

**JSPS A3 Foresight Program “Modeling and Simulation of
Hierarchical and Heterogeneous Flow Systems with
Applications to Materials Science VI”**

July 26-29, 2019

TOKYO ELECTRON House of Creativity
Sendai, Japan

Organized by

Yasumasa Nishiura (Tohoku University, Japan)
Hyeonbae Kang (Inha University, Korea)
Pingwen Zhang (Peking University, China)

Sponsored by

Japan Society for the Promotion of Science
National Natural Science Foundation of China
National Research Foundation of Korea

Tohoku Forum for Creativity, Tohoku University

Advanced Institute for Materials Research, Tohoku University
AIST-TohokuU Mathematics for Advanced Materials-OIL

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Program



日本学術振興会
Japan Society for the Promotion of Science

A3 foresight workshop

“Modeling and Simulation of Hierarchical and Heterogeneous Flow Systems with Applications to Materials Science VI”

Date: July 26 (FRI) – July 29 (Mon), 2019
Venue: TOKYO ELECTRON House of Creativity
Sendai, Japan

Schedule: July 26 (Fri)

19:00 – Welcome Reception and Discussion @ Hotel Bel Air Sendai

Schedule: July 27 (Sat)

09:00 – 09:20 Registration at 3rd floor of TOKYO ELECTRON House of Creativity

Chair: Pingwen Zhang

09:20 – 09:30 Opening

09:30 – 10:20 1 : Edgar Knobloch (University of California at Berkeley, USA)

Crystallization from a supercooled melt: some questions

10:20 – 10:50 2 : Shuonan Wu (Peking University, China)

A class of new upwinding finite element schemes for convection-dominated PDEs with applications to magnetohydrodynamics multi-physics systems

10:50 – 11:10 Coffee break

Chair: Hisashi Okamoto

11:10 – 11:40 3 : Kai Jiang (Xiangtan University, China)

An adaptive accelerated proximal gradient method for computing stationary states of phase field crystal models

11:40 – 12:10 4 : Young-Pil Choi (Inha University, Korea)

A hydrodynamic model for synchronization phenomena

12:10 – 14:00 Lunch at Combination room, 5th floor of AIMR main building

Chair: Hiroshi Kokubu

- 14:00 – 14:30 **5 : Douglas Zhou (Shanghai Jiao Tong University, China)**
The structure, dynamics and function of neuronal networks
- 14:30 – 15:00 **6 : Chohong Min (Ewha womans university, Korea)**
Augmented Hodge decomposition in fluid-solid interaction
- 15:00 – 15:20 **Coffee break**

Chair: Takashi Sakajo

- 15:20 – 15:50 **7: Eun Bo Shim (Kangwon National University, Korea)**
Three-Dimensional Heart Model–Based Screening of Proarrhythmic Potential by
in Silico Simulation of Action Potential and Electrocardiograms
- 15:50 – 16:20 **8: Zhenning Cai (National University of Singapore, China)**
One-dimensional Study of Gauge Cooling Technique for Complex Langevin
Method
- 16:20 – 16:35 **9 : Ruishu Wang (Jilin University, China)**
Weak Galerkin finite element method for linear elasticity problem
- 16:35 – 18:00 **Discussion**
- 18:00- **Dinner and discussion @ Restaurant Hagi**

Schedule: July 28 (Sun)

Chair: Jinhae Park

- 09:30 – 10:20 **10: Lei Zhang (Peking University, China)**
Construct the Solution Landscape beyond the Energy Landscape
- 10:20 – 10:50 **11 : Shinji Nakaoka (Hokkaido University, Japan)**
Application of energy landscape analysis for cellular differentiation process
- 10:50 – 11:10 **Coffee break**
- 11:10 – 11:40 **12 : Myeongmin Kang (Chungnam National University, Korea)**
A novel variational model for single image dehazing
- 11:40 – 13:30 **Lunch at Combination room, 5th floor of AIMR main building**

Chair: Lei Zhang

- 13:30 – 14:00 **13 : Ippei Obayashi (RIKEN, Japan)**
Data Analysis by Persistent homology and Machine learning

14:00 – 14:30 **14: Dan Hu (Shanghai Jiao Tong University, China)**
A Saddle-Point-Transition-Path-Umbrella-Sampling Framework for Free Energy Calculation

