Current and Future Computational Approaches to Quantum Many-Body Systems 2024 (CompQMB2024)

Date: 2024. Sep. 24-27
Venue: Lecture room A632, ISSP, University of Tokyo

Support
-FY2023-2025 MEXT -KAKENHI- Grant-in-Aid for Transformative Research Areas (B)
"Computational materials science based on quantum-classical hybrid algorithms"

-FY2023-2028 JST ASPIRE "Forging a global research network for quantum information and quantum biology"

Program

Sep. 24 (Tuesday)
10:00-11:00 "Deep variational free energy for hydrogen systems", Xinyang Dong
11:00-11:15 Free Discussion
11:15-12:15 "Vision Transformer Neural Quantum States for Impurity Models", Yi Lu

12:15-13:45 Lunch

13:45-14:45 "Variational autoregressive networks and its applications in statistical physics and quantum error-correcting codes", Pan Zhang
14:45-15:00 Free Discussion

15:00-16:00 “Applications of quantum computation and tensor networks to lattice gauge theory”, Etsuko Itou
16:00-16:15 Free Discussion
16:15-17:15 “Theory to Enable Practical Quantum Advantage”, Balint Koczor
17:15-17:30 Free Discussion
17:30-18:30 “Electronic structure simulations beyond the reach of exact diagonalization with quantum-centric supercomputing”, Mario Motta

Sep. 25 (Wednesday)
10:00-11:00 “Spectroscopy and complex-time correlations using minimally entangled typical thermal states”, Alexander Wietek
11:00-11:15 Free Discussion
11:15-12:15 “Quantum simulation of strongly correlated electrons through spin-coupled initial states”, Daniel Marti-Daficik

12:15-13:45 Lunch (**Group photo**)

13:45-14:45 “Computing solution space properties of combinatorial optimization problems via generic tensor networks”, Jin-Guo Liu
14:45-15:00 Free Discussion
15:00-16:00 Poster flash talks
16:00-18:30 Poster session w/ refreshments
18:30-20:00 Free Discussion

Sep. 26 (Thursday)
10:00-11:00 “Recent Developments in Applications of Quantum Computing to Chemistry and Materials Science”, Robert Izsak
11:00-11:15 Free Discussion
11:15-12:15 “Discontinuous Galerkin Hartree-Fock calculations for predicting accurate electronic structures of mesoscopic-scale metal-semiconductor junctions with millions of atoms”, Wei Hu

12:15-13:45 Lunch

13:45-14:45 “Recent progress with iPEPS: layered systems, incommensurate order, and spectral functions”, Philippe Corboz

14:45-15:00 Free Discussion
15:00-16:00 “Decomposing imaginary time Feynman diagrams via sum-of-exponentials approximation”, Jason Kaye
16:00-16:15 Free Discussion
16:15-17:15 Internal meeting

Sep. 27 (Friday)
10:00-11:00 “TBA”, Kun Chen
11:00-11:15 Free Discussion
11:15-12:15 “Thermal pure matrix product state in 2D: tracking thermal equilibrium from paramagnet down to the Kitaev spin liquid state”, Matthias Gohlke

12:15-13:45 Lunch

13:45-14:45 “Purification-based quantum simulations via clustering property”, Hideaki Hakoshima
14:45-15:00 Free Discussion
15:00-15:15 Closing
15:15-16:15 Free Discussion

Abstract

Sep. 24 (Tuesday)

“Deep variational free energy for hydrogen systems”, Xinyang Dong

Hydrogen, being the first element in the periodic table, is the most abundant elements in the Universe. Dense hydrogen systems exhibit a variety of fascinating physical phenomena, including liquid-liquid transition and metallization. Accurate prediction of the phase diagram of dense hydrogen has long been a challenge for computational methods. In this talk, I will present a neural network-based deep variational free energy approach to address the liquid-liquid phase transition problem in dense hydrogen systems. This method combines a deep generative model, normalizing flow, with a fermionic electron wave function neural network. The joint optimization of these two neural

networks enables accurate calculation of the variational free energy. Using this approach, our results indicate that the phase transition point shifts to higher density comparing to those predicted by Deep Potential molecular dynamics simulations.

