2024 KIAS School of Computational Sciences Workshop

ABSTRACTS

March 27 (Wed) ~ 29 (Fri), 2024

Sono Belle Byeonsan

2024 KIAS School of Computational Sciences Workshop

March 27 - 29, 2024 **Sono Belle Byeonsan**

<table>
<tr><th></th><th>March 27 (Wed)</th><th>March 28 (Thur)</th><th>March 29 (Fri)</th></tr>
<tr><td>07:30-09:00</td><td rowspan="10">KIAS -> Sonobelle Byeonsan
(Bus departs at 10:00)

Lunch at 12:00</td><td>Breakfast</td><td>Breakfast</td></tr>
<tr><td>09:00-10:00</td><td rowspan="3">Seminar
(20min × 4)</td><td>Seminar
(20min × 3)</td></tr>
<tr><td>10:00-10:10</td><td rowspan="2">Break (Check out)</td></tr>
<tr><td>10:10-10:20</td></tr>
<tr><td>10:20-10:30</td><td rowspan="2">Break</td></tr>
<tr><td>10:30-11:00</td><td rowspan="2">Seminar
(20min × 3)</td></tr>
<tr><td>11:00-11:30</td><td rowspan="2">Seminar
(20min × 3)</td></tr>
<tr><td>11:30-12:00</td><td>Break</td></tr>
<tr><td>12:00-13:00</td><td>Lunch</td><td>Lunch</td></tr>
<tr><td>13:00-14:00</td><td rowspan="5">Excursion</td><td rowspan="6">Sonobelle Byeonsan -> KIAS
(Bus departs at 13:30)</td></tr>
<tr><td>14:00-15:00</td></tr>
<tr><td>15:00-17:00</td><td>Self Check-in & Registration</td></tr>
<tr><td>17:00-18:00</td><td>Seminar
(20min × 3)</td></tr>
<tr><td>18:00-18:20</td><td>Break</td></tr>
<tr><td>18:20-19:00</td><td>Seminar
(20min × 2)</td><td rowspan="2">Banquet</td></tr>
<tr><td>19:00-20:00</td><td>Dinner</td></tr>
</table>

* Check in (15:00 ~), Check out (~ 11:00)

* Seminar Room (Rose Hall, 1st floor of West Tower)

* Breakfast - Poongyeong Maru (1st floor of West Tower)

Program

March 27 (Wed)

Time	Speaker	Title
17:00-17:20	Eunok Bae	Recursive QAOA for solving MAX-CUT problem
17:20-17:40	Eunwoo Lee	Quantum error correction for 7 year olds
17:40-18:00	Minki Hhan	Quantum Complexity for Discrete Logarithms and Integer Factorization
18:00-18:20	Break	
18:20-18:40	Eftaxias Giorgos	Could observed correlations be stronger than any quantum ones?
18:40-19:00	James Moran	Understanding the role of non-Gaussianity in coherent state discrimination

March 28 (Thur)

Time	Speaker	Title
09:00-09:20	Choong Hyun Kim	Hund correlations in ruthenate thin films
09:20-09:40	Sungmo Kang	Electronic Structures of Ternary Compounds GeSbTe Based on Machine Learning Empirical Pseudopotentials
09:40-10:00	Kunihiro Yananose	More is different, moiré is different
10:00-10:20	Gangmin Son	Hidden multiscale organization and robustness of real multiplex networks
10:20-11:00	Break	
11:00-11:20	Ji Woong Yu	An investigation of anomalous water dynamics using a machine learning force field
11:20-11:40	Daeseong Yong	Algorithmic Approach to the Optimal Computation of Chain Propagators of Branched Polymers in Polymer Field Theory Simulations
11:40-12:00	YeongKyu Lee	Influences of Charge-Mediated Interactions on Electrolytes and Understanding Electrostatic Effects of Systems

March 29 (Fri)