14:30 – 14:50 **Coffee break**

Chair: Yasumasa Nishiura

14:50 – 15:40 **15 : Seonhee Lim (Seoul National University, Korea)**
Volume entropy and information flow in brain networks: in case of tinnitus in subjects with hearing loss

15:40 – 16:10 **16 : Naoya Fujiwara (Tohoku University, Japan)**
Complex networks of human mobility and their applications

16:10 – 18:00 **Poster Session**

18:10 **Courtesy bus to the restaurant**

18:30- **Banquet at Shoukeikaku**

Schedule: July 29 (Mon)

Chair: Hyeonbae Kang

9:30 – 10:00 **17 : Soojung Kim (Soongsil University, Korea)**
Nematic liquid crystal flows in an applied magnetic field

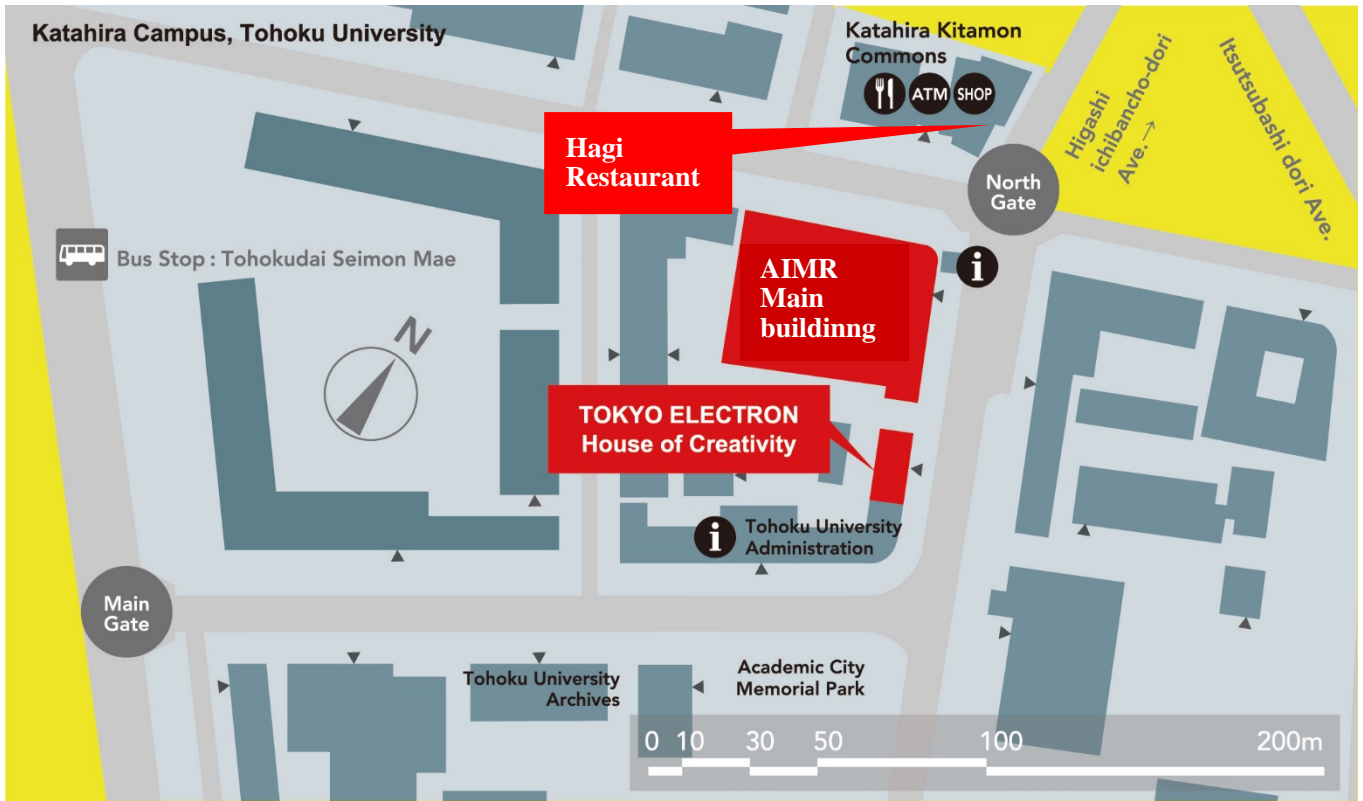
10:00 – 10:30 **18 : Tomoki Uda (Tohoku University, Japan)**
Constructing Reeb graphs from discrete data and its application to topological flow data analysis