“Vision Transformer Neural Quantum States for Impurity Models”, Yi Lu

We employ an adapted Vision Transformer (ViT) to model quantum impurity models, optimizing it with a subspace expansion scheme in the natural-orbital representation that outperforms conventional variational Monte Carlo in both accuracy and efficiency. Benchmarks against matrix product states in single- and three-orbital Anderson impurity models show that ViT-based neural quantum states achieve comparable or superior accuracy with far fewer variational parameters. We also compute dynamical quantities using by introducing a restricted excitation space, yielding accurate core-level X-ray absorption spectra. These results highlight the potential of ViT-based neural quantum states for efficient and accurate modeling of quantum impurity models.

“**Variational autoregressive networks and its applications in statistical physics and quantum error-correcting codes**”, Pan Zhang

In this presentation, Pan Zhang will introduce the variational autoregressive network (VAN) and its applications in the field of statistical mechanics. VAN leverages autoregressive neural networks to construct a normalized variational distribution across numerous discrete variables, with the objective of minimizing the variational free energy through policy gradients. In the realm of equilibrium statistical physics, VAN demonstrates its prowess by closely approximating the target Boltzmann distribution and accurately estimating the free energy. When addressing non-equilibrium statistical mechanics, VAN adeptly simulates the temporal progression of the joint distribution governed by a master equation. Pan Zhang will also showcase a recent work, qecGPT, which adapts the VAN framework to tackle Bayesian inference challenges encountered in the decoding process of quantum error-correcting codes.

“Applications of quantum computation and tensor networks to lattice gauge theory”, Etsuko Itou

In recent years, numerical analyses for lattice gauge theories using quantum computation and tensor network have attracted much attention among high-energy physicists as an alternative to lattice Monte Carlo methods. In this talk, I would like to discuss what kind of models and physical observables we aim to calculate and what we are now able to do.

“Theory to Enable Practical Quantum Advantage”, Balint Koczor

Quantum computers are becoming a reality and current generations of machines are already well beyond the 50-qubit frontier. However, hardware imperfections still overwhelm these devices and it is generally believed the fault-tolerant, error-corrected systems will not be within reach in the near term: a single logical qubit needs to be encoded into potentially thousands of physical qubits which is prohibitive.

Due to limited resources, in the near term, hybrid quantum-classical protocols are the most promising candidates for achieving early quantum advantage and these need to resort to quantum error mitigation techniques. I will explain the basic concepts and introduce hybrid quantum-classical protocols are the most promising candidates for achieving early quantum advantage. These have the potential to solve real-world problems---including optimisation or ground-state search---but they suffer from a large number of circuit repetitions required to extract information from the quantum state. I will finally discuss areas where quantum computers may have the potential to deliver advantage in the near term.

“Recent Developments in Applications of Quantum Computing to Chemistry and Materials Science”, Robert Izsak

Riverlane focuses on quantum error correction and fault-tolerant algorithms, prioritizing the development of algorithms for chemistry, material science and fluid dynamics applications. This contribution will provide a summary of the most relevant of our papers published in the last three years, including those on embedding, the cost analysis of pharmaceutical and solid-state algorithms, electron correlation, the adaptation of classical techniques, such as the projector augmented wave method, to quantum computers, first-quantization-based methods and some of our work on early fault tolerant algorithms. If time allows, fluid dynamics applications will be mentioned. Finally, some conclusions will be drawn on the trends and prospects of quantum computing in these application areas.

