JSPS A3 Foresight Program "Modeling and Simulation of Hierarchical and Heterogeneous Flow Systems with Applications to Materials Science III"

November 14-16, 2016
TOKYO ELECTRON House of Creativity
Sendai, Japan

Organized by

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

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Sponsored by

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 III"

Date: November 14 (Mon) – November 16 (Wed), 2016
Venue: TOKYO ELECTRON House of Creativity
Sendai, Japan

<u>Schedule:</u>   <u>November 14 (Mon)</u>

08:30 – 09:20   **Registration at 3rd floor of TFC**

Chair: Pingwen Zhang

09:20 – 09:30   **Opening**

09:30 – 10:20   **1 : Hyeonbae Kang (Inha University, Korea)**
The spectral theory of the Neumann-Poincare operator, plasmon resonance, and anomalous localized resonance; a survey

10:20 – 10:50   **2 : Kazunori Ando (Ehime University, Japan)**
Analysis of plasmonic resonance on smooth domains using the spectral properties of the Neumann-Poincaré operator

10:50 – 11:10   **Coffee break**

11:10 – 11:40   **3 : Karel Svadlenka (Kyoto University, Japan)**
Mathematical challenges in tissue formation related to interface network dynamics

11:40 – 12:10   **4 : Xueying Huang (Xiamen University, China)**
3D Thin-Layer Structure Only Models for Coronary Atherosclerotic Plaques

12:10 – 14:00   **Lunch at Hagi restaurant**

Chair: Yasumasa Nishiura

14:00 – 14:50   **5 : Ruo Li (Peking University, China)**
On Hyperbolic Moment Models for Kinetic Equation

14:50 – 15:20   **6 : Emerson G. Escolar (Tohoku University, Japan)**
An Introduction to Quiver Representation Theory for Topological Data Analysis

15:20 – 15:40   **Coffee break**

15:40 – 16:10   **7 : Lei Zhang (Peking University, China)**
Recent Developments in Computational Modeling of Nucleation in Phase Transformations

16:10 – 16:40   **8 : Ah-Ram Kim (Handong Global University, Korea)**
Killing of escaped living modified organisms: Integrating a suicidal circuit into bacteria

16:40 – 17:10   **9 : Yuan Yao (HKUST & Peking University, China)**
Linearized Bregman Path Algorithms — Statistical Consistency and New Applications

Schedule: November 15 (Tue)

Chair: Hyeonbae Kang

09:30 – 10:20   **10 : Hisashi Okamoto (Kyoto University, Japan)**
Some applications of very accurate numerical methods in fluid mechanics

10:20 – 10:50   **11 : Sung-Ik Sohn (Gangneung-Wonju National University, Korea)**
Fluid-structure interactions and vortex dynamics

10:50 – 11:10   **Coffee break**

11:10 – 11:40   **12 : Donghyun You (Pohang University of Science and Technology, Korea)**
Continuum modeling of nonlinear deformation and aggregation of red blood cells

11:40 – 12:10   **13 : Masao Doi (Beihang University, China)**
Variational Principle in Dynamics

12:10 – 13:00   **Lunch at Hagi restaurant**

Chair: Lei Zhang

13:30 – 14:20   **14 : Seung Yeal Ha (Seoul National University, Korea)**
Collective synchronization of classical and quantum oscillators

| 14:20 – 14:50 | **15 : Hui Zhang (Beijing Normal University, China)** |
| | Mathematical problems in soft matter like hydrogel |

| 14:50 – 15:10 | **16 : Hisashi Naito (Nagoya University, Japan)** |
| | Carbon structures and trivalent discrete surfaces |

15:10 – 15:30	**Coffee break**
15:30 – 17:30	**Poster Session**
18:30-	**Banquet**

Schedule: November 16 (Wed)

Chair: Hisashi Okamoto

| 10:00 – 10:30 | **17 : Jinhae Park (Chungnam National University, Korea)** |
| | A study of ferroelectric liquid crystals in a thin film |

| 10:30 – 11:00 | **18 : Jun-ichi Fukuda (National Institute of Advanced Industrial Science and Technology, Japan)** |
| | Exotic ordered structures of a spatially confined chiral liquid crystal |