10:30 – 10:45 **Coffee break**

10:45 – 11:00 **19 : Lingchao Zheng (Peking University, China)**
A Nonlinear Moment Model for Radiative Transfer Equation in Slab Geometry

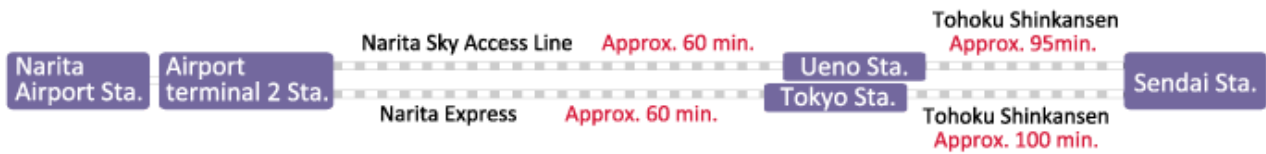
11:00 – 12:00 **Concluding remarks and Closing**

12:00 – 13:00 **Farewell Lunch at Combination room, 5th floor of AIMR main building**



Access

From Narita Airport



From Haneda Airport



From Sendai Airport



From Sendai Sta.

By taxi from Sendai Station

Approx. 10 min. by taxi from the West Exit on the first floor of Sendai Station

By foot from Sendai Station

Approx. 15 min. walk from the West Exit of Sendai Station

Abstracts

Crystallization from a supercooled melt: some questions

Edgar Knobloch

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University of California at Berkeley

The phase-field model, also known as the conserved Swift-Hohenberg equation, provides a useful model of crystallization that is derivable from the more accurate dynamical density functional theory (DDFT). I will survey the properties of this model focusing on spatially localized structures and their organization within a so-called snaking or bifurcation diagram [1]. I will highlight the role played by conserved mass and discuss the role played by these structures in the thermodynamic limit. I will then discuss dynamic crystallization via a propagating crystallization front in both one and two spatial dimensions [2,3]. Two types of fronts can be distinguished: pulled and pushed fronts, with different properties. I will demonstrate, via direct numerical simulation, that the crystalline structures deposited by a rapidly moving front are not in thermodynamic equilibrium and so become disordered as they age. I will conclude with a discussion of a two-wavelength generalization of the model that exhibits quasicrystalline order in both two and three dimensions [4] and the associated spatially localized structures with different quasicrystalline motifs [5]. I will compare the results with related results obtained from DDFT with a two-scale particle-particle interaction potential [6,7]. The possible role of metastable spatially localized structures in nucleating crystallization will be highlighted. Throughout the talk I will emphasize open questions that remain to be addressed in more detailed studies.

References

- [1] U. Thiele, A. J. Archer, M. J. Robbins, H. Gomez and E. Knobloch. Phys. Rev. E 87, 042915 (2013)
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- [7] A. J. Archer, A. M. Rucklidge and E. Knobloch. Phys. Rev. E 92, 012324 (2015)

A class of new upwinding finite element schemes for convection-dominated PDEs with applications to magnetohydrodynamics multi-physics systems

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In this talk, we present a new class of upwinding finite element schemes developed for convection-dominated PDEs discretized on unstructured simplicial grids in both 2 and 3 dimensions. The convection can be any one of the following operators: gradient, curl and divergence. The derivation of this scheme makes use of some intrinsic properties of differential forms and in particular some crucial identities from differential geometry. An essential feature of these constructions is to properly average the PDE coefficients on the sub-simplexes. Both theoretical analysis and numerical experiments show that the new upwinding finite element schemes provide an accurate and robust discretization in many applications and in particular for simulation of magnetohydrodynamics systems when the magnetic Reynolds number R_m is large.

Reference

[1] S. Wu, J. Xu, Simplex-averaged finite element methods for $H(\text{grad})$, $H(\text{curl})$ and $H(\text{div})$ convection-diffusion problems, in revision, arXiv:1810.04857, 2018.