Sep. 25 (Wednesday)

"Spectroscopy and complex-time correlations using minimally entangled typical thermal states", Alexander Wietek

Tensor network states have enjoyed great success at capturing aspects of strong correlation physics. However, obtaining dynamical correlators at non-zero temperatures is generically hard even using these methods. Here, we introduce a practical approach to computing such correlators using minimally entangled typical thermal states (METTS). While our primary method directly computes dynamical correlators of physical operators in real time, we propose extensions where correlations are evaluated in the complex-time plane. The imaginary time component bounds the rate of entanglement growth and strongly alleviates the computational difficulty allowing the study of larger system sizes. To extract the physical correlator one must take the limit of purely real-time evolution. We present two routes to obtaining this information (i) via an analytic correlation function in complex time combined with a stochastic analytic continuation method to obtain the real-time limit and (ii) a hermitian correlation function that asymptotically captures the desired correlation function quantitatively without requiring effort of numerical analytic continuation. We show that these numerical techniques capture the finite-temperature dynamics of the Shastry-Sutherland model - a model of interacting spin one-half in two dimensions.

"Quantum simulation of strongly correlated electrons through spin-coupled initial states", Daniel Marti-Daficik

The performance of quantum algorithms for eigenvalue problems, such as computing Hamiltonian spectra, depends strongly on the overlap of the initial wavefunction and the target eigenvector. This limits the power of quantum computers for solving challenging quantum chemistry problems, as typical initial states with a simple description have an overlap with the target Hamiltonian eigenstate that diminishes exponentially in the number of strongly correlated electrons. In this talk, we present a framework for understanding and approximating the low-energy wave functions in strongly correlated molecular systems in terms of a few spin-coupled states that are highly entangled but highly structured. We also provide efficient quantum circuits for initial state preparation. Our approach avoids the need for expensive classical or quantum heuristics. Instead, we exploit symmetries to directly encode the dominant entanglement structure of the simulated system on quantum computers. For a range of popular quantum algorithms, including quantum phase estimation and several variational quantum algorithms, we

demonstrate that using spin-coupled initial states drastically reduces the quantum resources required to compute strongly correlated ground and excited states.

“Computing solution space properties of combinatorial optimization problems via generic tensor networks”, Jin-Guo Liu

We introduce a tensor network based framework to analyse the solution space of a broad class of combinatorial optimization problems and probabilistic inference problems. We show how these tools can help the scientific discovery in the field of quantum computation.

Sep. 26 (Thursday)

"Electronic structure simulations beyond the reach of exact diagonalization with quantum-centric supercomputing", Mario Motta

We present [1] quantum computations of electronic structure that go beyond problem sizes amenable to current state-of-the-art exact diagonalization. Our results are obtained in a quantum-centric supercomputing architecture, using 6400 nodes of the Fugaku supercomputer to assist an IBM Heron quantum processor. We simulate the N2 triple bond breaking in a correlation-consistent cc-pVDZ basis set, and the active-space electronic structure of methyl-capped [2Fe–2S] and [4Fe–4S] clusters, using 58, 45 and 77 qubits respectively, with quantum circuits of up to 10570 (of which 3590 are 2-qubit gates) quantum gates.

[1] https://arxiv.org/abs/2405.05068

"Discontinuous Galerkin Hartree-Fock calculations for predicting accurate electronic structures of mesoscopic-scale metal-semiconductor junctions with millions of atoms", Wei Hu

The evaluation of the exact Hartree-Fock exchange in hybrid density functional theory (DFT) is a crucial ingredient for accurately predicting electronic structures in molecules and solids. However, its application is currently limited to 5K atoms on leadership supercomputers due to its ultra-high computational complexity O(N4). Herein, we propose a new discontinuous Galerkin Hartree-Fock (DGHF) method for large-scale hybrid functional electronic structure calculations. We present a massively parallel DGHF implementation on exascale supercomputers to reduce the high computational scaling of constructing the HFX matrix from O(N4) to O(N). We showcase how DGHF can be used to predict accurate electronic structures of complex metal-semiconductor junctions with 2.5M atoms (17.2M electrons) using 35.9M cores on exascale Sunway supercomputer. This is the first time high-accuracy hybrid functional electronic structure calculations enable us to simulate next-generation electronic devices at mesoscopic scale (200 nm).

