2022 KIAS School of Computational Sciences Workshop

ABSTRACTS

August 29 (Mon) ~ 31 (Wed), 2022

Phoenix Seopjikoji, Jeju

2022 KIAS School of Computational Sciences Workshop

August 29(Mon)~31(Wed), 2022 Phoenix Seopjikoji, Jeju

<table>
<tr><th></th><th>August 29 (Mon)</th><th>August 30 (Tue)</th><th>August 31 (Wed)</th></tr>
<tr><td>07:00-09:30</td><td rowspan="8">Aiport -> Resort (Phoenix Seopjikoji)

Shuttle Bus
Airport B-Zone Parking Lot #1, #2
1회차: 12:00
2회차: 16:00</td><td>Breakfast</td><td>Breakfast</td></tr>
<tr><td>09:30-10:30</td><td>Seminar
(20min x 3)</td><td>Seminar
(20min x 3)</td></tr>
<tr><td>10:30-11:00</td><td>Break</td><td>Break (Check out)</td></tr>
<tr><td>11:00-11:20</td><td rowspan="2">Seminar
(20min x 3)</td><td>Seminar
(20min x 1)</td></tr>
<tr><td>11:20-12:00</td><td>Group Discussion</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="3">Excursion

1. Jeolmul Natural Recreation Forest
2. Woljeongri Beach</td><td rowspan="6">Resort (Phoenix Seopjikoji) -> Airport
Shuttle Bus
Orange build. at CU
1회차: 10:30
2회차: 14:30</td></tr>
<tr><td>14:00-15:00</td></tr>
<tr><td>15:00-17:30</td><td>Self Check-in & Registration</td></tr>
<tr><td>17:30-18:00</td><td rowspan="2">Seminar
(20min x 4명)</td><td rowspan="2">Banquet</td></tr>
<tr><td>18:00-19:00</td></tr>
<tr><td>19:00-20:00</td><td>Dinner</td></tr>
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* Check in (14:00 ~), Check out (~ 11:00)
* Seminar Room - Wind Hall, 2Fl
* Meal at Seopjikoji - Haerang (1fl. Orange bldg., Bella Terrace)

Program

August 29 (Mon)

17:30-17:50	Dildar Hussain	Deep Learning in DXA Image Segmentation and Analysis
17:50-18:10	Irving Rondon	Modeling generalized growth laws using statistical physics
18:10-18:30	Jeeun Lee	Quantum Security of Block Cipher Modes of Operation
18:30-18:50	Spyridon Kechrimparis	Computational Mechanics, Causal Asymmetry and Ambiguity of Simplicity

August 30 (Tue)

09:30-09:50	Sudo Yi	Structure of international trade hypergraphs
09:50-10:10	Hyun gyu Lee	A generalized economic model for wealth exchange for studying wealth distribution; from extreme inequality to a fair distribution
10:10-10:30	Andrus Allan Giraldo Munoz	A Bifurcation and Numerical Continuation approach to selective extinction in Complex Mutualistic Networks
10:30-11:00	Break	
11:00-11:20	Jaeseong Oh	Combinatorial interpretations
11:20-12:00	Group Discussion	

August 31 (Wed)

09:30-09:50	Rokyeon Kim	Machine learning universal empirical pseudopotentials for density functional theory calculations
09:50-10:10	Changwon Park	Commensurate-Incommensurate Structural Phase Transition in Crystal; Interatomic potential approach
10:10-10:30	Minjae Kim	DFT+U+V as an efficient method for GW
10:30-11:00	Break	
11:00-11:20	Narina Jung	Swimming in complex fluids
11:20-12:00	Group Discussion	

Talk No. 1

Deep Learning in DXA Image Segmentation and Analysis

Dr. Dildar Hussain
School of Computational Sciences
Korea Institute for Advanced Study
2022 School of Computational Sciences Workshop

Abstract: Medical image segmentation can be a time-consuming task, and recent advances in segmentation techniques using Deep Learning are making it easier for routine tasks to be completed. Considering dual-energy X-ray absorptiometry (DXA) images many existing techniques are unable to accurately distinguish between bone and soft tissue. For the most part, this failure stems from bone shape variability, noise and low contrast in DXA images, inconsistent X-ray beam penetration producing shadowing effects, and person to-person variations.

