}{c} f_0 K_1\left(\frac{r}{\lambda}\right) \hat{\theta}$. Total current is sum of these current and an external current. Figure 1 shows an example of vortex distribution and current distribution.

We will discuss relations between global vortex motion and current distribution.

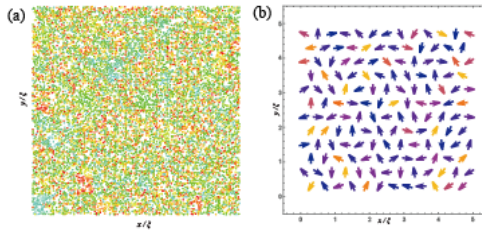


Figure1: Distributions of vortices (a) and current (b) in a $5 \xi_0 \times 5 \xi_0$ square superconducting plate. Number of vortices is 10000.

Poster 1 (No. 130) – Orthogonal and antiparallel vortex tubes and energy cascades in quantum turbulence

Tsuyoshi Kadokura, Hiroki Saito

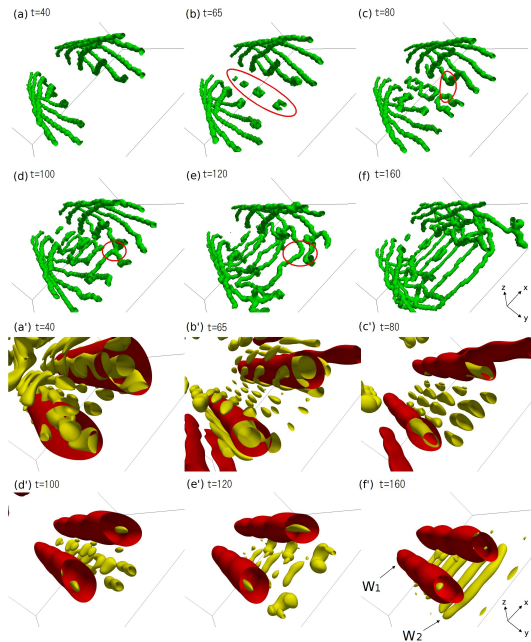
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We investigate the dynamics of energy cascades in quantum turbulence by directly observing the vorticity distributions in numerical simulations of the Gross-Pitaevskii equation. By Fourier filtering each scale of the vorticity distribution, we find that antiparallel vortex tubes at a large scale generate small-scale vortex

tubes orthogonal to those at the large scale, which is a manifestation of the energy cascade from large to small scales. We reveal the dynamics of quantized vortex lines in these processes[1].

[1] Tsuyoshi Kadokura and Hiroki Saito, Phys. Rev. Fluids **3**, 104606 (2018).



Poster 1 (No. 132) – Statistical properties of Hall MHD turbulence with a high magnetic Prandtl number

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Statistical properties of magnetohydrodynamic (MHD) turbulence with a high magnetic Prandtl number (Pr_M) under influences of the Hall term are studied by means of numerical simulations of homogeneous, isotropic, and incompressible Hall MHD turbulence driven by a random force.

We carry out numerical simulations for a range of Pr_M from 1 to 100. Our numerical simulations of $Pr_M = 100$ show a new power law in the kinetic energy spectrum which has not been reported in literatures of MHD turbulence. Based on an order estimate of the energy budget in the spectral space, we consider that this new power law is formed by a balance between the Lorentz force and the viscous dissipation while the Lorentz force is enhanced due to the Hall effect as we have reported partially in our earlier work [1]. We confirm formation of this new scaling regime by numerical simulations of a larger number of grid points.

Some typical quantities representing a statistical nature of turbulence such as the probability density functions of the enstrophy density and the current density and alignment of the velocity field to the magnetic field are studied. By investigating these natures at the scaling regime as well as the new scaling regime reported in [1], we report a new nature of a high magnetic Prandtl number Hall MHD turbulence.

- [1] H. Miura, J. Yang, and T. Gotoh, “Hall magnetohydrodynamic turbulence with a magnetic Prandtl number larger than unity”, Phys. Rev. E **100**, 063207 (2019).

Poster 1 (No. 156) – Crossover Phenomena in the 2D Random-Bond Blume-Capel Model

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It has been rigorously established that the addition of an infinitesimal amount of quenched disorder in two dimensions smoothes a first-order phase transition to become continuous. However, many open questions remain, such as regarding the universality class of the emerging continuous transition and the nature of the resulting crossover from first to second-order transition. Addressing such questions, we present some preliminary results in the ex-first-order regime of the 2D random-bond Blume-Capel model, employing a parallel version of the multi-canonical sampling method. We identify a crossover length-scale L^* , above which the continuous nature of the transition is observed and present its scaling behaviour as a function of temperature and disorder strength.

Poster 1 (No. 172) – Weakly relativistic effect in the formation of ion-acoustic solitary waves in dusty plasma

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Role of streaming speeds of positive ions (u_{i0}), relativistic electrons (u_{e0}) together with the immobile dust charge (Z_d) to form dust-ion acoustic compressive and rarefactive relativistic solitons in this multi-species plasma model for immobile dusty plasma are investigated. In this new investigation of dust-ion acoustic waves with positive ions and relativistic electrons in presence of immobile dust, it is noteworthy to mention that only compressive KdV solitons are seen to produce for some pairs of initial streaming of ions and relativistic electrons. Whereas for some other pairs of ion and relativistic electron streaming speeds, rarefactive solitons

of either increasing or decreasing character are seen to produce. The presence of dust charge of immobile dust, present in the plasma plays very crucial role to form compressive and rarefactive KdV solitons which is a salient feature of this theoretical investigation.

Poster 1 (No. 190) – Scaling of the Random-Field Ising Model in Two Dimensions

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As one of the simplest models of magnetic systems with quenched disorder, the random-field Ising model shows surprisingly rich critical behavior. Due to its complex free-energy landscape, it is only recently that large-scale numerical simulations have been able to shed some light even on basic questions in three and higher dimensions, such as universality, critical scaling and dimensional reduction. The two-dimensional model has received less attention, but is no less fascinating. We solve a long-standing puzzle by presenting compelling numerical evidence for the scaling behavior of the correlation length ξ . Results for two lattice geometries, square and triangular, consistently support the form $\xi \sim \exp[A/h^2]$, where h denotes the random-field strength, in line with early theoretical work, but at variance with some more recent numerical and analytical results. We also investigate the more widely used break-up length scale of the system, which we however find to be afflicted by much stronger scaling corrections and hence a rather less useful quantity. Finally, we discuss the self-averaging properties of the correlation length.

Poster 1 (No. 197) – Phenomenological simulation on intermediate states in a type-I superconducting wire

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When a critical current is applied to a type-I superconducting wire, superconductivity becomes inhomogeneous. London proposed a periodic structure of intermediate state. The critical current does not exceed the current that produces the critical magnetic field which is Silsbee's rules. If the current is larger than the critical current, surface magnetic field exceeds the critical field, and then superconductivity is destroyed around the surface. In this case, if the current flows only around small superconducting region, the current density increases and the magnetic field around the region exceeds further the critical field, therefore this layered structure is not stable. In this study, in order to clarify whether the London's intermediate state actually exists and what kind of structure the intermediate state can be stable. We solve following the Ginzburg-Landau equation,

$$\alpha\psi + \beta|\psi|^2\psi + \frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right)^2 \psi = 0.$$

With the finite element method, we impose at both ends of the wire following boundary condition for constant external current,

$$\mathbf{A} = -\frac{4\pi}{c} \frac{2\pi\lambda(T)^2}{\Phi_0} \times \frac{\mathbf{j}_{input}}{|\psi^{new}|^2}.$$

In Fig.1 we show the order parameter structure in a square wire $30\xi_0 \times 10\xi_0 \times 10\xi_0$ under an external current $\frac{j}{j_0} = 1.0$. We will discuss dependence of this structure on the current density and temperature.

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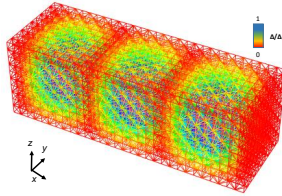


Fig.1. Three dimensional order parameter structure

Poster 1 (No. 209) – Molecular Dynamics Simulation on Vortex Dynamics in a Dirty Superconductor

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When an AC current is applied to vortices in a dirty superconductor under a magnetic field, vortices are driven by periodic locally shear force, collide with each other, and self-organize to avoid future collision. This is called random organization. Depending on the amplitude of AC current, the vortex arrangement may or may not return to its original state. This is called reversible-irreversible phase transition [1]. Okuma et al. found that when vortices in an amorphous superconductor are disordered by applying a weak DC current, applying an AC current, vortices are gradually organized. These disordered and organized vortices coexist [2]. However, distributions of organized and disordered regions have not been observed experimentally. In order to confirm above speculation, we investigate AC or DC driven vortex dynamics in a dirty superconductor with the molecular dynamics method. In our molecular dynamics method, we consider an impurity potential, which is treated with the finite element method. The force due to the impurity potential is given by $\mathbf{f}_{\text{imp}} = -\sum_{i=1}^3 (V_{\text{imp}i}^e \nabla N_i^e(x, y))$ where $V_{\text{imp}i}^e$ is the value of the impurity potential of the i th node of the e th element, and $N_i^e(x, y)$ is the area coordinate. In Fig.1, we show an example of time development of voltage due to the vortex motion under an AC driving force.

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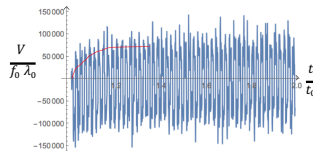


Figure 1. Time development of voltage due to vortex movement under an AC driving force with angular frequency $\omega = \frac{50}{t_0}$, where $t_0 = \frac{\eta\lambda_0}{f_0}$. The red curve outlines the voltage relaxation.

Poster 1 (No. 233) – Universality aspects of the two-dimensional spin-1 Baxter-Wu model in a crystal field

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We investigate the universality aspects of the two-dimensional spin-1 Baxter-Wu model in the presence of a crystal-field coupling Δ . We employ extensive numerical simulations of two types which provide us with complementary results: Wang-Landau entropic sampling simulations at fixed values of Δ and a parallelized variant of the multicanonical approach at constant temperatures T and crossing the phase boundary along the $\Delta - T$ phase diagram. A detailed finite-size scaling analysis at the regime of second-order phase transitions of the $\Delta - T$ phase diagram indicates that the transition belongs to the universality class of the 4-state Potts

model. Previous controversies with respect to the nature of phase transition are resolved and attributed to the presence of strong finite-size effects, especially as one approaches the pentacritical point of the model.

Poster 1 (No. 235) – DFT-NEGF Study of Electron Transfer Property in Graphene Nanoribbon Double Barrier System

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The hexagonal boron nitride (h-BN) which has an analogous structure with a graphene shows wide bandgap ($\sim 5\text{eV}$) and becomes an electrical insulator. For bond lengths of C-C in graphene and B-N in h-BN are close to each other, they form heterojunctions. Some graphene nanoribbon (GNR) shows electrical conductivity, then, a double barrier structure can be created by embedding two narrow h-BN nanoribbons (BNNRs) in the GNR. It is expected that the GNR/BNNR double barrier structures have resonant levels like semiconductor resonant diodes such as AlGaAs/GaAs double barrier diodes. In this paper, we present computational evaluations of electron transfer properties of GNR/BNNR heterojunctions, nano-sized double barrier systems. First, we perform band calculations of structural optimized nanoribbons of GNR/BNNR heterojunctions by the density functional theory (DFT) method. Next, the $I - V$ characteristics of the heterojunctions are evaluated by the non-equilibrium Green's function (NEGF) method.[1] The $I - V$ characteristics show flat behavior in a certain bias voltage region. These behaviors are different from those of the AlGaAs/GaAs diodes. Transmission functions are also determined and an energy gap at the Fermi level and some sharp peaks in the gap are observed. Since the spacing of the peaks is dependent on the separation length of BNNR barriers, it can be seen that the GNR/BNNR double barrier heterojunctions have resonant states. We calculate the partial density of states (PDOS) of the double barrier system. From the PDOS analysis, it is also shown that the behaviors of the electron transfer properties due to the matching of the eigenstates between the heterojunction and the electrodes.