"Recent progress with iPEPS: layered systems, incommensurate order, and spectral functions", Philippe Corboz

Infinite projected entangled-pair states (iPEPS) have become a state-of-the-art tool to study strongly correlated systems in 2D. In this talk, I report on recent progress in extending the iPEPS toolbox: (1) Simulation of weakly coupled 2D layers, with

applications to SrCu2(BO3)2, (2) extensions to states with incommensurate spin-spiral order, enabling an unbiased study of the quantum spin liquid phase in anisotropic triangular lattice Heisenberg model, and (3) the computation of spectral functions based on the iPEPS excitation ansatz and real-time evolution.

“Decomposing imaginary time Feynman diagrams via sum-of-exponentials approximation”, Jason Kaye

I will describe a new algorithm to evaluate imaginary time Feynman diagram integrals of low to intermediate order with controllable, high-order accuracy, and at low temperatures. The central idea is to approximate certain factors in the integrand as sums of exponentials, and use separation of variables to decompose the multiple integrals into sequences of nested one-dimensional products and convolutions, which can be computed efficiently using the discrete Lehmann representation. As a first application of the idea, I will focus on the bold hybridization expansion of a quantum impurity model. I will also discuss the AAA algorithm for rational approximation, which in this case is used to obtain compact sum-of-exponentials approximations of hybridization functions, but which may be more broadly useful in the problem of fitting spectral densities by sums of simple poles.

Sep. 27 (Friday)

"Thermal pure matrix product state in 2D: tracking thermal equilibrium from paramagnet down to the Kitaev spin liquid state", Matthias Gohlke

We show that the matrix product state (MPS) provides a thermal pure quantum state (TPQ) representation in equilibrium in two spatial dimensions over the entire temperature range. We start off by illustrating TPQ-MPS on the Kitaev honeycomb model as a prominent, non-trivial example hosting a quantum spin liquid ground state. Our method is able to qualitatively capture the double-peak in the specific heat. Then, application to other two-dimensional quantum systems will be discussed.

"Purification-based quantum simulations via clustering property", Hideaki Hakoshima

Quantum simulators are being built to surpass the classical computers in studying quantum many-body phenomena, yet current technology still suffers from experimental limitations such as insufficient cooling and external noise.

To overcome this issue, we propose localized virtual purification (LVP) which exploits the geometrical locality of target systems. We perform rigorous analysis for the cooling of thermal states and error mitigation of ground-state simulation, and show that the LVP breaks current limitations. Our work bridges fundamental concepts in quantum many-body physics and practical quantum simulation, and thus provides a significant impact in condensed matter physics, statistical physics, and quantum technology.