Time	Speaker	Title
09:00-09:20	Mancheon Han	Finding eigenstate properties using the quantum computer through the Quantum Zeno Monte Carlo
09:20-09:40	Taehee Ko	Randomized quantum-classical hybrid approaches for ground-state and energy computation
09:40-10:00	Johan Jonsson	Calculating X-ray spectra for strongly correlated materials
10:00-10:30	Break	
10:30-10:50	Cheolwon Heo	Recognizing even-cycle and even-cut matroids
10:50-11:10	Sunyo Moon	A brief introduction to the Laplacian matrix of graphs
11:10-11:30	Jungho Ahn	How complex is your graph?

Talk No. 1

Recursive QAOA for solving MAX-CUT problem

Eunok Bae*
School of Computational Sciences, Korea Institute for Advanced Study, Seoul 02447, Korea

Quantum approximate optimization algorithms are hybrid quantum-classical variational algo- rithms designed to approximately solve combinatorial optimization problems such as the MAX- CUT problem. In spite of its potential for near-term quantum applications, it has been known that quantum approximate optimization algorithms have limitations for certain instances to solve the MAX-CUT problem, at any constant level p. Recently, the recursive quantum approximate opti- mization algorithm, which is a non-local version of quantum approximate optimization algorithm, has been proposed to overcome these limitations. However, it has been shown by mostly numerical evidences that the recursive quantum approximate optimization algorithm outperforms the original quantum approximate optimization algorithm for specific instances. In this talk, I briefly introduce the recent work on analytical proof that the recursive quantum approximate optimization algorithm is more competitive than the original one to solve the MAX-CUT problem for complete graphs with respect to the approximation ratio.

Talk No. 2

Quantum error correction for 7 year old

Eunwoo Lee
School of Computational Sciences, Korea Institute for Advanced Study, Seoul 02447, Korea

In this talk, I will explain basics of quantum error correction to as broad audience as possible.

Talk No. 3

Quantum Complexity for Discrete Logarithms and Integer Factorization

Minki Hhan
School of Computational Sciences, Korea Institute for Advanced Study, Seoul 02447, Korea

Shor's algorithms for discrete logarithm and integer factorization are arguably the most influential quantum algorithms. Surprisingly, no known lower bound exists for these problems, even for the restricted settings, unlike the other important quantum algorithms such as Grover's and Simon's. In recent works, I gave the first quantum lower bounds for these problems in the idealized models that assume the algorithms only use the group/ring elements in a black-box way. This model encompasses almost all known algorithms, and our lower bounds match the complexity of Shor's algorithms. We also discuss the relation between a recent breakthrough of Regev's improved integer factoring algorithm.

Talk No. 4

Could observed correlations be stronger than any quantum ones?

Eftaxias Giorgos

This talk will tell a brief story about the interplay among the realms of nonlocality distillation, communication complexity and the axiomatization of quantum theory, with an eye to illuminating our current research objectives.

Talk No. 5

Understanding the role of non-Gaussianity in coherent state discrimination

James Moran

Coherent states are prototypical Gaussian states in quantum mechanics and quantum optics. Here ‘Gaussian’ refers to their distribution on the phase space. Two different coherent states are never orthogonal, meaning that no measurement scheme can perfectly discriminate between them without error. The minimal achievable error in this context is known as the Helstrom bound. It was shown definitively in [M. Takeoka and M. Sasaki, Phys. Rev. A 78, 022320 (2008)] that non-Gaussian operations are required to achieve the Helstrom bound, though the form which these operations take is not specified. In this talk we will investigate different types of non-Gaussian measurements, from photon-counting to non-Gaussian unitary operations followed by Gaussian measurement, to see how different forms of non-Gaussianity can help one approach, and in some cases achieve, minimum-error discrimination of two coherent states.