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Poster 1 (No. 242) – Efficiency of equilibration with three event-based algorithms in hard disk melting

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The physical properties in “equilibrium” are calculated using the particle positions and velocities after the “equilibration” in the molecular simulation. Although the “equilibration” is just preliminary overhead on the research, it often requires a long computational cost, especially in high-density and large-scale systems. The performance of equilibration between methods from arbitrary non-equilibrium states in the many-body systems has been investigated in the history of molecular simulation, which is recognized as a crucial issue. In 2009, Event-Chain Monte Carlo (ECMC) [1] was invented in the hard disk systems and has actively been applied to the many typical models studied in statistical physics from the viewpoints of its high performance. In such a direction, a novel variant of ECMC with the collision rule of particle velocities, called Newtonian-ECMC (NEC) [3] was developed recently. NEC shows clear advantages in the diffusion coefficient and melting process in hard-sphere systems than other conventional methods. To clarify the microscopic mechanism and its performance between event-based algorithms [1, 3, 2], we focus on the non-equilibrium response during the equilibration process induced by a disturbance of the homogeneous expansion of the simple hard disk systems. In the case of Event-Driven Molecular Dynamics (EDMD), we observed the anomalous slow equilibration around the co-existence phases toward the liquid states in large-scale simulation [4]. In the present work, we compared the results of EDMD with Straight-ECMC (SEC) and NEC cases systematically. We also observed anomalous slow equilibration in SEC and NEC; however, we detected distinct differences between methods in the performance and functional forms of relaxation of physical properties. The clear relations between the relaxing mechanism and algorithm (i.e., the procedure of updating particle information) would be clarified and presented at the conference.

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Poster 1 (No. 245) – Automated Complex for Investigation of the Dusty Plasma Properties

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Dusty plasma [1] is the system where micron-sized particles are suspended in a partially ionized gaseous environment consisting of neutral (atoms/molecules) and charged particles (electrons and ions). The interest in dusty plasma is related with the widespread occurrence of dusty plasma in nature and in plasma technologies (installations for plasma etching in the production of microcircuits in electronics, plasma-chemical reactors, etc). The question of how the different forces (force due to magnetic field, friction force and Brownian force) influence the dynamic, transport and structural properties of the ensemble of charged particles is of great interest [2,3]. Particular attention is drawn to the case of the strong correlation, i.e. when the interparticle interaction energy exceeds the kinetic energy of particles. This work is dedicated to creating the developed automated complex of computer programs for the simulation and investigation of the physical properties of magnetized dusty plasma. Computer simulation of the system was carried out on the basis of molecular dynamics method, taking into account the influence of the external uniform magnetic field. To integrate the equations of motion, the velocity Verlet scheme was used, which is indispensable for simulating physical processes in real time [4]. The particles of the system interact by the Yukawa potential. The complex was developed in the Borland Delphi7 object-oriented programming environment, using additional components. Moreover, the complex consists of several subprograms supporting investigation of the dynamic and structural properties of dusty plasma. The program interface provides the ability to set task parameters, monitor the progress of calculations, and save the resulting calculations in appropriate format. Furthermore, the complex allows visualize the movement of particles in two dimensional and three dimensional spaces. The authors acknowledge support from the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan under Grant number AP09058005.

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Poster 1 (No. 246) – Molecular Dynamic Study of the Relationship between Li-ion Migration and Disordering of Hydride Complexes in $\text{LiCB}_9\text{H}_{10}$

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All-solid-state battery is one of the most promising candidates to resolve the intrinsic drawbacks of current lithium-ion batteries, such as electrolyte leakage, flammability, and limited energy density. Recently, a class of complex hydrides like $\text{LiCB}_9\text{H}_{10}$ is paid considerable attention because of its high ionic conductivity and stability against metal anode [1]. Conductivity measurement and structure analysis suggest that the disordering of hydride complexes plays a critical role of this high ionic conductivity, whereas the exact relationship between Li-ion conduction and the disordering has not been clarified yet. Therefore, to reveal the relationship between them, here, we conducted *ab initio* and Neural-net potential molecular dynamic simulations (AIMD and NNP-MD). From the observation of Euler angle (θ) of CB_9H_{10} and mean squared displacement (MSD) of Li ions during AIMD simulation at 200-1000K, it is found that Li-ion migration is induced by the rotation of CB_9H_{10} . In fact, the correlation coefficient between Euler angle of CB_9H_{10} and $\sqrt{\text{MSD}_{\text{Li}}}$ is about 0.9. Therefore, to discuss the relationship more quantitatively, NNP-MD simulations at various temperatures have been conducted. The calculated self-diffusion coefficient of Li, D_{Li} is comparable with that obtained from pulse-field-gradient NMR measurement [2]. In addition, $\log(D_{\text{Li}})$ is linearly proportional to $\log(\tau)$ (reorientational time constant for CB_9H_{10}).

Acknowledgement: This work was supported by JSPS KAKENHI Grant-in-Aid for Scientific Research on Innovative Areas “Hydrogenomics”, No. JP18H05513, JP18H05518, and JP18H05519.

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Poster 1 (No. 247) – QCD software development and performance of Fugaku and ARM architectures

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The supercomputer "Fugaku" was jointly developed by Fujitsu Limited and RIKEN, and is the latest supercomputer installed at the RIKEN Center for Computational Science in Kobe, Japan. In the recent Top500, HPCG, and HPL-AI benchmark rankings, it has been ranked No. 1 in the world for two consecutive terms (June 2020 and November 2020). The CPU installed in Fugaku is a 48-core + 2 assistant core processor called A64FX, which is an extension of the Arm v8-A instruction set architecture for high-performance computing, and was developed by Fujitsu as the processor for Fugaku. The CPU consists of four "core memory groups" (CMGs) of 12 cores, and the L2 cache is shared by the 12 cores in the CMG. The main memory per node is 32GiB. The interconnect is a Tofu interconnect D. In this talk, we will present an overview of Fugaku, development of QCD code for A64FX and its performance, and large-scale benchmark results on Fugaku.

Poster 1 (No. 256) – Geometrical clusters of the multi-replica Ising model

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We study the geometrical clusters in stacks of q independent copies of the two-dimensional Ising ferromagnet. By means of Monte Carlo simulations and a finite-size scaling analysis, we estimate the critical temperature and the critical exponents characterizing the transition. For two replicas a percolation transition occurs at the same temperature as for one replica (corresponding to the standard Ising problem), but with different exponents for the percolation strength and the

average cluster size. With increasing number of replicas, stronger and stronger deviations are observed. Implications of our simulations and scaling arguments for the case of general q are discussed.

Poster 1 (No. 262) – The Role of Resampling in Population Annealing

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Population Annealing (PA) is a population-based algorithm that can be used for equilibrium simulation of thermodynamic systems with a rough free energy landscape. It is known to be more efficient in doing so than standard Markov chain Monte Carlo alone. The algorithm has a number of parameters that can be fine-tuned to improve performance. While there is some theoretical and numerical work regarding most of these parameters, there appears to be a gap in the literature concerning the role of resampling in PA, which this work attempts to bridge.

The $d = 2$ Ising model is used as a benchmarking system for this study. At first various resampling methods are implemented and numerically compared using a GPU PA implementation. In a second part the exact solution of the Ising model is utilized to create an artificial PA setting with effectively infinite Monte Carlo updates at each temperature as well as an infinite population. This allows one to look at resampling in isolation from other parameters.

We identify when resampling choices affect the simulation outcome and obtain some results that are model-independent. Further, we name two resampling methods that appear preferable over the widely used multinomial resampling.

Poster 1 (No. 269) – Population annealing with weighted averages: A case study for the Ising model

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Originally proposed by Hukushima and Iba [1], population annealing (PA) is a highly parallelizable sequential Monte Carlo algorithm that shares similarities with simulated annealing and parallel tempering. The method is based on a population of replicas designated to sample the equilibrium distribution at each temperature in the cooling schedule. Every change in temperature is accompanied by a resampling step where the number of each replica's descendents in the consecutive population is proportional to the relative Boltzmann weight. The correlations induced by resampling are counterbalanced by an equilibration routine applied at every temperature employing, e.g., a Markov-chain Monte Carlo (MCMC) method [3][4].

In practise, there is a bound on the number of replicas that can be handled in parallel. If no PA run with population size MR can be performed on the given hardware, one might consider averaging over M independent runs of size R . However, the M smaller populations have implicitly been normalized differently in the PA process which makes averaging non-trivial. Machta [2] proposed a weighted average based on the free energy estimator to account for this problem.

We investigate the consequences of employing these weights to PA data of the two-dimensional Ising model in comparison to the exact solutions available [5]. In particular, we present an analysis of the scaling of bias and statistical errors with respect to M and the number of MCMC sweeps per spin θ . We also discuss in which cases weighted averages may be applied successfully and compare to criteria given by Machta [2] and Wang *et al.* [6].

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Poster 1 (No. 278) – Diffusional characteristics of Newtonian Event-Chain Monte Carlo in hard disk systems

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Equilibration and relaxing time of the physical properties in time correlation functions have been investigated as fundamental issues in the history of molecular simulation. Recently, the combined algorithm of the event-chain Monte Carlo (ECMC) [1] and event-driven molecular dynamics (EDMD) [2], called Newtonian ECMC (NEC)[3], was proposed. The particle positions in NEC are updated as sequential collisions (i.e., event-chain) with chain length like ECMC; however, its direction obeys collision rule based on the particle velocities like EDMD. In the hard-sphere systems, the NEC outperformed other algorithms in the efficiency of the diffusion coefficient, nucleation rate, and melting process, which was recently extended to anisotropic hard particles without approximations [3]. However, the optimal performance strongly depends on the parameter (i.e., chain length), the physical properties, and the system size, where its microscopic mechanism is still elusive. To figure out the key factors of the relaxing time, we investigate NEC in the two-dimensional hard disk systems systematically as the simplest but untrivial case. We especially focus on diffusional characteristics per event or CPU hour, such as diffusion coefficient and pair dispersion (i.e., a separation distance of two particles in time where they are located as neighbors at the initial time). Figure 1 compares the results of methods on (a) the chain length dependence of diffusion coefficient and (b) pair dispersion in time with optimal chain length. Based on the event, NEC has a fair advantage on diffusion coefficient for a wide range of chain length; however, ECMC (xy-direction version) is the highest performance of pair dispersion. We address the microscopic mechanism of the above contradictory situation, which will be presented at the conference.