In recent years, deep learning technology has been used for analyzing medical images in various fields, and it shows excellent performance in segmentation and registration. Large number of papers has been presented recording the success of deep learning in the field. This work explores the feasibility of using state-of-the-art deep learning semantic segmentation models, fully convolutional networks (FCNs), SegNet, and U-Net to distinguish femur bone from soft tissue. We investigated the performance of deep learning algorithms with reference to some of our previously applied conventional image segmentation techniques (i.e., a decision-tree-based method using a pixel label decision tree [PLDT] and another method using Otsu's thresholding) for femur DXA images, and we measured accuracy based on the average Jaccard index, sensitivity, and specificity. Deep learning models using SegNet, U-Net, and an FCN achieved average segmentation accuracies of 95.8%, 95.1%, and 97.6%, respectively, compared to PLDT (91.4%) and Otsu's thresholding (72.6%). Thus we conclude that an FCN outperforms other deep learning and conventional techniques when segmenting femur bone from soft tissue in DXA images. Accurate femur segmentation improves bone mineral density computation, which in turn enhances the diagnosing of osteoporosis.

Talk No. 2

Modeling generalized growth laws using statistical physics.

Rondon Irving

Korea Institute for Advanced Study, Seoul 02455, Korea

In this talk, we briefly present the problem of modeling general universal laws growth using statistical physics and thermodynamics for systems out of equilibrium.
A general growth model based on non-extensive statistical physics is presented. The obtained equation is expressed in terms of nonadditive q entropy. We show that the most common unidimensional growth laws such as power law, exponential, logistic, Richards, Von Bertalanffy, Gompertzian behavior can be obtained. The new evolution equation resembles the "universality" behavior presented and discussed using experimental tumor growth data. It is shown that for early times the model follows a power law growth classify different growth. Several examples are presented and discussed. Finally, we present some work in progress and connection with superstatistics that consider time fluctuations dynamics that can be related with this model. Some discussion and potential applications using machine learning are presented.

Talk No. 3

Quantum Security of Block Cipher Modes of Operation

Jeeun Lee

Korea Institute for Advanced Study, Seoul 02455, Korea

In this talk, I will investigate the quantum security of modes of operation in block ciphers which are widely used cryptographic primitives, and introduce many quantum concepts that are extended from the classical ones. First, for a systematic study, quantum adversaries are classified as Q0, Q1, or Q2 depending on their ability to perform quantum computation. Then the underlying block ciphers are assumed as pseudorandom functions which are Q0, Q1, or Q2 secure. Also, modes of operation to be investigated, CBC, IGE, CFB, OFB, and CTR, are defined and represented in the quantum circuit. Next, our desired security notions are considered in terms of quantum version of indistinguishability (IND) and chosen-plaintext attack (CPA) with quantum security games. Finally, the security of each mode in Q0-, Q1-, or Q2-secure block ciphers is analysed and compared in these various quantum security game scenarios.

Talk No. 4

Computational Mechanics, Causal Asymmetry and Ambiguity of Simplicity

Spyridon Kechrimparis

Korea Institute for Advanced Study, Seoul 02455, Korea

Computational mechanics is concerned with the study of minimal causal representations of stochastic processes. A surprising phenomenon is *causal asymmetry*: the memory required to optimally predict the future is in general different from the memory to retrodict the past. Another interesting phenomenon has been termed *ambiguity of simplicity:* the question of which one of two given processes is simpler can assume different answers depending on whether a classical or quantum description is employed. I will give an introduction to the field and overview open problems and recent progress.