Talk No. 6

Hund correlations in ruthenate thin films

Choong Hyun Kim

Hund's coupling, instead of Hubbard interaction, is a new knob to manipulate the physical properties of strongly correlated materials. For example, the role of Hund's coupling in unconventional superconductors such as Fe-pnictide or Sr2RuO4 has been re-examined from the perspective of the newly proposed correlated metallic phase called Hund's metal. Among them, ruthenates have an appropriate size of Hubbard interaction and Hund's coupling, making them a suitable system for studying Hund's correlation physics. In particular, when ruthenates are grown as a single-layer thin film, bandwidth, crystal field, etc. can be effectively controlled, and various emergent phases can be observed. In this talk, we present a systematic theoretical study on the novel metallic and insulating properties of various ruthenates films by means of density functional theory plus dynamical mean-field theory (DMFT). Our study suggests the possibility of ruthenate film as a new platform to study the characteristics of Hund correlation.

Talk No. 7

Electronic Structures of Ternary Compounds GeSbTe Based on Machine Learning Empirical Pseudopotentials

Sungmo Kang, Rokyeon Kim and Young-Woo Son*

Korea Institute for Advanced Study, Seoul 02455, Republic of Korea
* E-mail: hand@kias.re.kr

Germanium-antimony-telluride (GST) compounds have long been recognized as one of candidate materials for nonvolatile phase-change memory due to high read and write speed and low power consumption. In this study, we present electronic structure calculations of ternary GST compounds using a machine learning empirical pseudopotential method (ML-EPM) [Kim and Son, arXiv:2306.04426 (2023)]. The newly developed ML-EPM method overcomes poor transferability of traditional EPM by ML while retaining its merit such as formal simplicity and less demanding resources. We extend a previous use of ML-EPM from binary to ternary compounds. With a training set of ab initio electronic structures of various GST compounds and their rotation-covariant descriptors, we successfully generate versatile and transferable empirical pseudopotentials of Ge, Sb and Te, respectively. We demonstrate that, using the MLEPM, computed electronic energy bands and wavefunctions of unlearned GST compounds without cumbersome self-consistency show good agreements with results from first-principles calculations. This agreement holds even for GST crystal structures with distinctive local atomic environments or more extended systems compared to those in training dataset.

Talk No. 8

More is different, moiré is different

Kunihiro Yananose

“More is different” by P.W.Anderson is a famous quotation in condensed matter physics. This points out the limitation of the reductionism and the emergence of entirely new properties at each level of complexity of the science. The moiré pattern, which is appearing due to the twist of 2-dimensional materials, i.e., rotational misalignment of two atomically thin layers, has been attracting considerable attention as a new manifestation of “more is different.” In this talk, I will introduce the ‘moiré physics’ and discuss several computational challenges and approaches related to it.

Talk No. 9

Hidden multiscale organization and robustness of real multiplex networks

Gangmin Son

The structure of many systems of interacting elements, including the Internet and the brain, is represented by complex networks, which are networks far from both lattices and classical random graphs. The so-called hidden geometry paradigm enables the investigation of complex networks at different scales. In this talk, I will show that this idea can be applied to multiplex networks to uncover their multiscale organization and its role in robustness. In particular, we discover clans, groups of nodes that preserve local geometric arrangements across layers. Furthermore, we reveal the intimate relationship between clans and mutual connectivity, which leads to an ambivalent role of clans: making a system fragile yet less prone to complete shattering. Finally, we find that clans can enhance overall robustness. Our findings highlight potential pitfalls in evaluating and controlling the breakdown of multiplex systems.

Talk No. 10

An investigation of anomalous water dynamics using a machine learning force field

Ji Woong Yu

Parametric models, known as force fields, play a critical role in the computational simulation of atomic interactions, each designed to accurately reflect the chemical properties of specific atomic species. Despite the prevalence of water, current force field models exhibit limitations in comprehensively modeling its behavior, particularly within salt solutions. A notable challenge in computational science is the consistent underperformance of in-silico models in replicating the dynamic behavior of water in salt solutions, which contrasts sharply with experimental findings. Specifically, while kosmotropic salts are observed to decelerate and chaotropic salts to accelerate water dynamics in accordance with the Hofmeister series, many force fields fail to adequately mirror these effects.