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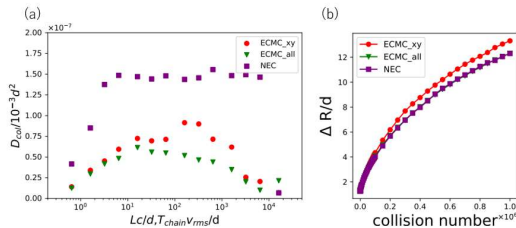


Figure 1 The comparison of the three methods based on collision numbers in the liquid state of hard disk system: (a) The chain length (L_c or $T_c v_{rms}$ in units of particle diameter d) dependence of the diffusion coefficients D_{col} and (b) pair dispersion $\Delta R/d$ as a function of collision number are shown. Note that v_{rms} is the root mean square velocity.

Poster 1 (No. 287) – Convective non-locality: the impact of boundary layers on the convection dynamics in 2D stellar hydrodynamic simulations

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Turbulent convection is a common process in stellar interiors which has a critical impact on long-term stellar evolution. For instance, the penetration of convective material into stably stratified layers (i.e. convective overshooting) can lead to important exchange of angular momentum and transport of chemical elements. Stellar convection however is a strongly non-local phenomenon – it is driven by

perturbations at the boundaries. So, the radial extent of the simulation domain is expected to have a significant impact on the convection zone's properties.

To investigate and quantify this we perform a series of 2D simulations of a sun-like star with different radial truncations using reflective boundaries with a constant flux corresponding to about one solar luminosity. The simulations are carried out with MUSIC – a multi-dimensional, fully compressible time-implicit hydrodynamical code designed to produce global simulations of stellar and planetary interiors.

Because of the mean hydrostatic temperature and density stratification, including more of the outer convective layers is associated with stronger perturbations at the outer simulation boundary. This leads to a significant increase in the convective intensity, as characterised by e.g. the velocity dispersion and the entropy perturbations and hence the effective Nusselt number, throughout the bulk of the convection zone, as well as the depth of the overshooting layer. It is also linked to a significant decrease in the convective time scale near the lower convective boundary, which leads to a faster relaxation of that layer. The location of the inner simulation boundary has a smaller impact, as long as a significant part of the stably stratified zone is included.

Poster 1 (No. 294) – The unstable analysis of soliton compression in Silicon photonic crystal

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Soliton solution to the perturbed nonlinear Schrödinger equation, for describing the wave in the photonic crystal, can be found by the sine-cosine expansion method. This method provides both bright and dark soliton solutions. The instability of the perturbed soliton in the perpendicular direction to the wave motion will be shown from the growth rate. The time evolution of the unstable soliton will be transformed into the higher dimensional solitons.

Poster 1 (No. 298) – Percolation Properties of Spin Glasses

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In the Ising model there exists a direct connection between percolation of Fortuin-Kasteleyn clusters and the ferromagnetic phase transition. Percolation of Fortuin-Kasteleyn clusters in spin glasses occurs at a higher temperature than the spin-glass transition [1, 2, 3]. Even when looking at the Fortuin-Kasteleyn percolation in two replicas simultaneously the percolation temperature remains above the critical one [5].

Here, we focus on percolation in two and more replicas. To be more concrete, we are interested in the CMR representation of L. Chayes J. Machta and O. Redner [4] as well as the two-replica Fortuin-Kasteleyn representation of C. M. Newman and D. L. Stein [5]. The latter approach decreases the temperature of percolation notably and an extension of it to more than two replicas further lowers the percolation threshold. To investigate the characteristics of these percolation transitions and their physical relevance we perform Monte Carlo simulations of the two dimensional Ising spin glass. A better understanding of these phenomena might help to develop efficient cluster algorithms for spin glasses at low temperatures.

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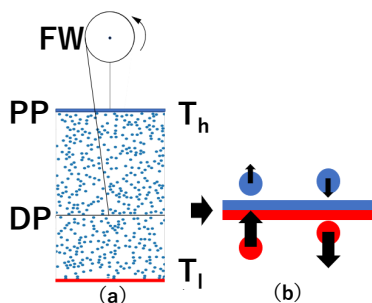
Poster 1 (No. 305) – Molecular dynamics study on the nano-scale β -type Stirling engine

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The Stirling Engine (SE) is one of the devices constructed based on the thermodynamic cycles, where the difference of temperature generated the rotation of the flywheel. Its importance in the age of SDGs would be significant due to SE's wide applicability and compactivity. The arbitrary (stochastic) heat resources in contact with the part of systems generate the work (i.e., energy). Recently, the nano-scale (α -type) SE in particle systems has been investigated via Molecular Dynamics (MD) simulation [1], which surveys the condition of stable flywheel rotation and the thermal efficiency by changing particle number and temperature difference. Besides, the β -type of SE has a couple of advantages over the α -type, which has much compactivity since two pistons, i.e., displacer (DP) and power (PP) pistons, are located on the same axis. In this study, we focus on the nano-scale " β -type" SE, especially on constructing the relevant model of DP. We performed the MD on the two-dimensional model with a couple of hundreds of particles and calculated the thermal efficiency. We would clarify the minimal necessary condition of stable rotation in the limit of both lower particle and smaller difference of temperature to confirm the validation of the thermodynamic cycles. The comparison of the results with the past literature will be summarized, which will be presented at the conference.

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(a) The schematic view of our nano-scale (β -type) SE in two dimensions is shown. The flywheel (FW) is driven by particles as the work fluids via power piston (PP) and displacer piston (DP), which are put between two heat walls at

the temperature T_h and T_l . (b) The particle pass through our DP, which has two heat walls worked as the regenerators.

Poster 1 (No. 307) – Numerical Analysis of Electronic state of CNT/BNNT Heterojunction

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With high electron mobility and thermal conductivity of the carbon nanotube (CNT), it is expected to build high-speed nano-devices with low electricity consumption operation. Boron nitride nanotubes (BNNTs) which have analogous structures with CNTs show wide bandgaps ($\sim 5\text{eV}$) and become electrical insulators. For bond lengths of C-C in CNT and B-N in BNNT are close to each other, CNT and BNNT of the same chirality combine and form heterojunctions. We are interested in electrical properties of the heterojunctions, especially metallic-CNT/BNNT junctions. In this paper, I-V characteristics of CNT/BNNT heterojunctions are numerically investigate with the density functional theory (DFT) method and the non-equilibrium Green's function (NEGF) method.[1] First, we perform band calculations of structural optimized double barrier junctions, and next, the I-V characteristics of the heterojunctions are calculated. The $I-V$ characteristics show flat behavior in a certain bias voltage region. These behaviors are different from those of the semiconductor based double barrier diodes. Transmission functions are also determined and an energy gap centered on the Fermi level and some sharp peaks in the gap are observed. Since the spacing of the peaks is dependent on the separation length of BNNT barriers, it can be seen that the GNR/BNNT double barrier heterojunctions have resonant states. By the PDOS analysis, we also find that the behaviors in the transmission function due to the matching of the eigenstates between the heterojunction and the electrodes.

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Poster 1 (No. 328) – Li on a C-H divacancy in graphane

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Density functional theory calculations are performed to study the interaction between Li atoms and the C-H vacancy single and bilayer graphane systems to enhance the performance for lithium-ion batteries (LIBs). The energetic stability, structural and electronic properties of different Li configurations are examined. We find that the two Li atoms prefer to alternatively adsorb on the C-H divacancy with a relatively high binding energy. The density of states plots reveals that this kind of structure is metallic with a pronounced sharp peak crossing the Fermi level, contributed by the Li states. The calculated equilibrium redox potential associated with the movement of Li atoms into and out of the graphane layers is relatively high. The Li capacity is also calculated and compared with the available experimental and theoretical data of other materials.

Poster 1 (No. 357) – Critical properties of the three-dimensional three-state random-field Potts model

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Unlike the random-field Ising model, an exact ground-state algorithm for the random-field Potts model (RFPM) with more than two states does not exist. Using a computationally efficient graph-cut method, however, we solve the ground state problem approximately in polynomial time. Combining this technique with a sophisticated extrapolation method, we can guarantee results that are representative of the exact ground-state behavior up to reasonably large system sizes. A comprehensive study is carried out to predict the critical behavior for the case of the 3-state model in three dimensions from such approximate ground-state calculations. In particular, we determined the magnetization, Binder cumulant, specific heat, as well as the connected and disconnected susceptibilities for many ran-

dom initial conditions and extrapolated them to the limit of quasi-exact solutions. These results are used to (precisely) locate the critical point and to calculate (accurately) the critical exponents that characterize the singular behavior near the phase transition.

Poster 1 (No. 400) – Structural and dynamical properties of randomised mixed labyrinth fractals

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In order to predict the structure of synthesized dendritic structures, like nano antennas or polymer brushes, or of porous structures, like sponges, and dynamical processes therein randomised mixed labyrinth fractals (RMLF), a special subclass of Sierpinski carpets, are analysed here. We make various combinations of two labyrinth patterns at different mixing ratios. Our main interest is, if and how the mixing ratio of the combinations effects the resulting shortest path- and random walk dimension of the obtained RMLF.

For more general Sierpinski carpets, it is known that the mass of the fractal patterns (active sites), the number of contact points (infinitely ramified) and the length of the shortest path have a significant impact on the resulting random walk dimension [1]. An open question is if and how the different path lengths within the patterns influence the random walk dimension. So we define labyrinth pattern combinations, where only the path lengths but not the number of active sites or number of contact points change due to the different mixing ratios. We show that for these RMLF one can determine both dimensions directly by utilizing the path matrix of the corresponding patterns [2]. Furthermore, we discuss the various effects of the mixing ratio for the different pattern combinations on the shortest path- and random walk dimension [3].

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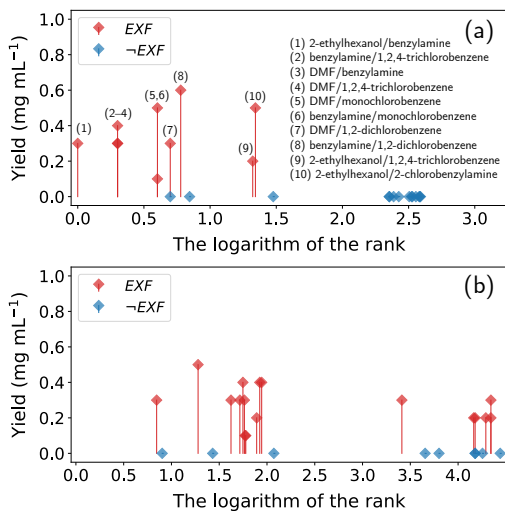
Poster 2 (No. 14) – Application of evidence theory to recommend solvent mixtures for chemical exfoliation of graphite

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Chemical exfoliation of graphite is an effective method to produce graphene of relative high quality, where the choice of solvents plays an important role in the product yield and quality [1]. Here, we present a data-driven approach to systematically investigate synergistic effects of solvents and recommend new solvent mixtures for the liquid-phase exfoliation of graphite. To overcome the challenges with numerous solvent-mixture candidates and limitations of existing data, the evidence theory [2] is used to develop an evidence-based recommender system for recommending solvent mixtures. The proposed system measures similarities between solvent combinations and utilizes the similarities to recommend potential solvent mixtures. We use leave-one-out cross-validation on an experimental data set of single solvents and binary solvent mixtures to evaluate the recommendation capability of the proposed system. Figure 1(a) shows that solvent mixtures with high graphene yield are recommended with higher ranking than the non-exfoliating solvent mixtures [3]. Furthermore, we experimentally validate 14 most strongly recommended ternary solvent mixtures and confirm that 11 of them exfoliate graphite to produce graphene (Fig. 1 b) [3].