Talk No. 5

Structure of international trade hypergraphs

Sudo Yi

Korea Institute for Advanced Study, Seoul, Korea

We study the structure of the international trade hypergraph consisting of triangular hyperedges representing the exporter-importer-product relationship. Measuring the mean hyperdegree of the adjacent vertices, we first find its behaviors different from those in the pairwise networks and explain the origin by tracing the relation between the hyperdegree and the pairwise degree. To interpret the observed hyperdegree correlation properties in the context of trade strategies, we decompose the correlation into two components by identifying one with the background correlation remnant even in the exponential random hypergraphs preserving the given empirical hyperdegree sequence. The other component characterizes the net correlation and reveals the bias of the exporters of low hyperdegree towards the importers of high hyperdegree and the products of low hyperdegree, which information is not readily accessible in the pairwise networks. Our study demonstrates the power of the hypergraph approach in the study of real-world complex systems and offers a theoretical framework.

Talk No. 6

A generalized economic model for wealth exchange for studying wealth distribution; from extreme inequality to a fair distribution

Hyun Gyu Lee

Korea Institute for Advanced Study, Seoul 02455, Korea

Unequal distribution of wealth is a consequence of enormous amounts of decision-making processes between individuals. Pinpointing the exact cause of the wealth inequality is almost impossible because not only of the sheer number of individuals, but also of the unpredictability of how a human makes economic decisions. However, rather recent and successful attempts to understand economic phenomena via principles of physics (so-called 'econophysics') frequently assumes dramatically simple microscopic processes comprising a macroscopic system.

One of such attempts to understand the unequal wealth distribution, which can also be represented by the seemingly universal Pareto's law (i.e., the probability distribution of wealth has power-law form), has been made by Bouchaud and Mézard in 2000. In the work, they assumed a system in which each individual exchanges a fixed proportion of his/her own wealth with their neighbors, and the wealth itself can multiply by a random factor each time. After writing down this into a set of stochastic differential equations, the authors discovered that the analytical solution for the equilibrium probability distribution was indeed power-law. Furthermore, they presented a generalized version of this distribution by tuning parameters for the equations, thus arriving at a spectrum of wealth distribution between two extremes of inequality; power-law and delta-function (perfect equality).

Meanwhile, early attempts to understand the inequality mechanism by prescribing exchange rules to a finite number of agents came to rise from the 1980s, and later the so-called Yard-sale model provided an agent-based approach to the wealth inequality. Boghosian's work in 2014 where he showed analytical long-time solutions to the Yard-sale model, and many others via numerical methods revealed that the model also produces power-law distribution. The exchange rule utilized in the model inherently places advantage to wealthy individuals, leading to a time-irreversible process in which the wealthier grows even wealthier. A generalized version of Yard-sale, on the other hand, would probably assume an additional exchange rule which counters this time-irreversible effect, distributing wealth to a greater population.

In our work, we introduce a parameter to realize this effect, and suggest a generalized Yard-sale model in an effort to draw parallel with the work by Bouchaud and Mézard. Furthermore, we report several scaling behaviors which can be significant in statistical mechanics' perspective.

Talk No. 7

A Bifurcation and Numerical Continuation approach to selective extinction in Complex Mutualistic Networks

Andrus Giraldo

Korea Institute for Advanced Study, Seoul 02455, Korea

In this talk, the problem of interest is the species abundance and extinction of a plant-pollinator empirical ecological network. A generalized Mutualistic-Competitive Lotka-Volterra equation is used to model its dynamical behavior, where some plants and pollinators have a mutualistic relation, and uniform intra-group competition exists. We consider two parameters in the Lotka-Volterra equation representing the strength of mutualism and competition. Thus, some species can go extinct under particular combinations of these two parameters.

Using a dynamical system approach, we will show in this talk how we transform the species extinction problem into a bifurcation problem that can be readily solved using numerical continuation techniques. By doing so, we systematically build the species survival's bifurcation (phase) diagram as a function of the mutualism and competition parameters. Furthermore, we unveiled the spontaneous existence of multistability, where different extinction scenarios emerge due to Hopf bifurcations.

Talk No. 8

Combinatorial interpretations

Jaeseong Oh

Korea Institute for Advanced Study, Seoul 02455, Korea

A combinatorial interpretation promotes a numerical quantity to one with more structure. I will explain what combinatorial interpretation is and why we seek combinatorial interpretations. The main examples are binomial coefficients and Catalan numbers.