An adaptive accelerated proximal gradient method for computing stationary states of phase field crystal models

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In this talk, we will present an adaptive accelerated proximal gradient (APG) method for computing stationary states of phase field crystal models, which can be formulated as an energy minimization problem. The energy functional is discretized by different discretization schemes dependent on the physical problem. For periodic crystals, the Fourier pseudospectral method is applied, while for quasicrystals, the projection method is adopted. Thus the original infinite nonconvex minimization problem is approximated by a finite dimensional nonconvex minimization problem. The convergence of the adaptive APG method is estimated. Extensive numerical experiments, including several three dimensional periodic crystals in Landau-Brazovskii model and two dimensional quasicrystals in Lifshitz-Petrich model, demonstrate that our method is efficient, fast and robust.

A hydrodynamic model for synchronization phenomena

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In this talk, we present a new hydrodynamic model for synchronization phenomena which is a type of pressureless Euler system with nonlocal interaction forces. For the proposed system, we first establish local-in-time existence and uniqueness of classical solutions. For the case of identical natural frequencies, we provide synchronization estimates under suitable assumptions on the initial configurations. We also analyze critical thresholds leading to finite-time blow-up or global-in-time existence of classical solutions. Finally, we numerically investigate synchronization, finite-time blow-up, phase transitions, and hysteresis phenomena.

The structure, dynamics and function of neuronal networks

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In this talk, I will describe how mathematics can play important roles in revealing the relationship among the structure, the dynamics and the function of neuronal networks. First, I will present our modeling work about how to establish an effective point neuron model which is capable of capturing the nonlinear dendritic integration of real neurons, therefore, one can efficiently simulate the real neuron dynamics without taking into account the complicated morphology of real neurons. Then I will discuss how to infer the network connectivity structure by measuring the output signals of neuronal networks. By solving this inverse problem, one can build up the large-scale computational neuronal network model of certain cortical regions. Finally, I will focus on the early visual pathway of primates and use our modeling, analysis and simulation, in comparison with experimental observations, to understand the coding principle of the primary visual cortex.

Reference

- [1] S. Li, N. Liu, X. Zhang, D.W. McLaughlin, D. Zhou and D. Cai, “*Dendritic computations captured by an effective point neuron model*”, Proc. Natl. Acad. Sci., USA, in revision.
- [2] Y. Zhang, Y. Xiao, D. Zhou and D. Cai, “*Spike-triggered regression for synaptic connectivity reconstruction in neuronal networks*”, Front. Comput. Neurosci., 11, 101, (2017).
- [3] S. Li, N. Liu, X. Zhang, D. Zhou and D. Cai, “*Bilinearity in spatiotemporal dendritic integration of synaptic conductance inputs*”, PLoS Comput. Biol., 10 (12), e1004014, (2014)
- [4] D. Zhou, A.V. Rangan, D.W. McLaughlin and D. Cai, “*Spatiotemporal dynamics of neuronal population response in the primary visual cortex*”, Proc. Natl. Acad. Sci., USA, 110 (23), 9517-9522, (2013).
- [5] D. Zhou, Y. Xiao, Y. Zhang, Z. Xu and D. Cai, “*Causal and structural connectivity of pulse-coupled nonlinear networks*”, Phys. Rev. Lett., 111 (5), 054102, (2013).

Augmented Hodge decomposition in fluid-solid interaction

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The Hodge decomposition plays an important role to understand and simulate incompressible fluid flows. We introduce an augmented Hodge decomposition for the system of incompressible fluid and rigid solid. It is an orthogonal decomposition whose pressure Poisson equation has non-local Robin boundary condition. The boundary value problem with the non-local condition turns out to be very similar to the Neumann condition. Using Heaviside function, the complicated boundary value problem can be efficiently formulated [1]. In this talk, we present our recent analysis [2] that shows the first order convergence of an approximate solution of the decomposition

Reference

[1] Frederic Gibou and Chohong Min, Efficient symmetric positive definite second-order accurate monolithic solver for fluid/solid interactions, *Journal of Computational Physics*, Volume 231, Issue 8, 20 April 2012, Pages 3246-3263