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Stem plots of screened binary solvent mixtures (a) and new ternary solvent mixtures (b) that are randomly selected for the sake of validation. Red and blue points indicate results corresponding to exfoliating and non-exfoliating mixtures, respectively.

Poster 2 (No. 25) – The experience of using of versions of binary correlation function approximations by proposed sets of functions for purposes of the structural quasicrystal analysis and model computations by means of variational principle of a functional of the equilibrium free energy of simple liquids

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Versions for applying binary correlation function approximations that uses sets of:

- “displaced Gaussian functions that averaged in 3-dimensional space” [1, 2]:

$$\psi_{m,k}(\vec{r}) = \left\langle e^{-\frac{(\vec{r}-\vec{a}_m)^2}{\sigma_k^2}} \right\rangle_{\vec{n} \cdot \vec{a}_m} = \frac{\sigma_k^2 \cdot e^{-\frac{(r^2+a_m^2)}{\sigma_k^2}} \cdot sh\left(2 \cdot \frac{r \cdot a_m}{\sigma_k^2}\right)}{2 \cdot r \cdot a_m};$$

- Hermite functions [2];

based on the quasicrystal model approach [1, 2] for purposes of performing of the structural analysis and computations of consistent thermodynamic properties of simple liquids by means of variational principle of the free energy functional in classical equilibrium statistical mechanics [2, 3] is considered. A preliminary comparison with the results of the molecular dynamics method is carried out.

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Poster 2 (No. 51) – Microscopic insights into dynamic disorder in the conformational changes of the protein

Yoshihiro Matsumura, Shinji Saito

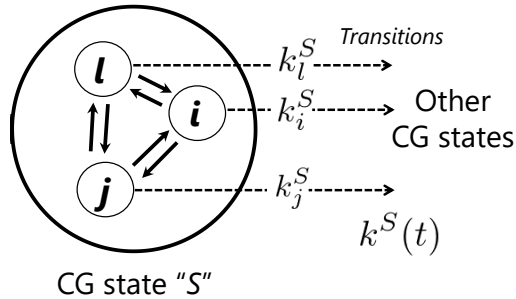
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Understanding the dynamic disorder behind a process, i.e., the dynamic effect of fluctuations that occur on a timescale slower or comparable with the timescale of the process, is essential for elucidating the dynamics and kinetics of complicated molecular processes in biomolecules and liquids. Despite numerous theoretical studies of single-molecule kinetics, our microscopic understanding of dynamic disorder remains limited. In the present study, [1] we investigate the microscopic aspects of dynamic disorder in the isomerization dynamics of the Cys14–Cys38 disulfide bond in the protein BPTI, which has been observed by nuclear magnetic resonance. We use a theoretical model with a stochastic transition rate coefficient, [2] which is calculated from the 1-ms-long time molecular dynamics trajectory obtained by Shaw et al. [3] The isomerization dynamics are expressed by the transitions between coarse-grained (CG) states consisting of internal states, i.e., conformational sub-states (see image below). In this description, the rate for the transition from the coarse-grained states is stochastically modulated due to fluctuations between internal states. Our analysis of the rate modulations behind the survival probability, in relation to the fluctuations between internal states, reveals the microscopic origin of dynamic disorder.

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Poster 2 (No. 63) – Radiative-rate calculations of erbium-like ions Lu IV, Hf V and Ta VI of interest in fusion

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There is a growing need in atomic data for elements which could be used in thermonuclear fusion installations. Lutetium ($Z = 71$), hafnium ($Z = 72$) and tantalum ($Z = 73$) would be candidates as plasma-facing materials in controlled nuclear fusion devices [1, 2]. In addition, the last two of them are also produced in neutron-induced transmutation of tungsten ($Z = 74$) and tungsten-alloys that will compose the divertors in future tokamaks [3]. As a result, their sputtering may generate ionic impurities of all possible charge states in the deuterium-tritium plasma that could contribute to radiation losses in fusion reactors. Therefore, the identification of emission lines and the knowledge of spectroscopic parameters from all ionization stages of these elements have potential important applications in this

field.

In the present work, we report the theoretical determination of radiative properties (transition probabilities and oscillator strengths) in Lu IV, Hf V and Ta IV belonging to the isoelectronic sequence of Er I, for allowed lines falling in the spectral range from ultraviolet (UV) to infrared (IR).

In view of the lack of experimental radiative parameters available for Lu IV, Hf V and Ta IV, the accuracy of the data obtained in our work has been assessed by comparing two independent theoretical approaches, i.e. the semi-empirical Hartree-Fock with relativistic corrections method (HFR) [4] and the *ab initio* multiconfiguration Dirac-Hartree-Fock with subsequent relativistic configuration interaction method (MCDHF-RCI) [5, 6].

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Poster 2 (No. 67) – Dynamics of spin-1 magnets from numerical simulations

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Spin-1 magnets allow for dipolar and quadrupolar moments on a single site, providing novel properties as seen in spin nematic phases [1], Fe-based superconductors [2] and cold atom systems [3]. Unfortunately, such unconventional phases can be

found hard to probe experimentally, and therefore require new theoretical tools to describe and interpret their ground state and excitation properties. In this talk, we present a new Monte Carlo and Molecular Dynamics scheme, which can be used to study thermodynamic and dynamic properties of spin-1 magnets. The extension of the problem from its $SU(3)$ symmetry to a $U(3)$ symmetry allows us to treat dipolar and quadrupolar fluctuations on equal footing. Within this framework we can define Metropolis updates in the space of $U(3)$ matrices, and numerically integrate the equations of motion for given thermodynamically equilibrated ensembles. We benchmark our numerical implementation by studying the ferroquadrupolar phase of the spin-1 bilinear-biquadratic (BBQ) Hamiltonian on the triangular lattice, and find a perfect match to analytical flavour-wave theory and low-temperature expansion. Furthermore, the investigation of thermodynamic properties of the model revealed a topological phase transition, originated in the proliferation of vortex – anti-vortex pairs. We show that our method does not only provide a way to visualize the annihilation process of topological defects in spin-nematic phases, but can also be used to explore thermodynamic and dynamic properties at finite temperatures, certainly helpful to identify and characterize spin-1 magnets in experiments.

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Poster 2 (No. 82) – Dynamical analysis for protein folding simulations using relaxation mode analysis

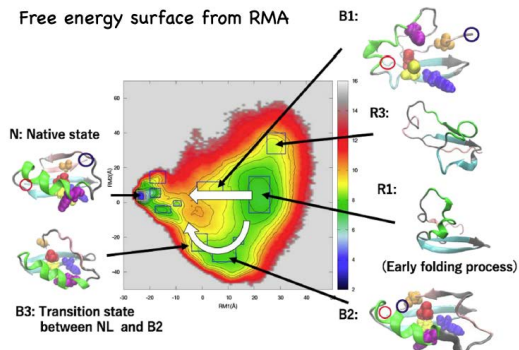
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Molecular dynamics simulation is a powerful method for investigating the structural stability, dynamics, and function of proteins at the atomic level. In recent years, it has become possible to perform simulations on time scales of the order of milliseconds using special-purpose system. It becomes to be necessary to develop dynamical analysis method to automatically extract reaction coordinates

that identify characteristic states in simulations. Relaxation mode analysis (RMA) have been developed to investigate dynamics and kinetics of spin [1], polymer [2], and protein simulations [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. RMA approximately extracts slow modes and rates from simulations. RMA was applied to folding simulations [3, 5, 9, 11] and several-microsecond-scale molecular dynamics simulations [4, 8, 12]. New methods related to RMA were also developed such as PCRMA [4], Markov state RMA [5], and PDRMA [8]. Here, we introduce RMAs and show the results of protein simulations of a designed mutant of protein G, NuG2, [9] for which folding simulations were previously performed by Lindorff-Larsen et al. [10]. RMA clarified two main folding pathways.

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Poster 2 (No. 86) – Molecular dynamics simulation for LIM2 domain mutants in FHL1 protein

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Reducing body myopathy is one of hereditary myopathies caused by mutations in the *FHL1* gene, which encodes a protein named four and a half LIM domains 1 (FHL1). FHL1 contains 4.5 LIM domains, and each LIM domain contains two zinc fingers in which 4 amino acids (4 cysteines or 3cysteins and one histidine) bind zinc. These zinc fingers are important structures to maintain the LIM domain. The mutations in *FHL1* selectively damage the zinc finger structures in the LIM2 domain.

We performed molecular dynamics (MD) simulations examining for stability and dynamic property of the variant of LIM2 domain using wild type and mutant of LIM2 domain (PDBID: 1X 63). The force fields for the zinc residue and its binding residues were prepared with quantum computing [2], and the force fields for the other amino acid residues were defined by AMBER99SBILDN. We prepared zinc-binding or non-binding models, and preformed 500 ns MD simulations

for each model. We found that the non-binding models tend to maintain the wild-type structure. On the other hand, in the zinc-binding models, the structure of main chain was fluctuated widely, which changed the position, shape, and dynamic properties of the zinc finger loops.

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Poster 2 (No. 87) – Application of plasma simulation and theory to heavy ion cancer therapy

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The radial dose (RD); that is, the dose as a function of r , is employed to estimate cell survival rates in treatment planning systems for heavy ion cancer therapy, where r is the perpendicular distance from the incident ion path. Two types of radial dose distributions are available in radiology and radiation biology. Despite the fact that the region near the incident ion path is the most important in terms of biological effects, different features exist between these two types of conventional RD distributions in this region. Following the proposal of these distribution models, computers have undergone tremendous development. Therefore, we decided to develop a simulation model that is closer to reality than the conventional models. Because the energy deposition of secondary electrons creates the RD, it is necessary to develop a simulation model for the motion of secondary electrons that is as close to reality as possible. The difference between these two types of conventional distributions is caused by the effect of plasma produced near the incident ion path. In the one distribution proposed from theory, the effect of plasma is considered, however, the target (free electron gas) treated in this theory is far from the reality. On the other hand, plasma is not created in the other distribution obtained from simulations using binary collision models. Because the computers were very slow when these models were proposed, we guess that plasma could not be treated. By

effectively using present super-computers, we developed a new simulation model in which plasma is created. Only our model almost reproduced the trend of the measurement trend of secondary electron yield as a function of stopping powers [1]. The results obtained from these conventional models are independent of stopping powers. We propose a new distribution using RD obtained from our simulations [2]. Further, we confirmed that the electron density in plasma solved by a plasma theory agrees well with our simulation results [3].

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Poster 2 (No. 88) – Dynamics of photoinduced entanglement generation between remote electron-phonon systems

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We numerically study the dynamics of quantum entanglement generation between remote electron-phonon systems by photoirradiation employing a model of multiple spins and boson modes.

Generation of quantum entanglement is a key to realize various quantum information devices. It is particularly important that irradiation of light induces quantum entanglement between systems without direct interaction[1,2]. Theoretically, irradiation of classical light to remote systems corresponds to "local operations and classical communication" in the terminology of quantum information science, and no entanglement generation is obtained between them. Hence, the quantum mechanical nature of light is essential to understand the entanglement generation mechanism[3]. On the other hand, considering that quantum entanglement plays an important role in quantum many-body physics[4], the coherent dynamics of remote systems is an appropriate reference to study general quantum many-body states under photoirradiation, i.e., it gives us an insight on the photoinduced entanglement in interacting many-body systems.