Talk No. 9

Machine learning universal empirical pseudopotentials for density functional theory calculations

Rokyeon Kim

Korea Institute for Advanced Study, Seoul, Korea

Traditional empirical pseudopotentials allow for efficient calculations of electronic band structures. Such potentials, however, were not able to reproduce wave functions and related quantities, and transferability to different environments is difficult to achieve. Here, we introduce a method to generate empirical pseudopotentials from density functional theory calculations with machine learning. The use of these empirical pseudopotentials produces not only band structures, but also wave functions, total energies, forces, and so on. It also enables us to address structures with thousands of atoms by bypassing the self-consistent loop. We apply the method to Si, Ge, and SiO_2, finding excellent agreement with density functional theory results. We also discuss how to improve the transferability of empirical pseudopotentials via machine learning.

Talk No. 10

Commensurate-Incommensurate Structural Phase Transition in Crystal; Interatomic potential approach

Changwon Park

School of Computational Sciences, Korea Institute for Advanced Study, Hoegiro 85, Seoul 02455, Korea

Abstract

In a crystal, temperature not only changes its volume but also often breaks its symmetry. In some crystal, intriguingly, the period of symmetry-broken structure is sometimes larger than the lattice constant (charge density wave) and the period itself undergoes a phase transition between lattice-commensurate and lattice-incommensurate ones. This commensurate-incommensurate phase transition is quite ubiquitous that a few models are independently suggested in different fields. Unfortunately, for crystals, the model is still phenomenological that there is no known way to calculate the model parameters from first-principles.

For a layered crystal hexagonal-$TaSe_2$, I successfully reproduced its temperature-dependent phase diagram from first-principles interatomic potential. The only approximation is the mean-field treatment of temperature. This suggests that the (adiabatically calculated) interatomic potential is the correct and sufficiently accurate microscopic descriptor for charge density wave. For a comprehensive understanding, I will demonstrate how commensurate-incommensurate phase transition takes places in anharmonic spring chain.

Talk No. 11

DFT+U+V as an efficient method for GW

Minjae Kim[1], Bo Gyu Jang[1], Sang-Hoon Lee[1], Young-Woo Son[1]

[1]*Korea Institute for Advanced Study, Seoul 02455, Korea*

The density functional theory (DFT) is an essential tool for the computation of physical properties of materials. Even though this tool is efficient in description of the quasiparticle band structures and structural properties, there is a limitation mainly due to the approximation in Kohn-Sham potentials for the exchange-correlation functional. From the exchange-correlation functional, the many-body problem of materials is map to the effective single particle equation. In this talk, we show that the DFT with corrections on the exchange-correlation functional from extended Hubbard interactions (U for on-site, V for inter-site), DFT+U+V, is an efficient and accurate method for the computation of materials properties, can be regarded as an approximation of the GW method. We prove that the extended Hubbard interactions can map onto the local and nonlocal static self-energy of the GW approximation. This mapping suggests that the DFT+U+V, which is a parameter-free, self-consistent pseudohybrid functional method of with an appropriate implementation of the spatial variation of screenings, is a proper method for descriptions of physical properties of materials. We show that the DFT+U+V method is accurate in descriptions of energy band gap, effective mass, work function, absorption spectra, and renormalized optical phonon frequency for bulk silicon, monolayer black phosphorus, and NiO, relying on the precise description of the dielectric screenings of materials.

Talk No. 12

Swimming in complex fluids

Narina Jung

Korea Institute for Advanced Study, Seoul 02455, Korea

The locomotion of animals is essential for their survival and also determines their modes of life. The swimming mechanism of aquatic animals involves a wide range of different coordinations, underpinned by diverse physical principles. In addition to periodically deforming parts of their bodies, they exploit the properties of the liquid for efficient swimming. They even change swimming strategies to deal with obstacles or other swimmers nearby. In this presentation, we discuss the swimming mechanisms of some aquatic animals in various time and length scales and specific features of swimmers in particular environments.