[2] Gangjoon Yoon, Seick Kim and Chohong Min, A Stable And Convergent Method For Hodge Decomposition Of Fluid-Solid Interaction, *Journal of Scientific Computing* August 2018, Volume 76, Issue 2, pp 727-758

Three-Dimensional Heart Model–Based Screening of Proarrhythmic Potential by *in Silico* Simulation of Action Potential and Electrocardiograms

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Abstract

The proarrhythmic risk is a major concern in drug development. The Comprehensive *in vitro* Proarrhythmia Assay (CiPA) initiative has proposed the JT_{peak} interval on electrocardiograms (ECGs) and qNet, an *in silico* metric, as new biomarkers that may overcome the limitations of the hERG assay and QT interval. In this study, we simulated body-surface ECGs from patch-clamp data using realistic models of the ventricles and torso to explore their suitability as new *in silico* biomarkers for cardiac safety. We tested three drugs in this study: dofetilide (high proarrhythmic risk), ranolazine, and verapamil (QT increasing, but safe). Human ventricular geometry was reconstructed from computed tomography (CT) images, and a Purkinje fiber network was mapped onto the endocardial surface. The electrical wave propagation in the ventricles was obtained by solving a reaction-diffusion equation using finite-element methods. The body-surface ECG data were calculated using a torso model that included the ventricles. The effects of the drugs were incorporated in the model by partly blocking the appropriate ion channels. The effects of the drugs on single-cell action potential were examined first, and three-dimensional (3D) body-surface ECG simulations were performed at free C_{max} values of 1x, 5x, and 10x. In the single-cell and ECG simulations at 5x C_{max}, dofetilide, but not verapamil or ranolazine, caused arrhythmia. However, the non-increasing JT_{peak} caused by verapamil and ranolazine that has been observed in humans was not reproduced in our simulation. Our results demonstrate the potential of 3D body-surface ECG simulation as a biomarker for evaluation of the proarrhythmic risk of candidate drugs.

Keywords: 3D heart model, ECG simulation, hERG, QT, Torsade de Pointes

One-dimensional Study of Gauge Cooling Technique for Complex Langevin Method

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We study the mechanism of the gauge cooling technique to stabilize the complex Langevin method in the one-dimensional periodic setting. In this case, we find the exact solutions for the gauge transform which minimizes the Frobenius norm of link variables. Thereby, we derive the underlying stochastic differential equations by continuing the numerical method with gauge cooling, and thus provide a number of insights on the effects of gauge cooling. A specific case study is carried out for the Polyakov loop model in $SU(2)$ theory, in which we show that the gauge cooling may help form a localized distribution to guarantee there is no excursion too far away from the real axis.

Weak Galerkin finite element method for linear elasticity problem

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In this report, the weak Galerkin finite element (WG) method is used to solve the linear elastic equation. The linear elastic equation is a classical model equation. Due to its complex structure and the fact that some of its physical quantities need to meet certain conditions, many difficulties are encountered in the numerical calculation of the linear elastic equation. Among the three issues that scholars are generally concerned about are: 1. The speciality of the definition of strain tensor leads to the numerical format is difficult in satisfying the coercive property; 2. The numerical solution of the linear elastic problem has a certain parameter dependence, and the parameter is unbounded when the elastic body tends to be incompressible; Stress tensor has symmetry due to Newton's third law, while the numerical format that maintains the stress tensor symmetry is very difficult to construct. This report talks about the WG method to answer the above three questions separately.

Construct the Solution Landscape beyond the Energy Landscape

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In mathematics, physics, and chemistry, an energy landscape is a map of the energy function across the configuration space of the system, which can provide the information such as local minima. In this talk, we propose an efficient algorithm to construct the solution landscape, which is a directed graph consisting of all critical points of the energy function. The solution landscape shows a global and intrinsic properties of the system that is beyond the energy landscape. As an illustration, we apply the Landau-de Gennes theory to study the defects in nematic liquid crystal. We show how to build the complete solution landscape of nematic liquid crystals in a 2D square to advance our understanding on the mathematical models. The joint work with Pingwen Zhang (PKU), Jianyuan Yin (PKU).