We focused on the phonon properties by dividing the entire electron-phonon-photon state $|\Phi(t)\rangle$ into phonon states $|\eta_n(t)\rangle$ and the electron-photon states $|\theta_n(t)\rangle$ by the Schmidt decomposition as $|\Phi(t)\rangle = \sum_n \lambda_n(t) |\eta_n(t)\rangle |\theta_n(t)\rangle$. Numerical calculations on the time-evolution of the singular values $\lambda_n(t)$ and $|\eta_n(t)\rangle$ show that light irradiation induces weak entanglement between different electron-phonon systems at first, and that creation of entangled phonons follows to construct strongly entangled phonon states. The calculated results also show that the quantum mechanical nature of light should be taken into account even in directly interacting systems in order to design quantum control methods in transient regime.

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Poster 2 (No. 98) – Molecular Dynamics simulations of ring polymers in a slit geometry of two parallel walls.

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We have used molecular dynamics simulations to obtain the monomer density profiles for linear polymers and ring polymer chains of 360 monomers length with different topologies such as: 0_1 , 3_1 , 6_1 , 7_1 , and 9_1 in a slit of two parallel walls with one attractive and another repulsive surface. We have used Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software to perform simulations with Verlet integration algorithm. The interactions between

monomers were simulated as Lennard-Jones 12-6 potential, for bonds we have used Finitely Extensible Nonlinear Elastic (FENE) potential and the interaction with the walls took into account via Lennard-Jones 9-3 potential. The number of adsorbed monomers on the surface decreases with increasing of the entanglement of polymer. As the number of monomers on the surface decreases so there is more of them in the space between the walls. For higher temperatures polymer chains start desorbing from the surface of the wall which might be explained intuitively by increased fluctuations of the polymers. These results are important for better understanding nature of the depletion forces which arise in a slit geometry of two parallel walls with mixed b.c.

Poster 2 (No. 100) – Excitation and transport of bound magnon clusters in frustrated ferromagnetic chain

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By exploiting density-matrix renormalization group methods, we study magnetic and transport properties of a frustrated quantum spin chain with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange interactions in an applied magnetic field. In high magnetic fields, there appear a series of spin multipole liquid ground states such as quadrupole, octupole, and hexadecapole, which are two-, three-, and four-magnon bound states, respectively. Since the low-energy excitation is governed by multi-magnon bound states, we envisage that bound magnon clusters would carry spin current. We will report detailed analyses of multipole excitation spectra and current correlation functions, and discuss how the magnon clusters contribute to the transport.

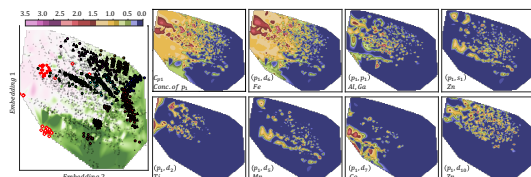
Poster 2 (No. 101) – Active learning in discovery $\text{SmFe}_{12-x-y}\text{A}_x\text{B}_y$ magnets A, B as Mo, Zn, Co, Cu, Ti, Al, Ga

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We examined the problem of exploring potentially stable $\text{SmFe}_{12-x-y}\text{A}_x\text{B}_y$ structures with A, B as Mo, Zn, Co, Cu, Ti, Al, Ga, and $x + y \leq 4$, using an active learning approach. Using first-principle calculation, we estimate the formation energy of the 4062 $\text{SmFe}_{12-x-y}\text{A}_x\text{B}_y$ structures to handle as the experimental dataset. Optimal active learning designs are investigated in three abilities: (1) to build accurate stability predictors using most finite training data, (2) ability to recall most likely stable structures, and (3) ability to interpret the exploration process. In evaluating the prediction ability, the mean absolute prediction errors (MAE) of all active learning designs show that the lowest values vary between 2.1×10^{-2} (eV/atom) and 1.8×10^{-2} (eV/atom). Notably, the formation energy-embedded Orbital Field matrix representation [1] has the greatest impact on the performance of active learning designs. MAE of embedded representation designs outperforms all corresponding systems using the non-embedding method by 1.7 times on average. In the experiment of finding the most likely stable structures, all active learning designs present the success recall rate increased by 1.3-to 2.3 times compared to the random search strategy. Finally, we manifest correlations on the embedding space that most likely stable $\text{SmFe}_{12-x-y}\text{A}_x\text{B}_y$ structures comprise post-transition substituted element connections and vice versa.

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Distribution of $\text{SmFe}_{12-x-y}\text{A}_x\text{B}_y$ structures on embedding spaces, which are learned by referring to the OFM features [1] (p_1, p_1) (upper panel) and (f_6, d_{10}) (lower panel), observed formation energy ΔE of queried structures.

Poster 2 (No. 112) – Thermodynamic folding transition of a small protein molecule

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Proteins are polymers formed by linearly polymerized amino acids. Proteins are known to spontaneously fold into unique three-dimensional structures in aqueous solutions, and their native structure is believed to be determined by the information of amino acid sequences only. The protein folding problem is one of the most challenging and important problems in natural sciences[1]. The "ab-initio" method based on molecular simulations provides a powerful and promising route to solve the problem. However, it is difficult to perform sufficient sampling with a limited computational time using conventional molecular dynamics and Monte Carlo methods because the energy landscape of proteins is characterized by a huge number of local energy minima separated by high barriers in configurational space. The generalized-ensemble algorithms have been developed to overcome this type of problems. In the present study, we performed the folding simulation of a small protein molecule, called chignolin, using a method of the generalized-ensemble, the multicanonical replica-exchange method (MUCAREM)[2]. Configurational sampling was performed by our generalized hybrid Monte Carlo (GHMC) method[3, 4]. The GHMC method uses equations of motion to efficiently generate trial configurations. We calculated thermodynamic quantities of the chignolin molecule to characterize the folding transition. Figure 1 shows the heat capacity of the chignolin as a function of temperature. The heat capacity shows the maximum at 344 K indicating the temperature of the folding transition T_f of the chignolin. Our simulation result is found to be in good agreement with the experimental estimate of the temperature of the folding transition (311-316 K)[5]. We will present more detailed analysis of the folding transition at the conference.

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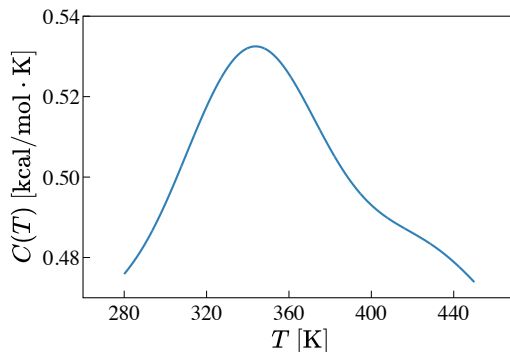


Fig.1: The heat capacity $C(T)$ of the chignolin as a function of temperature T .

Poster 2 (No. 122) – Molecular Modeling of Ionic Liquids and their Analogues via Self-Consistent Scheme with MD and DFT Methods

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The development of atomistic force fields has remain important for the improvement of molecular dynamics (MD) calculations of various soft materials. In particular, electrolytes systems complicate the Coulomb interaction in condensed phase by inducing many-body effects of polarization and charge transfer.[1,2] The usage of polarizable force field is then a theoretical methodology for the exact treatment of Coulomb interaction, and charge scaling method is also an alternative approach for the modification of force field. Meanwhile, the scaling parameter remains empirically-determined for non-polarizable force fields of ionic liquids. Therefore we recently suggest a self-consistent modeling scheme combining MD and density functional theory (DFT).[3] This strategy is a useful tool to incorporate the effective interaction in condensed phase by theoretically quantifying the atomic charge distributions of molecules under the periodic boundary condition. This work demonstrates the self-consistent scheme to accurately evaluate

structural and transport properties of ionic liquid and their analogues.[3,4] The atomic charges of cation and anion determined with the Blochl charge analysis systematically improves the computational accuracy of electrical conductivity and viscosity over various ionic liquids and their analogues. The self-consistent shame thus addresses the transferability of nonpolarizable force field into functional self-assembled materials.

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Poster 2 (No. 127) – Machine Learning the 2D Percolation Transitions

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The percolation model is one of the simplest models in statistical physics displaying a phase transition [1]. A classical lattice is occupied randomly with a given probability at each site (or bond). A phase transition from a non-percolating to a percolating state appears around a probability p_c , the so-called percolation threshold. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques allow to detect phase transitions directly from images of computed quantum states [2,3]. Here, we implement ML/DL techniques to identify the percolation threshold in 2D by identifying the connectivity properties of percolation clusters. We employ a standard image classification strategy with a multi-layered convolutional neural network. In addition, we also work directly with the numerical “raw data”. The implementation is carried out in Python with the ML/DL libraries of Pytorch [4]. We pay special attention to the question of whether these DL methods can indeed identify percolation, i.e. spanning clusters, or are just

counting occupation densities.

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Poster 2 (No. 128) – Machine Learning Methods applied to the 2D Ising Model

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The Ising model is one of the most studied models in statistical physics. It is well known to exhibit an ordering transition in two dimensions (2D). Snapshots of magnetic configurations taken above and below the phase transition show clear differences in the distribution of spins. Recently, machine-learning methods have been shown to be successful in identifying and classifying such differences across many types of images, and also to the 2D Ising model [1-3]. Here, we study the performance and the limits of such classification models. In particular, we investigate how accurately the temperature of a given configuration can be classified from just the image. We use the TensorFlow environment as the main machine-learning environment and train with various neural network architectures. With respect to transfer learning between different variants of the model [2,3], we suggest classification according to spin-spin correlation length as more appropriate

than according to temperature.

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Poster 2 (No. 139) – Coarse-grained model for protein-nucleotide interaction

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Association/dissociation of protein molecules promotes or inhibits protein function in living cells. We have developed a coarse-grained model for interaction between protein molecules for long-time and large-scale simulations to investigate association/dissociation processes of protein complex. By using the Langevin dynamics simulation with our coarse-grained model, we have shown complex formation process of a small protein tetramer [1, 2], a potential candidate of unfolded intermediate during activation of a cyclin-dependent kinase [3], and electron transfer reaction constant from cytochrome f to plastocyanin [4]. In addition, the association/dissociation process of heat shock protein 90 (HSP90) and ADP has been elucidated by using all-atom molecular dynamics (MD) simulations [5].

In this work, coarse-grained model for protein-nucleotide interaction are developed and applied to long-time Langevin simulations for HSP90 and ADP. Free energy profile is calculated as a function of distance between ADP and 18 amino acid sidechain analogues (excluding Gly and Pro) by using all-atom MD simulations combined with the thermodynamic integration method. Then, the coarse-grained potential function and parameters are determined from the free energy profile obtained from the all-atom MD simulations. The coarse-grained potential is applied to the Langevin dynamics simulation for HSP90 and ADP. Free energy profile as a function of the distance between HSP90 and ADP is calculated and compared

with free energy profile obtained from our previous all-atom MD simulation.

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Poster 2 (No. 157) – Higher Order Auxiliary Field Quantum Monte Carlo Methods

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The auxiliary field quantum Monte Carlo (AFQMC) method has been a workhorse in the field of strongly correlated electrons for a long time and has found its most recent implementation in the ALF package (*alf.physik.uni-wuerzburg.de*). The utilization of the Trotter decomposition to decouple the interaction from the non-interacting Hamiltonian makes this method inherently second order in terms of the imaginary time slice. We show that due to the use of the Hubbard-Stratonovich transformation (HST) a semigroup structure on the time evolution is imposed that necessitates the introduction of a new family of complex-hermitian splitting methods for the purpose of reaching higher order. We will give examples of these new methods and study their efficiency, as well as perform comparisons with other established second and higher order methods in the realm of the AFQMC method.