Poster list https://qc-hybrid.github.io/CompQMB2024/assets/posters.pdf

No	Name	Title
1	Shota Kanasugi	Subspace-based local compilation of variational quantum circuits for large-scale quantum many-body simulation
2	Rihito Sakurai	Learning Fourier-based parametric option price using tensor cross interpolation
3	Hao-Ti Hung	Dynamical Quantum Phase Transition and Thermal Equilibrium in the Lattice Thirring Model
4	Junwei Feng	Large-scale Discontinuous Galerkin Real-Time Time-Dependent Density Functional Theory
5	Tatsuya Sakashita	Fast and accurate decoder for the XZZX code using simulated annealing
6	Tao-Lin Tan	Quantum many-body scars as caged eigenstates via destructive interference in Hilbert space
7	Akira SaiToh	Simulated bulk-ensemble search revisited in the current machine environment
8	Wei-Lin Tu	Generating Function for Projected Entangled-Pair States
9	Daniel Donghyon Ohm	Benchmarking a PEPS Random Quantum Circuit Sampling Algorithm
10	Bo THOMSEN	Accelerating the Study of Nuclear Quantum Effects in water with Self-Learning Path Integral Monte Carlo
11	Yuya Nakagawa	Averaging gate approximation error and performance of Unitary Coupled Cluster ansatz in Pre-FTQC Era
12	Hirofumi Nishi	Probabilistic imaginary-time evolution with quantum error detection for spin qubits
13	Hiroshi Watanabe	Optimizing a generalized single-qubit gate and a controlled gate.
14	Ken Inayoshi	Nonequilibrium Green's function method with quantics tensor trains
15	Luca Erhart	Chebyshev Approximated Variational Coupled Cluster for Quantum Computing
16	Hiroyoshi Kurogi	Quantum subspace compiling of the time-evolution operators for molecular systems by using sequential optimizers
17	Ken Okada	Classically optimized variational quantum eigensolver with application to topological phases
18	Pranay Patil	MPS approach to disordered Heisenberg chain
19	Yifan Ke	DeepH + HONPAS: Machine Learning-Assisted Hybrid Functional Calculations
20	Yuhei Ikeda	Application of adaptive quantum-selected configuration interaction method to ab initio extended Fermi-Hubbard model
21	Sanghyun Park	Degeneracy-engineered zero-temperature Mott transition in two-orbital Hund systems
22	Norifumi Matsumoto	Quantum many-body simulation of finite-temperature systems with sampling a series expansion of a quantum imaginary-time evolution
23	Shuhei Kashiwamura	Bayesian Parameter Estimation of Quantum Spin Models for the One-dimensional Quantum Magnet Azurite by a Surrogate-Assisted Monte Carlo Method
24	Takahiro Misawa	Compensated Ferrimagnets with Colossal Spin Splitting in Organic Compounds
25	Satoshi Morita	Multi-impurity method for bond-weighted tensor renormalization group
26	Kota Ido	Measurement of an excitation spectrum and a topological property using variational Monte Carlo method
27	Yuichiro Yoshida	Ab initio extended Hubbard model of short polyenes for efficient quantum computing
28	Riki Toshio	Accelerating Materials Simulation with Partially Fault-Tolerant Quantum Computing
29	Seongyeon Youn	Origin of the correlated gaps in twisted bilayer graphene
30	Jun Takahashi	NP-hardness of Sign-Problem Curing with Clifford Circuits
31	SungBin Lee	Projected entangled pair states simulation of noiseless random quantum circuits
32	Atsushi Hariki	DFT+DMFT study on correlated altermagnets
33	Koji Inui	Inverse Hamiltonian design of highly entangled quantum many-body systems
34	Haruki Shimizu	Tensor network simulations for non-orientable surfaces
35	Shizhe Jiao	Projected wavefunction extrapolation scheme to accelerate plane-wave hybrid functional-based Born–Oppenheimer molecular dynamic simulations
36	Tianchun Wang	Quantum Krylov Method for Electronic Structure Simulations
37	Hidemaro Suwa	Semiclassical dynamical simulation of weak Mott insulators
38	Beomjoon Goh	Role of On-site Coulomb Interaction in Electronic Raman Spectrum of Sr3Ir2O7
39	Yufan Yao	Combining PWDFT with DeePMD for hybrid functional enabled ab initio molecular dynamics within plane waves
40	Koudai Sugimoto	DC electric field-driven discretization of single-particle excitation spectra in the Mott insulator
41	Hidehiro Saito	Engineering exact quantum many-body ground states in 1D and 2D
42	Han Yan	Hyperbolic fracton model as a toy model of holography
43	Kenji Homma	Extracting conformal data from frustrated classical spin model via tensor network renormalization algorithm
44	Hirone Ishida	Low-rank quantics tensor train representations of Feynman diagrams for multiorbital electron-phonon models
45	Khinevich Viktor	Wave Function Refinement via Quantum Power Lanczos Method Using Generalized Quantum Signal Processing
46	Ryosuke Akashi	Electron-phonon GW0 theory based on the intermediate representation
47	Motoharu Kitatani	Optimizing superconductivity: from cuprate via nickelate to palladates
48	Synge Todo	MateriApps - a Portal to Materials Science Simulation
49	Hiroshi Shinaoka	Multiscale Space-Time Ansatz for Correlation Functions of Quantum Systems Based on Quantics Tensor Trains
50	Tomoya Shiota	Universal Neural Network Potentials as Descriptors : Predicting Chemical Properties of Molecules and Nanomaterials
51	LingYun Wan	Wigner crystals under high magnetic fields and Cartan quantum algorithm