Application of energy landscape analysis for cellular differentiation process

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Tissues and organs in the body are composed of lineage-specific cells. Lineage-specific cells are given rise from a stem cell population via a cellular differentiation process. An energy landscape in cell biology is a geometric representation of a potential energy function which defines cell fate change via cellular differentiation. Although a concept of energy landscape has been employed to explain cellular differentiation processes qualitatively, reconstruction of energy landscape based on measured data has appeared recently.

In this talk, I would like to introduce an application of energy landscape analysis to single-cell RNA sequencing data. Based on the energy landscape analysis, we find the existence of multiple states at which the potential energy function is minimized. Each of these states represents a feasible configuration state and give us useful information on cellular differentiation. We also discuss the possibility of theoretical extension to the existing energy landscape analysis to apply to a variety of different datasets.

A novel variational model for single image dehazing

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In haze weather, outdoor images are often degraded by haze, causing a change of image contrast and color values. In this talk, we introduce a novel variational model for the restoration of a single color image degenerated by haze. The proposed model extends the total variation based model. To deal with various haze images, the proposed model also involves the inter-channel correlation term between the channels. This additional term permits both color and gray-valued transmission maps, which enable broader applications of the proposed model. In addition, a convergence analysis of the proposed minimization problem is also provided. To realize the proposed model, we adopt an alternating minimization algorithm, and then the alternating direction method of multipliers is employed for solving subproblems. Its convergence is also proved. Numerical experiments are demonstrated to validate the superiority of the proposed model with comparison with the state-of-the-arts models.

Reference

- [1] K. He, J. Sun and X. Tang, “Single image haze removal using dark channel prior”, IEEE transactions on pattern analysis and machine intelligence, Vol. 33, 2011 pp. 2341-2353.
- [2] W. Wang, C. He and X. G. Xia, “A constrained total variation model for single image dehazing”, Pattern Recognition, Vol. 80, 2018, pp. 196-209.

Data Analysis by Persistent homology and Machine learning

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RIKEN

Persistent homology is a homology theory based on *persistence* and was developed for data analysis. Persistent homology enables us to characterize the shape of data quantitatively. Machine learning enables us to find characteristic patterns behind the data. The combination of persistent homology and machine learning enables us to find *characteristic geometric patterns* from data. In this presentation I will introduce the data analysis method [1] by persistent homology and machine learning, and show some applications of the method to materials science [2].

Reference

- [1] Ippei Obayashi, Yasuaki Hiraoka, and Masao Kimura. Persistence diagrams with linear machine learning models. *Journal of Applied and Computational Topology* 1, 3-4, 421–449. (2018)
- [2] M. Kimura, I. Obayashi, Y. Takeichi, R. Murao, and Y. Hiraoka. Non-empirical identification of trigger sites in heterogeneous processes using persistent homology. *Scientific Reports* 8, 3553. (2018)

A Saddle-Point-Transition-Path-Umbrella-Sampling Framework for Free Energy Calculation

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For many complex rare event dynamics, multiple reaction coordinates may be involved in describing the transition mechanism. In the study of such complex rare events, expensive multi-dimensional sampling are required for traditional free energy calculation methods. In this talk, we propose a Saddle-Point-Transition-Path-Umbrella-Sampling framework for free energy calculation. Following this frame work, the free energy calculation for complex rare event dynamics becomes a one-dimensional umbrella sampling along the transition path, which reduces the computational cost greatly.

We will introduce a Finite-Temperature Dimer Method to find saddle points on the free energy surface efficiently. Then a relaxation dynamics can be used to obtain the transition path in the phase space approximately. With multi-dimensional umbrella potentials of the reaction coordinates, we can obtain sample data along the transition path. A newly developed free energy analysis method Welsam (Weighted least square analysis method) is then used to obtain the free energy profile along the transition path.