Poster 2 (No. 177) – Optical and magnetic signatures of topological edge states in a dimerised donor chain

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The topological state in one dimension is interesting, but rarely explored in combination with electron correlations [1]. Meanwhile, one-dimensional hydrogen chains are increasingly attracting attention owing to their simplicity and natural link to strongly correlated electronic systems [2]. However, such hydrogen chains would be extremely difficult to prepare in practice; a more realistic alternative is to form chains of hydrogenic dopants in semiconductors such as silicon, making use of the techniques of atomic-scale lithography [3], as a way to provide a platform to study exotic electronic states.

Here we have studied the excited states of one-dimensional dimerised chains of hydrogenic donors in silicon, by using time-dependent Hartree-Fock and density-functional theories [4] and adopting the methodology previously used for uniform donor chains [5]. We find that tuning the inter-donor distances can induce a phase transition from an anti-ferromagnetic ground state to a topological phase supporting spin-polarised edge states and having no spins in the bulk. Significant changes in the optical spectra accompany this transition, with a robust $1s \rightarrow 2p$ ‘atomic’ transition providing a signature for the phase transition and the existence of the edge states. By contrast, the bulk of the chain becomes spinless as the topological states form, inducing a reduction in the bulk energy gap and a decrease of the excitation energies in the optical spectra. The inclusion of physics beyond the Su-Schrieffer-Heeger-Hubbard model [6] (long-range electron correlations and basis states beyond the $1s$ manifold) has a critical effect on the results and leads to the novel prediction of a change in optical response related to a topological phase transition. Our results provide a theoretical foundation for using artificial donor linear arrays in semiconductors to form a topological edge state for a one-dimensional many-body system by design.

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Poster 2 (No. 198) – Simulation study of the function of the domain swapping in the HSP90 chaperone cycle

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Molecular dynamics simulation is a useful tool for understanding the fluctuations and characteristics of biomolecules. Recently, it has become possible to perform the calculations of large-scale systems and long-time calculations. Heat Shock Protein 90 (HSP90), one of the molecular chaperons, has been known as a target protein for anticancer drugs. It has an essential function in folding and stabilizing various client cancer-related proteins. HSP90 forms a homodimer, and it consists of three domains, N-terminal domain (NTD), Middle domain (MD), and C-terminal domain (CTD). In the HSP90 chaperone cycle, when the ATP and the client protein bind to the HSP90NTD, a partial exchange of domains, called the domain swapping, occurs at the HSP90NTD domain swapping region. After that, the co-chaperone binds to the HSP90, and the chaperone cycle processes. In our previous study, we developed a new HSP90 inhibitor that binds to the HSP90NTD [1]. Moreover, we found that this inhibitor interacts with the domain swapping region. In this study, to investigate how the interaction of this inhibitor with the domain swapping region is related to the inhibition of the HSP90 chaperone cycle, we performed several molecular dynamics simulations.

We have compared the molecular dynamics simulation of the ATP + co-chaperone p23 + HSP90 system with the domain swapping and that without the domain swapping. It showed that the domain swapping induces the stable interaction between HSP90 and the p23, while the lack of the domain swapping enhances the dissociation of the p23 from HSP90NTD. We found that the homodimer structure of the interface helices in the HSP90NTD is frequently lifted with an unstable state, leading to the dissociation of the p23. The lifting motion of the interface helices would be controlled by domain swapping. However, without domain swapping, the instability of the interface helices affected the entire HSP90NTD, and it led to the dissociation of the p23. Therefore, domain swapping is very important for the stable binding of the p23 in the HSP90 cycle. The new HSP90 inhibitor

that we developed interacts with the domain swapping region of HSP90, and it would lead to difficulty binding of co-chaperone. It may lead to the inhibition of the HSP90 chaperone cycle.

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Poster 2 (No. 199) – Deep attention model for extracting material structure-property relationships

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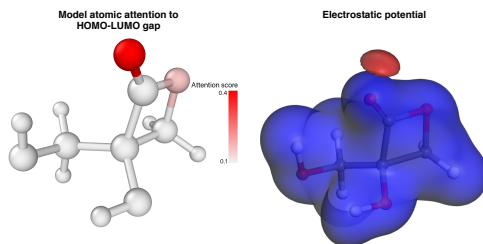
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Recent efforts in materials informatics (MI) include the applications of data mining and machine learning methods to materials science to build predictive models from data or extract useful knowledge toward accelerating materials discovery [1]. In this field, the development of material descriptors is very important since most MI methods depend on materials representation. An appropriate representation can produce good prediction results and enhance the interpretability of the machine learning models. In this work, we introduce an attention neural network model to represent the structures and predict the target physical property of material molecules and crystalline structures in materials science. The model can capture information on atoms and their local environments by taking into account self-consistently long-range interactions. The representation is learnt and updated by critical information of local structures and target physical properties via an attention mechanism. The proposed model was evaluated on three benchmark datasets including Qm7 [2], Qm9 [3], and Latxb [4]. The experimental results show that the predictive performance of the proposed model outperforms the WaveScatt [5] and the orbital-field matrix (OFM) [6]. Moreover, the obtained quantitative contribution of each local structure to the properties of the materials is useful for understanding the structure-property relationships of the materials.

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The left image shows the attention score of the HOMO-LUMO gap produced by the proposed model, while the right one indicates the highest electrostatic potential of $C_4H_6O_4$ (Qm9) from simulation. The result verifies the consistency between the model and DFT calculation.

Poster 2 (No. 207) – Effect of phase string on single-hole dynamics in the two-leg Hubbard ladder

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Optical measurements in doped Mott insulators have discovered the emergence of spectral weights at mid-infrared (MIR) upon chemical doping and photodoping [1, 2]. MIR weights may have a relation to string-type excitation of spins, which is induced by a doped hole generating misarranged spins with respect to their sublattice. There are two types of string effects: one is an S^z string that is repairable by quantum spin flips [3, 4, 5, 6] and the other is a phase string

irreparable by the spin flips [7]. We investigate the effect of S^z and phase strings on MIR weights. Calculating the optical conductivity of the single-hole Hubbard model in the strong-coupling regime and the t - J model on two-leg ladders by using time-dependent Lanczos and density-matrix renormalization group, we find that phase strings make a crucial effect on the emergence of MIR weights as compared with S^z strings [8]. Our findings indicate that a mutual Chern-Simons gauge field acting between spin and charge degrees of freedom, which is the origin of phase strings, is significant for obtaining MIR weights. Conversely, if we remove this gauge field, no phase is picked up by a doped hole. As a result, a spin-polaron accompanied by a local spin distortion emerges and a quasiparticle with a cosine-like energy dispersion is formed in single-particle spectral function. Furthermore, we suggest a Floquet engineering to examine the phase-string effect in cold atoms.

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Poster 2 (No. 212) – Four-body variational calculation of muonic molecules in an electron cloud

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A muonic molecule consisting of a negative muon (μ) and two nuclei of hydrogen, e.g. $pp\mu$, $dd\mu$ and $dt\mu$, has a compact structure whose size is more than 100 times

smaller than the hydrogen molecule. Since the muonic molecule is a positively charged ion, it behaves as a quasi-nucleus in atomic/molecular systems. The formation of the muonic molecules has been investigated both theoretically and experimentally in the studies of muon catalyzed fusion (μCF) [1] where the μ facilitates intramolecular nuclear fusion like a catalyst.

The $dt\mu$ is considered to be formed in the D_2 molecule resonantly in the collision between $t\mu(1s)$ and D_2 ($t\mu + \text{D}_2 \rightarrow [dt\mu]e\text{-de}$) by transferring the binding energy of $dt\mu$ to the rovibrational excitation energy of $[dt\mu]e\text{-de}$ [2]. A similar process for the excited $t\mu$ would be allowed, $t\mu(n=2) + \text{D}_2 \rightarrow [dt\mu^*]e\text{-de}$ where $dt\mu^*$ is a resonance state of $dt\mu$. The latter process appears in the μCF side-path model [3] and affects the muonic atom populations in μCF .

While the three-body properties (energy levels, structures and lifetimes) of the muonic molecules have been investigated precisely [4], the four-body properties of these muonic molecules in the electron cloud are still on discussion. In the case of $dt\mu$ in the electron cloud, the binding energy of $dt\mu$ slightly changes by the surrounding electron; however, a perturbative calculation [5] suggests a slow convergence of such energy shift and a variational calculation will be required. Furthermore, the resonant $dt\mu^*$ has much larger size than $dt\mu$, there expected to be a considerable change in the energy levels and structures from the three-body properties.

In this work we report our recent progress of the four-body treatment of the muonic molecules in the electron cloud. Based on a Gaussian expansion method (GEM) [6], a four-body system ($dt\mu e$) is expanded in terms of Gaussian basis functions defined in several different Jacobian coordinate systems. The Schrödinger equation is converted to a generalized eigenvalue problem. Since the muonic molecules in the electron cloud are unstable against the Auger transitions, we deal with the transitions by a complex coordinate rotation method [7]. The complex coordinate rotated Hamiltonian results in the generalized eigenvalue problem for the non-Hermitian matrices. The complex eigenvalues are solved by using an implicitly restarted Arnoldi iteration method. We reveal that the energy level shifts of $dt\mu e$ [8] and $dt\mu^*e$ ($dd\mu^*e$) and their structure changes by the electron attachment.

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Poster 2 (No. 249) – Quantum criticality at finite temperature for two-dimensional JQ_3 models on the square and the honeycomb lattices

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We study the quantum criticality at finite temperature for three two-dimensional (2D) JQ_3 models using the first principles quantum Monte Carlo calculations (QMC). In particular, the associated universal quantities are obtained and their inverse temperature dependence are investigated. The considered models are known to have quantum phase transitions from the Néel order to the valence bond solid. In addition, these transitions are shown to be of second order for two of the studied models, with the remaining one being of first order. When the temperature dependence of the studied universal quantities is considered, a substantial difference between the two models possessing second order phase transitions and the remaining model is observed. Moreover, by using the associated data from both the models that may have continuous transitions, good data collapses are obtained for a number of the considered universal quantities. The findings presented here not only provide numerical evidence to support the results established in the literature regarding the nature of the phase transitions of these JQ_3 models, but also can be employed as certain promising criterions to distinguish second order phase transitions from first order ones for the exotic criticalities of the JQ -type models.

[1] arXiv:2102.04005

Poster 2 (No. 251) – Simulation study of shape change of growing lipid bilayer vesicles using DPD method

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Various shapes of vesicles have been analyzed from the viewpoint of theoretical physics. In particular, research on vesicle shape changes in non-equilibrium states using computers is developing. T. Ruiz-Herrero et al. analyzed the shape change of vesicles during the growth process by computer simulation using a triangular lattice membrane model [1]. They focused on characteristic shape changes such as tubulation and budding during division of L-form cells, which were mutant strains of bacteria which did not have a cell wall [2]. However, the shape of the vesicles observed was limited since the simulation was performed using a model which did not allow changes in topology.