This presentation will detail recent research on the comparative analysis of various force fields for water and salt solutions, including SPC/Fw+JC, iAMOEBA, MB-Pol, AIMD(BLYP-D3), and a novel machine learning force field (MLFF), DPMD. Emphasis will be placed on the analysis of the four-point susceptibility of water as a method to qualitatively distinguish between the effectiveness of these force fields. The research aims to not only elucidate the complex dynamics of water at the molecular level but also to demonstrate the significant potential of machine learning in refining and advancing computational models for more accurate simulations in the field of computational sciences.

Talk No. 11

Algorithmic Approach to the Optimal Computation of Chain Propagators of Branched Polymers in Polymer Field Theory Simulations

Daeseong Yong

Polymer field theory simulations are efficient theoretical tools for investigating the self-assembly of block copolymers. In order to perform simulations with branched polymers, it is crucial to eliminate duplicated computation of chain propagators. Until now, this has been done through researchers' experience and intuition, and not algorithmically. However, this has prevented developing an efficient open-source simulation software for diverse polymer systems, because we cannot manually optimize the computations for many polymer architectures. It should be done using an algorithm approach. In this talk, I will introduce an algorithmic approach to the optimal computation of chain propagators by serializing polymer architectures of corresponding chain propagators. Using the serialized information of chain propagators, duplicated computations can be successfully eliminated for an arbitrary mixture of acyclic branched polymers.

Talk No. 12

Influences of Charge-Mediated Interactions on Electrolytes and Understanding Electrostatic Effects of Systems

YeongKyu Lee

Understanding the electrostatic interactions within ion-molecular systems is essential for the advancement of future scientific technologies. To deepen our understanding of these interactions at the molecular scale, it is imperative to engage in both theoretical and numerical studies across diverse ion-molecular systems. This presentation will explore a wide range of ion-molecular systems, bridging theoretical foundations with practical applications. Additionally, it will highlight the correspondence between theoretical insights and numerical outcomes, emphasizing the significance of their interplay in unraveling the complexities of these systems.

Talk No. 13

Finding eigenstate properties using the quantum computer through the Quantum Zeno Monte Carlo

Han Mancheon1, *, Park Hyowon2,3, and Choi Sangkook1, †

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2Materials Science Division, Argonne National Laboratory,
3Department of Physics, University of Illinois at Chicago
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Solving quantum many-body system with the quantum computer can be much easier than with the classical computer. For example, the quantum phase estimation (QPE), which assumes fully fault-tolerant quantum computer, finds Hamiltonian eigenvalue and eigenvector within a polynomial complexity, with a cost of long circuit depth and many ancilla qubits. But quantum devices in past decade were noisy intermediate-scale quantum (NISQ) devices. The noise-resilience of the algorithm is most important factor to conduct computation with such device. The variational quantum eigensolver (VQE), is the representative of algorithms that tackles noise resilience. Though VQE can give reasonable results with NISQ devices, ansatz-based nature makes it to encounter the representability and the barren plateau issues. In this work, we invented an ansatz-free and noise resilient approach, the quantum Zeno Monte Carlo (QZMC). Our approach represents eigenvector by Monte Carlo summation, allowing eigenvector properties computation within a polynomial quantum time if the state is gapped. QZMC is classical-quantum hybrid realization of the Quantum Zeno effect, which is the phenomenon that repeated measurements slow down transitions of the state. We verified QZMC as follows. First, we demonstrated noise resilience of our method by applying it to a small system with NISQ devices. Second, we show that our algorithm can find the eigenvector properties of larger system with a polynomial cost by computing energy eigenvalues and spectral functions of the Hubbard model for various sizes. Because our algorithm is noise-resilient and can show polynomial computational complexity, we expect our algorithm can achieve quantum advantage with an early fault-tolerant quantum computer. In this work, we invented an ansatz-free and noise resilient approach, the quantum Zeno Monte Carlo (QZMC). Our approach represents eigenvector by Monte Carlo summation, computing eigenvector properties within a polynomial quantum time if the state is gapped. We verified QZMC as follows. First, we demonstrated noise resilience of our method by applying it to a small system with NISQ devices. Second, we show that our algorithm can find the eigenvector properties of larger system with a polynomial cost by computing energy eigenvalues and spectral functions of the Hubbard model for various sizes. Because our algorithm is noise-resilient and can show polynomial computational complexity, we expect our algorithm can achieve quantum advantage with an early fault-tolerant quantum computer.