Information

- ✓ Room
  - A632 Lecture room (大講義室) @ 6th floor ISSP
- ✓ Wi-Fi
  - SSID: CompQMB2024_WiFi
  - Password: is$P+qcHyB2024
  - eduroam is also available
- ✓ Light snacks, such as sandwiches, will be provided at lunchtime, including a small selection of vegetarian options.

Campus map

For lunch, it is convenient to go to the following restaurants:

- Cafeteria
- Ikoi
- Hama (sushi restaurant)

Ikoi and Hama offer a small selection of vegetarian options.

NB: Cash is *not* accepted at "Cafeteria". To use Cafeteria, you should either buy a meal card or use transportation IC cards such as Suica or Pasmo.

Shuttle Bus

A free shuttle bus is available for travel between Kashiwa-no-ha Campus Station and Kashiwa Campus.

NB: When boarding the shuttle bus, please tell the driver that your visiting department is "ISSP".

UTokyo Students & Employee

UTokyo Kashiwa Campus ↔ Kashiwanoha Campus Station

SHUTTLE BUS

※ Shuttle bus also runs on the Kashiwa Open Campus Day.

Fare

Student : Free (Show your Student ID)

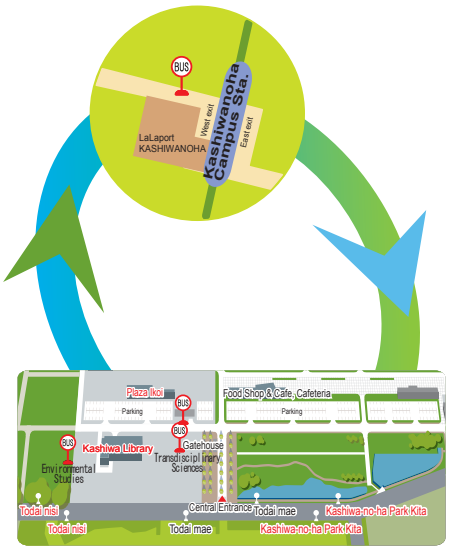
Employee : Prepaid Ticket

- Prepaid Ticket needed.
- Tickets are available at Coop Store in Kashiwa Campus.
- 1,700 JPY for 11 pieces (non-refundable).
- Cash is not acceptable.

Visitor : Free (Inform your visiting department)

Operating Time

8:00 am ～ 8:00 pm



From TSUKUBA EXPRESS Kashiwanoha Campus Sta.

Time	To Kashiwa Campus (Environmental Studies Transdisciplinary Sciences)					
8	00	10	20	30	40	50
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From Kashiwa Campus (Environmental Studies)

Time	To Kashiwanoha Campus Sta.						
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17	00	10	20	30	40	50	
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19	00	10	20	30	40	50	

※NOTE: Operated as Field Operational Test for Automated Driving Vehicle.Students, Visitors and Faculty stuff can also use these.
Maximum passengers in each bus are 17 persons. Any tickets are not required for these bus.

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THE UNIVERSITY OF TOKYO GRADUATE SCHOOL OF FRONTIER SCIENCES

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