In this study, we constructed a model that allowed changes in topology and analyzed these changes in the shape of growing vesicles. In the simulation, the dissipative particle dynamics (DPD) method was used, and lipid molecules were added to the system at regular time intervals to increase the surface area of the lipid membrane. The lipid molecule represented 10 hydrophobic groups and the hydrophilic group represented by 3 DPD particles, and the water molecule represented 3 molecules of water by 1 DPD particle [3]. After adding until the number of lipid molecules was doubled, the shape change of the vesicle during the relaxation process of free energy was analyzed. As a result, not only a shape change such as a transition from a sphere to a budding, but also a shape in which the inside of the vesicle was divided by a membrane were obtained.

In the presentation, we will discuss the relationship between the conditions for adding lipid molecules and the obtained vesicular shapes.

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Poster 2 (No. 260) – Theoretical Investigation of Complex Aspirin and Hydroxypropyl- β -cyclodextrin in Solvent Phase

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Aspirin is used for anti-inflammatory property that reacts by inhibition of prostaglandin synthesis and COX-II inhibitor. Long-term consumption of aspirin is associated with severe gastrointestinal side effects. If we can increase the solubility and bioavailability of the aspirin, we can reduce the gastrointestinal side effects [1]. Cyclodextrin has a lipophilic central cavity that able to form inclusion complexes with many drugs by taking up some lipophilic part of the drug molecules into its cavity [2]. In the pharmaceutical, cyclodextrin can improve the aqueous solubility, stability, dissolution rate, bioavailability, and/or local tolerance of drugs [3]. Hydroxypropyl- β -cyclodextrin has been investigated for the application model of cyclodextrin because it has the less toxicological potential [4].

In this Computational study, we investigated of Host-guest complexation between Aspirin and Hydroxypropyl- β -cyclodextrin. The structure and stabilization energy are calculated in the gas and solvent phases using Semiempiric PM3 and Density Functional Theory. The solvents are checked as water, ethanol, methanol, acetone, and chloroform. Some parameters such as the determination of thermodynamic parameter values, determination of DEF (Deformation Energy) value, determination of HOMO energy, LUMO energy, gap energy between HOMO and LUMO were analyzed to determine the stability of the complexes [5].

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Poster 2 (No. 264) – Alpha Clustering in Atomic Nuclei obtained by First Principles calculations and Characterization of the Hoyle state Reinforced by Statistical Learning technique

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A long-standing crucial question with atomic nuclei is whether or not the α clustering occurs there, and if so, how: Two protons and two neutrons can form an α particle (helium-4 nucleus), which may be the building block of some nuclei. This very fascinating idea is plausible because the α particle is particularly stable with a large binding energy. However, its direct experimental evidence has never been provided. In this talk, we shall computationally clarify this picture by means of the state-of-the-art quantum many-body simulations, that is *ab initio* No-Core Monte Carlo Shell Model[1, 2, 3, 4], formulated from first principles[5, 6, 7], utilizing supercomputers including K/Fugaku[8, 9]. The obtained physical quantities show agreement with experimental data. The appearance and variation of the α clustering are shown, by utilizing density profiles, for the nuclei beryllium-8, -10 and carbon-12. Beryllium-8 and -10 show clear patterns of the α clustering. The story is more complex and richer with the Hoyle state of the carbon-12 (^{12}C) nucleus[10, 11]. The Hoyle state is particularly important not only as an unsolved quantum many-body problem with atomic nuclei but also as a critical gateway to the birth of life formed with elements such as carbon, oxygen, *etc.* synthesized in stellar nuclear reactions [12]. A novel picture is presented for the Hoyle state: the quantum liquid and α -clustering are mixed, with the clustering component composed of three α clusters in triangular configurations. The evaluation of this mixing has been enabled by the present *ab initio* No-Core Monte Carlo Shell

Model calculations, while these calculations need advanced supercomputers like K/Fugaku[8, 9]. This new picture is further reinforced, in a completely independent manner without physical pictures, by the cluster analysis of the unsupervised statistical-learning technique[13].

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Poster 2 (No. 271) – Theoretical studies on association/dissociation process of plastocyanin in photosynthesis by a coarse-grained model

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Plastocyanin(PC) is one of type I copper proteins which have one copper ion in their active site. The function of the type I copper protein is electron transfer between proteins. In photosynthesis, PC transfers one electron from cytochrome *f* in cytochrome *b6f* complex to P700 in Photosystem I by diffusing in the lumen side of the thylakoid membrane. In order to investigate both association process and diffusion process of PC, coarse-grained simulation is efficient to simulate large system sizes on long time scale. In our pervious studies[1]-[5], we have developed coarse-grained intermolecular interaction including the hydrophobic interaction.

In this study, we investigate the association, self-assembly behaviour, and binding modes with complex configurations by using the presented simple coarse-grained model for describing intermolecular interaction between proteins in solvent. We discuss the association process of type I copper proteins PC for P700 in relation to the process for Cytochrome *f* by comparing some physical properties such as the binding modes between interacting proteins, the free energy landscape of the complex, and so on.

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Poster 2 (No. 279) – Statistics of the hopping motion approaching the glass transition in the binary hard disk systems

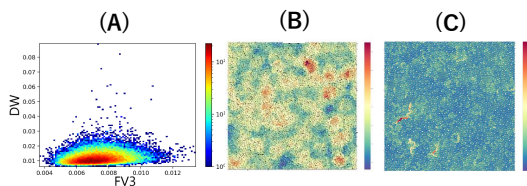
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Many theoretical attempts have focused on the origin of slow dynamics near the glass transition; however, our understanding is still controversial due to the severe limitation of both experiments and simulation. Recently, the state-of-art colloidal experiment can trace individual particles directly for a long time, revealing the dominant mechanism of the hopping motion as approaching the glass transition [1]. The quasi-voids scenario was proposed where many fragmented voids distributed in the regions within 2nd and 3rd neighborhoods create available space of a tagged particle as a first hopping motion by squeezing out the arrangement of dozens of particles cooperatively. After that, the successive hopping motion is induced as a string-like hopping chain by transferring the voids. To confirm the above scenario, we focus on the statistics of the hopping motion from both static and dynamic viewpoints. In the binary hard disk systems often used as a model system of the glass former materials, we systematically employ a replica ensemble with different initial velocity distribution (called the iso-configuration ensemble) by event-driven molecular dynamics method. We focused on the statistics of the hopping motion and the mobility of each particle (Debye-Waller (DW) factor) and investigated correlations with the free volume systematically, where any correlation between them has not been observed in the previous literature[2]. Figure 1 (A) shows a typical correlation diagram at sufficiently high density between the free volume averaged over within the 3rd shell (FV3) and DW. Figures 1(B) and (C) correspond to FV3 and DW for each particle, respectively. In general, the particle around the region with higher FV3 would be expected to have much mobility; however, we confirmed that this is not the case due to its directionality with large displacement. The detailed analyses will be presented at the conference.

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(A) The correlation diagram between free volume within the 3rd shell (FV3) and DW. The corresponding spatial snapshots of FV3 and DW are shown in (B) and (C), respectively.

Poster 2 (No. 281) – Interaction between PET tracer and the specific residues around the gate of the open form of Monoamine Oxidase B (MAO-B).

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Recently Monoamine Oxidase B (MAO-B) has been paid attention as one of the target proteins of the PET tracer to check Neurological disorders and Alzheimer's disease (AD). MAO-B is an enzyme that breaks down neurotransmitters such as dopamine in the brain. This protein forms a homodimer *in vivo* and is bound to the outer mitochondrial membrane. It is also related to Parkinson's disease (PD) and it has been known as a ligand-target for suppressing the progression of PD. It had been suggested by X-ray crystallographic study that the ligand enters from the loop near the membrane-binding site of MAO-B[1]. However, this entrance has a complicated structure, and the mechanism of the ligand-binding process has not been cleared yet. In addition, it has been reported that the activity of MAO-A depends on whether it is bonded or unbonded to biological membranes[2].

Therefore, we considered that the function of MAO-B would also be affected by the biological membrane.

In this study, we performed 2-microsecond molecular dynamics (MD) simulations on two structures, MAO-B in the solution and MAO-B with membrane environments, to estimate the effects of biological membrane. We found the entrance, which was suggested by the previous study, is not open enough, while the other loop regions have fluctuated mainly, and it seems the entrance to the ligand-binding site. Thus, the new entrance of MAO-B would be the ligand entrance of MAO-B.

We also performed docking simulations of PET tracers to estimate the binding mode, and we obtained the binding free energy by MD simulation and MMPBSA. We found the binding sites of a PET tracer, SMBT-1, for MAO-B, and we figured out the key residues of the binding in MAO-B. Four residues are catching the PET tracer by hydrophobic interactions.

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Poster 2 (No. 282) – Molecular dynamics simulation for large-scale water droplet systems using the tree method

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The wettability of hydrophobic surfaces have attracted great interest for fundamental research as well as practical applications such as self-cleaning surfaces, low friction surfaces, anti-fouling, and anti-icing.

Many types of strongly hydrorepellent surface have been developed to achieve superhydrophobicity. [1, 2, 3, 4, 5, 6]. In particular, the contact angle on the multi-scale hierarchical surface structures [1, 4] is greater than 165° due to the strong superhydrophobic effect. Because air is trapped between a droplet bottom and the surface, the droplet is in contact with the composite solid-air interface which results in lower free energy. This state of droplet is called the Cassie state,

the favorable state for the superhydrophobic surface compared to the Wenzel state in which the droplet is in contact with the surface without air pockets. Nanoscale structure can be fabricated onto a surface with microscale roughness to achieve the hierarchical surface.

The superhydrophobic effect for water droplets on rough surfaces were also investigated by molecular dynamics (MD) simulations. While many experimental results have shown that the hierarchical surface structures lead the superhydrophobic surface, detailed analyses using MD simulations have not been done. This is because large computational cost should be required to perform the hierarchical surface system. In MD simulations, fixed atoms are usually employed to construct pillared surfaces. The minimum size of pillars is about 1 nm to reproduce hydrophobic surfaces. When dual-scale roughness structures are constructed in MD simulations, small scale pillars are arranged on surfaces of large scale pillars. If the small pillar size is set 1 nm, the large pillar size must be more than 5 nm which is larger than the single-scale pillar size. Hence, sizes of the superhydrophobic plates constructed by the dual-scale pillars and water droplets for MD simulations should be much larger than single-scale pillared surfaces. Complex surface structures such as the dual-scale pillars greatly increase the computational cost of the MD simulations.

In this work, we demonstrate the applicability of the tree method [7] to perform MD simulations of large scale droplets. The tree method is widely used in astrophysical many-body simulations to reduce the computational cost of the force calculations. To implement this method in our simulation program [8], we use the high-performance library, Framework for Developing Particle Simulators (FDPS) [9, 10], which has the parallelized functions to use the tree method. Because the density distribution of the droplet system is not uniform, the tree method is suitable to perform MD simulations in parallel supercomputers. The FDPS enable us to perform MD simulations of the large scale droplets

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Poster 2 (No. 288) – Molecular Dynamics Simulation of the Complex of PDE5 and Evodiamine

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Alzheimer's disease is an irreversible, progressive brain disease that slowly impairs memory and thinking ability. The phosphodiesterase 5 (PDE5) protein inhibitor is one of the candidates for the cure for this disease. The indole alkaloid rutaecarpine and its derivatives have been shown to have inhibitory activity on PDE5[1]. Rutaecarpine is a compound found in a natural medicine called *Euodiaefructus*. This plant also contains an indole alkaloid called evodiamine, which has a similar structure to rutaecarpine. Therefore, we attempt to simulate the docking of PDE5 with evodiamine, which is also a component of *Euodiaefructus* and has a similar structure, and to simulate the structure of the complex.