Talk No. 14

Randomized quantum-classical hybrid approaches for ground-state and energy computation

Taehee Ko

In this talk, we present two quantum-classical hybrid approaches for the ground-state and energy computation of a Hamiltonian based on the random coordinate descent. The first approach is the incorporation of the random coordinate descent into the variational quantum eigensolver. We show rigorous analysis under a local PL condition and extensive numerical experiments for various quantum optimization problems, which demonstrate the efficiency of the random coordinate descent over the full gradient descent. As the second approach, we propose a new algorithm that can be combined with any existing quantum algorithm which prepares a matrix polynomial (e.g. quantum signal processing, quantum singular value transformation and so forth). In the fault-tolerant regime, the algorithm can converge to ground state with high probability to an arbitrary precision without further changing a given quantum circuit. We provide convergence properties of our algorithm and demonstrate its performance for transverse field ising model and Hubbard model.

Talk No. 15

Calculating X-ray spectra for strongly correlated materials

Johan Jonsson

X-ray spectroscopy is a family of very powerful and widely used experimental techniques capable of examining electronic and magnetic properties of materials. Advances in experimental techniques have increased the resolution achievable in X-ray measurements tremendously. This increase in detail from experiments has led to a need for theoretical models capable of calculating X-ray spectra with equally high details, especially for materials containing correlated electronic structures.

In this talk I will describe our efforts in developing a theoretical method capable of producing high quality X-ray spectra. Our method is based on Multiplet Ligand Field Theory (MLFT), which explicitly includes core-hole interactions and electron-electron interactions in the valence band, at the cost of having a large number of adjustable parameters. By combining MLFT with underlying electronic structure calculations, such as Density Functional Theory (DFT) and it's combination with Dynamical Mean-Field Theory (DFT + DMFT). The result is a powerful method that has far fewer adjustable parameters, similar to a DFT+DMFT calculation, and produces X-ray spectra that agree very well with experiments.

Talk No. 16

Recognizing even-cycle and even-cut matroids

Cheolwon Heo

Even-cycle matroids are elementary lifts of graphic matroids.
Even-cut matroids are elementary lifts of cographic matroids.
We give a polynomial time algorithm to check if a binary matroid is an even-cycle matroid.
We also give a polynomial time algorithm to check if a binary matroid is an even-cut matroid.
These algorithms rely on structural properties of the class of pinch-graphic matroids.

This is joint work with Bertrand Guenin at University of Waterloo.

Talk No. 17

A brief introduction to the Laplacian matrix of graphs

Sunyo Moon

Spectral graph theory is a branch of graph theory that studies the relation between the properties of a graph and the eigenvalues and eigenvectors of matrices associated with the graph, such as the adjacency matrix and the Laplacian matrix. In this talk, we introduce the definition of the Laplacian matrix and present its properties.

Talk No. 18

How complex is your graph?

Jungho Ahn

There are numerous graph parameters and each of them measures structural complexity of graphs in their own manner.
In this talk, we introduce several basic graph parameters with some applications.