Reference

- [1] H. Zhang, L. Qiu, and D. Hu, “*Finite-Temperature Dimer Method for Finding Saddle Points on Free Energy Surfaces*”, J. Comput. Chem., DOI: 10.1002/jcc.25824, (2019).
- [2] X. Guan, D. Wei, and D. Hu, “*Free Energy Calculation of Transmembrane Ion Permeation: Sample with a Single Reaction Coordinate and Analysis along Transition Path*”, J. Chem. Theory Comput. 15:1216-1225, (2019).
- [3] D. Hu, X. Guan, and Y. Wang, “*Weighted Least Square Analysis Method for Free Energy Calculation*”, J. Comput. Chem., 39(28):2397-2404, DOI: 10.1002/jcc.25580, (2018).
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Volume entropy and information flow in brain networks: in case of tinnitus in subjects with hearing loss

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ABSTRACT

Brain regions send and receive information through neuronal connections in an efficient way. However, when these brain networks are organized in an abnormal way, a symptom-generating pathologic network may be generated. In this regard, based on the fact that only some of subjects with hearing loss develop tinnitus, we conjecture that subjects with hearing loss and tinnitus (HL-T) may be different from subjects with hearing loss without tinnitus (HL-NT) with regard to the cortical network property. This assumption prompted us to conduct the current study comparing the HL-T group and the HL-NT group with regard to volume entropy and inflow using a relatively large quantitative electroencephalography (qEEG) data.

We use volume entropy and the weights on vertices and edges, as well as other type of entropy-like invariants in modeling the brain networks of various populations including tinnitus and hearing loss using EEG. Volume entropy of a metric graph, a global measure of information, measures the exponential growth rate of the number of network paths. On the other hand, weight vectors of nodes and edges, which are local measures of information, represent the stationary distribution of information propagation in brain networks.

Reference

[1] Seonhee Lim, “Minimal volume entropy”, Transactions of the American Mathematical Society, Vol. 360 (10), 2006, pp. 5089-5100.

[2] A. Mohan, D.D. Ridder, S. Vanneste “Emerging hubs in phantom perception connectomics”. NeuroImage: Clinical, Vol. 11 (2016), 181-194.

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Complex networks of human mobility and their applications

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Development of the network science has provided new insights into geographical systems [1]. As the interaction and the correlation of quantities between geographical regions are essential in the geographical systems [2], it is expected that tools developed in the network science are applicable to such systems. Geographical structures of human mobility in urban regions play a crucial role in the human society. Economic activities are based on the efficient transportation of people, spread of infectious diseases takes place due to heterogeneous individual mobility patterns, and reaction to rare events such as evacuations after disasters is identified as the change in mobility patterns. Therefore, the human mobility has been intensively studied in the network science [3].

Mobile devices provide us new possibilities of recording a huge amount of real data regarding the human activities. As for the human mobility, location information is available using GPS data or a location of a base station connected with a caller (Call Detail Records). Additional information may be available, e.g. tweet data for social networking services, receiver information which reflects friendship relations between users. Some aspects of the human mobility can be expressed as networks, e.g. origin-destination matrix of the traffic flow across regions.

In this talk, examples of the network analysis of the human mobilities and possible applications are presented. Features of contacts of people is revealed through the analysis of the human mobility data, where the percolation transition is present [4]. A disease can spread on this time-dependent contact networks. In addition to the numerical simulations, an analytical approach to estimate the final size of the infection from the network topology is presented. Based on this method, risk of infection can be computed. Extension to the networks of the longer time scale is discussed.

Quantification of the aggregated mobility flow between regions in the urban area is important for intuitively understanding the geographical structure of the human mobility. The mobility data can be aggregated within certain geographical units, e.g. grid squares. A network community detection algorithm is applied to the origin-destination matrix derived from the human mobility data [5]. Hierarchical communities detected by this algorithm consist of units which locate geographically close. Some borders between communities are characterized by natural objects such as mountains and rivers. Infrastructures such as railroads and bridges are also relevant to the community structures.

Finally, a generative model which reproduces the spatial population distribution and a possible application of these methods to the analysis of the public health data are discussed.

Reference

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- [3] H. Barbosa-Hilfo et al., Phys. Rep. 734, 1 (2018).
- [4] N. Fujiwara, A.R. Sonawane, K. Iwayama, and K. Aihara, arXiv:1512.01901.
- [5] S. Fujishima, N. Fujiwara, Y. Akiyama, R. Shibasaki, and H. Kaneda, CSIS Discussion Paper No. 150.