The structure of PDE5 was obtained from PDB (ID: IXOZ), and that of evodiamine was obtained from Zinc15 (ID: ZINC2031813). The structure of the complex was created with SwissDock. After short simulation with NVT and NPT ensemble, MD simulations of protein with or without the binding of evodiamine were performed using GROMACS for 100 ns. Amber99SB-ILDN was used for the force field of PDE5, and SwissPalm was used for the force field of evodiamine.

In the result of MD simulation, neither large structural changes such as unfolding were observed with nor without the binding of evodiamine. The radius of inertia of the structure bound with evodiamine was larger than that of the structure without evodiamine due to the spreading of the structures called M-loop and H-loop. In addition, the RMSF of the structure with evodiamine is larger than that of the structure without evodiamine. The fluctuations of M-loop and H-loop were particularly large. And the hydrogen bonds were formed between protein and ligand.

Detailed results, including the formation of hydrogen bonds, will be presented in the poster.

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Poster 2 (No. 295) – Theoretical Studies of Dissociation Process of Plastocyanin by PaCS-MD Simulation

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Plastocyanin is one kind of small type I blue copper proteins. Plastocyanin has 100 amino acids. [1]. The function of plastocyanin is well known as the electron transfer from cytochrome-f complex to photosystem I [2]. Recently, multi-subunit complex Plastocyanin has been developed as carriers of polyethylene glycol chain for biological drugs (biologics) aim [3].

In this study, we investigate the dissociation process of the complex plastocyanin using the Parallel Cascade Molecular Dynamics (PaCS-MD) simulation method [4]. PaCS-MD simulation is one of the molecular simulation methods use to generate conformational transition pathways. This method is one of the effective computational calculations which is using short cycle multiple independent molecular dynamics simulation to find the pathway. PaCS-MD simulation for the all-atom model has been used for two cases calculation which active site and amino acid residues of complex plastocyanin (PDB:2GIM). We obtain the equilibrium point of complex Plastocyanin is around 31.79Å after 15ns simulation time. On the other hand, the distance between complex plastocyanin that was solved by Schmidt et al [5] (PDB:2GIM) is 27.847Å.

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Poster 2 (No. 310) – Theoretical Study of Dynamics and Infra-Red Spectra of Myosins

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One of the issues relating to food safety is meat adulteration. This problem can be dangerous for some people because of allergies or the particular religions that prohibit the adherents from consuming certain animal meats. There are species detection methods such as DNA amplification, gas chromatography, Fourier transform infrared spectroscopy (FTIR), and electronic nose. Generally, all of that methods require a particular instrument and essentially reagent. Therefore, the following studies of the species detection method are necessary. The detection methods in processed meat products would be more sophisticated. Currently, to study food processing and safety, molecular dynamics (MD) simulation has been used [1]. MD simulations in food science will increase to solve fundamental problems which the currently available instrument could not achieve.

Our study focuses on myosin, which is one of the myofibrillar proteins in muscle. Myosin is a major component of meat. Myosin also had a vital function in the ability of muscle contraction and relaxation [2]. Our study aims to investigate the molecular dynamics of myosin and predict the Infra-Red (IR) spectra. There are differences in IR spectrum profiles of animal fats [3]. Our study applies the all-atom model MD simulation. The computational of spectral densities using time series data will be created from the trajectories, and custom spectral densities will be a plugin to compute the auto-correlated Fourier transform [4]. The following stage is to compare the IR spectra profiles of myosin from different species, specifically *Sus scrofa* (pig), *Gallus gallus* (chicken), and *Bos taurus* (cattle).

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Poster 2 (No. 315) – Construction of a neighbour linked list on a spherical surface

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In molecular simulations, neighbour lists or cell linked-lists are standard methods to reduce the cpu-time for short-range interactions. These have been optimised, as described by many authors, in Euclidean space using periodic boundary conditions. In many cases, however, the systems studied are confined to a spherical surface, *e.g.*, the diffusion of molecules or ions on colloid particles or small molecules moving in the membrane-like environment formed by liposomes.

For long-range interactions in bulk system, such as electrostatic interactions, an alternative to Ewald summation is to embed the system to the surface of a sphere in \mathbb{R}^4 , a method which was developed by Caillol et.al. [1, 2, 3].

In this work we present a method to construct a cell linked-list directly on a spherical surface. The starting point is the equal area partition algorithm described by Leopardi [4] and we show how to find the neighbouring cells for the 2-sphere and 3-sphere, denoted by \mathbb{S}^2 and \mathbb{S}^3 , depending on the interaction distance.

An important advantage with the presented method is the considerable smaller arrays since the memory requirement can otherwise be a limiting factor for large systems using a linked list in an Euclidean geometry. The results from Brownian dynamics simulations, looking at the diffusion of particles on \mathbb{S}^2 and \mathbb{S}^3 also show that constructing a linked-list directly on \mathbb{S}^2 reduces the cpu-time by a factor between 1.2 and 1.5 (depending on interaction distance and volume fraction) for a system with 15000 particles while on \mathbb{S}^3 , the corresponding gain is by a factor of 1.5 for the largest interaction distance investigated. The actual decrease in cpu-time when calculating the non-bonded interactions is actually substantially larger, but to make a rather conservative comparison, we have used Cartesian coordinates. Performing the simulations using angular coordinates instead would reduce the cpu-time when sorting the particles into the corresponding cells almost by a factor of two.

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Poster 2 (No. 318) – Generic circuit for a linear combination of unitary operators: Green’s functions and linear-response functions

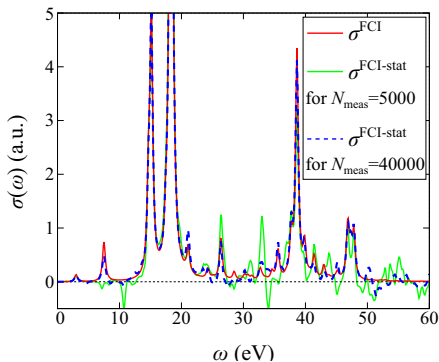
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Quantum chemistry calculations on quantum computers[1] for obtaining the ground-state energies have been realized by using photonic[2], superconducting[3, 4] and trapped-ion[5] quantum computers. The electronic Hamiltonian for an interacting system is mapped to that for the qubits comprising a quantum computer via some transformation, which leads to the Hamiltonian made up of Pauli tensors. In order for the quantum computation for electronic structure to come to practical use, quantum algorithms not only for the total energy but also for other various physical quantities have to be developed. In this study, we propose a scheme for the construction of a quantum circuit for an arbitrary nonunitary operator given as a linear combination of unitary operators. Depending on the outcome of a measurement on the ancillary qubits, the input state on which the nonunitary operator has acted will be obtained probabilistically. This state enables one to compute various kinds of physical quantities involving matrix elements of nonunitary operators. One of such quantities is the one-particle Green’s functions[6] and linear-response functions.[7] We performed simulations for obtaining them based on full configuration interaction calculations for molecules.

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Photoabsorption cross section of a carbon dimer from full configuration interaction calculations and that from simulation of quantum circuits.

Poster 2 (No. 371) – Multicriticality of the deconfined quantum critical point

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The square lattice JQ model [1] hosts a quantum phase transition between an antiferromagnetic and a dimerized (valence-bond solid) ground state. This enables a large-scale quantum Monte Carlo study of the deconfined quantum critical point (DQCP) which is theoretically predicted to separate the above two phases [2].

In our study [3], we consider two different perturbations to the DQCP, and numerically find out that both of them are relevant operators that were previously not considered. This has a two-fold implication; 1. the DQCP actually requires additional fine-tuning in order to be reached, which resolves an inconsistency that was pointed out from conformal bootstrap calculations before [4]. 2. the DQCP could be regarded as a multicritical point sitting at the edge of a newly found “helical valence-bond” phase.

In the poster, we will explain in detail about the perturbations, the new phase, and their implications.

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Poster 2 (No. 372) – \mathbb{Z}_2 topological order and first-order quantum phase transitions in systems with combinatorial gauge symmetry

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We study a generalization of the two-dimensional transverse-field Ising model, combining both ferromagnetic and antiferromagnetic two-body interactions, that hosts exact global and local \mathbb{Z}_2 gauge symmetries. Using exact diagonalization and stochastic series expansion quantum Monte Carlo methods, we confirm the existence of the topological phase in line with previous theoretical predictions. Our simulation results show that the transition between the confined topological phase and the deconfined paramagnetic phase is of first-order, in contrast to the conventional \mathbb{Z}_2 lattice gauge model in which the transition maps onto that of the standard Ising model and is continuous. We further generalize the model by replacing the transverse field on the gauge spins with a ferromagnetic XX interaction while keeping the local gauge symmetry intact. We find that in both models the \mathbb{Z}_2 topological phase remains stable, while the model with XX interaction exhibits ferromagnetic order at large XX . The topological–ferromagnetic quantum phase transition is also of first-order. For both models, we discuss the low-energy spinon and vison excitations of the topological phase and their avoided level crossings associated with the first-order quantum phase transitions.

Poster 2 (No. 377) – Unconventional U(1) to Z_q cross-over in quantum and classical q-state clock

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3D Clock models with a discrete Z_q symmetry show an emergent U(1) symmetry at the critical point. In the ordered phase, there exist distinct lengthscales associated with the development of U(1) order and the further discrete symmetry breaking to Z_q . We find here that the exponent associated with the second lengthscale is fundamentally different for spatially isotropic and anisotropic systems. Relevance to 2D quantum models through the quantum to classical mapping is discussed.

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About Coventry

Coventry is a city in the county of west midlands in England and is well known for its rich history of industry. By the 14th century, Coventry was the fourth largest town in England with an estimated population of 8,000. It was an important centre of the cloth trade, and throughout the Middle Ages was one of the most important cities in England. In the 18th and 19th centuries, Coventry became one of the three main UK centres of watch and clock manufacture. In 1885 in Coventry, Rover produced the first bicycle to include modern features such as a chain-driven rear wheel with equal-sized wheels on the front and rear. By the 1890s the cycle trade was booming and Coventry had developed the largest bicycle industry in the world. To this day, the bicycle is called “Rover” in Poland and western Ukraine. The first British motor car was made in Coventry in 1897 by The Daimler Motor Company Limited. Coventry’s darkest hour came during World War II when it was singled out for heavy bombing raids. The symbol of the mythical phoenix, which the University has adopted is a reminder of the way in which the city of Coventry rebuilt itself after Second World War. Today the city is a centre of post-war reconciliation. Coventry is also known for the legendary 11th century Lady Godiva who, according to legend, rode through the city on horseback clothed only in her long hair, in protest of high taxes being levied on the cityfolk by her husband Leofric, Earl of Mercia.

Coventry has won the title of UK City of Culture for 2021. In the course of the celebrations, a varied series of events are taking place, including exhibitions, concerts, arts festivals and special awards.

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Locations

Although CCP2021 cannot take place in Coventry due to the coronavirus pandemic, we include below a map of the relevant locations of a CCP that we had initially dreamed of when events with face-to-face were still considered natural and harmless.

Please come and visit us at Coventry one day!

- A Centre for Fluid and Complex Systems at the Design Hub**
- B Engineering, Environment and Computing Building**
- C Ibis Hotel Coventry Centre**
- D Ramada Hotel & Suites**
- E Coventry main station**
- F The Establishment Bar & Grill (now Slug & Lettuce)**