Nematic liquid crystal flows in an applied magnetic field

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Liquid crystal is an intermediate phase of matter between liquid and solid states. When a sufficiently strong external field such as magnetic and electric fields is applied to liquid crystals, the orientation of liquid crystals is easily aligned along the direction of the external field. In this talk, we consider global solutions to the Ericksen-Leslie system modeling the hydrodynamic flow of nematic liquid crystals. In the presence of an applied magnetic field, we discuss dynamical instabilities of global solutions to the Ericksen-Leslie system due to magnetic fields in dimension two.

Reference

- [1] Chen, Yuan; Kim, Soojung; Yu, Yong, Freedericksz transition in nematic liquid crystal flows in dimension two. *SIAM J. Math. Anal.* 50 (2018), no. 5, 4838–4860.
- [2] Kim, Soojung; Pan, Xing-Bin, Anisotropic nematic liquid crystals in an applied magnetic field, preprint.

Constructing Reeb graphs from discrete data and its application to topological flow data analysis

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Topological data analysis attracts researchers in many fields and it also plays important roles in fluid dynamics. Sakajo and Yokoyama have proposed a tree-representation theory for fluid dynamics in which we have one-to-one correspondence between labeled trees and generic 2D Hamiltonian flows under topological classification [1]. Since their theory is applicable to a wide range of physical phenomena, there is a rise in demand for an algorithm that converts given fluid data to tree-representations.

A Reeb graph of a real-valued function, which consists of certain topological features, is a central key to the conversion. Although there are several methods for constructing the Reeb graph in preceding studies, we propose a new discrete formulation so that the derived algorithm achieves certain mathematical properties. Because our formulation is based on persistent homology in topological data analysis, our algorithm admits a stability theorem. Furthermore, we also establish a consistency theorem that bridges a gap between discrete data and continuous data. Thanks to these nice properties we can effectively construct a tree-representation from discrete fluid data.

In this presentation, we give some application examples of tree-representations obtained by the proposed method.

Reference

- [1] T. Sakajo and T. Yokoyama, Tree representation of topological streamline patterns of structurally stable 2D Hamiltonian vector fields in multiply connected domains, *The IMA Journal of Applied Mathematics*, vol. 83 pp. 380--411 (2018) (doi: 10.1093/imamat/hxy005)
- [2] T. Uda, T. Yokoyama and T. Sakajo, Algorithms converting streamline topologies for 2D Hamiltonian vector fields using Reeb graphs and persistent homology, in print (in Japanese).

A Nonlinear Moment Model for Radiative Transfer Equation in Slab Geometry

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We study the approximation of the radiative transfer equation for a grey medium in the slab geometry by the moment method. We develop a novel moment model inspired by the classical P_n model and M_n model. The new model takes the ansatz of the M_1 model as the weight function and follows the primary idea of the P_n model to approximate the specific intensity by expanding it around the weight function in terms of orthogonal polynomials. The weight function uses the information of the first two moments, which brings the new model the capability to approximate an anisotropic distribution. Mathematical properties of the moment model are investigated, and particularly the hyperbolicity and the characteristic structure of the Riemann problem of the model with three moments are studied in detail. Some numerical simulations demonstrate its numerical efficiency and show its superior in comparison to the P_n model.

Poster Presentations

- P-1. Yasumasa Nishiura (Tohoku University)**
“Mathematical descriptors in materials science”
- P-2. Hiroshi Kokubu(Kyoto University)**
“Switching systems and global dynamics of regulatory networks”
- P-3. Takeshi Sakajo (Kyoto University)**
“Vortex Dynamics on the surface of a torus”
- P-4. Seirin-Lee Sungrim (Hiroshima University)**
“Regionality-based optimal policy to reduce empty houses, Akiya, in Japan”
- P-5. Takeshi Watanabe (Suwa University of Science)**
“Dynamics of multiple collision among traveling spots in a field with and without heterogeneity”
- P-6. Yoshiki Sugitani (Tohoku University)**
“Deep Learning with Imbalanced Datasets for Anemia Treatment in Hemodialysis Patients”
- P-7 Tomohiro Nakahara (Hiroshima University)**
“The effect of cell geometry on polarity formation”
- P-8 Joon-Hyun Song (Handong Global University)**
“Analysis of the robustness against mutations by the arrangement of superpositioning transcription factor binding sites”
- P-9 Yong-Gwan Ji (Inha University)**
“Spectral properties of the Neumann-Poincar'e operator and M"obius transformation”

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