11:00 – 11:10	**Coffee break**
11:10 – 12:00	**Discussion**
12:00 – 13:00	**Lunch at Hagi restaurant**
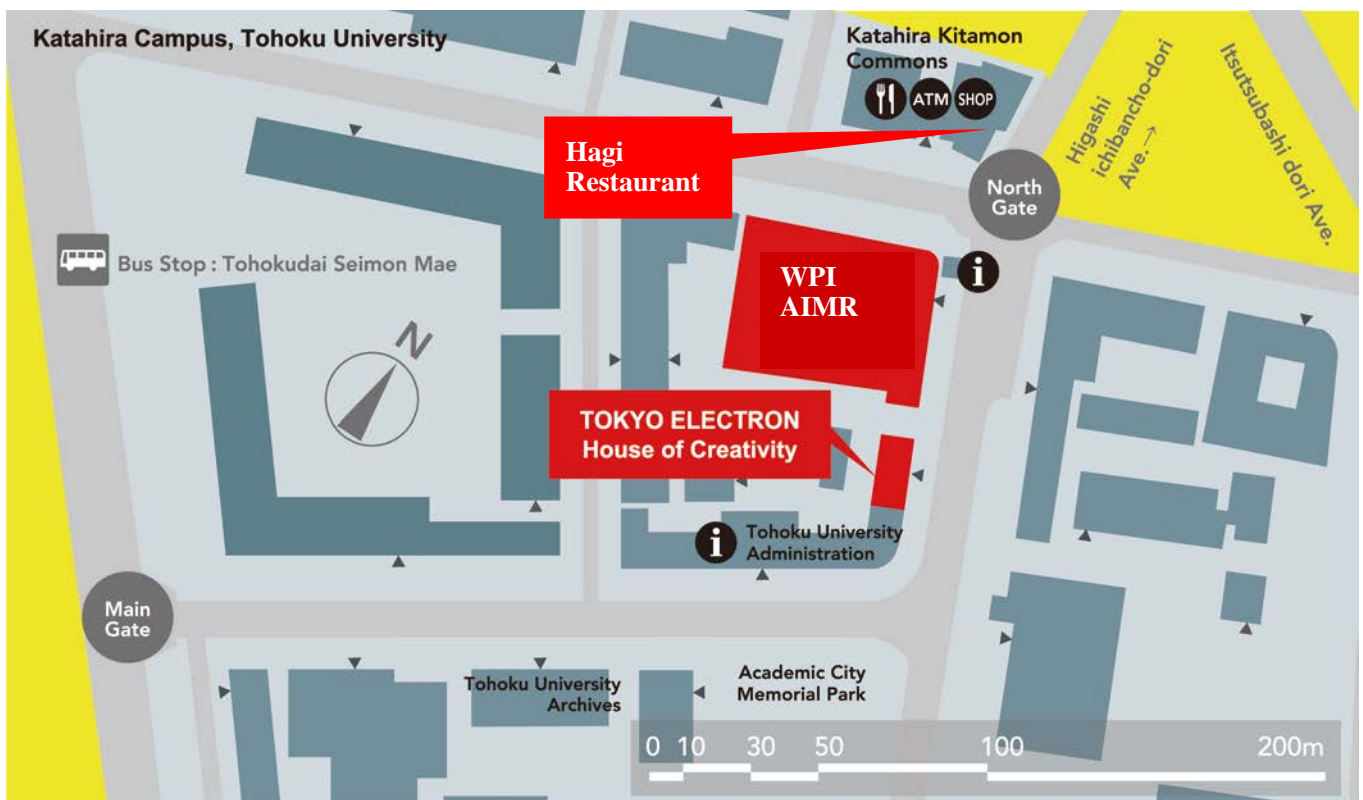
Abstracts

The spectral theory of the Neumann-Poincare operator, plasmon resonance, and anomalous localized resonance; a survey

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On the surface of dielectric materials with the negative dielectric constant a resonance occurs. This resonance is called the surface plasmon resonance and is underlying physical phenomenon of important imaging modalities such as SERS (surface enhanced Raman spectroscopy). It turns out that the Plasmon resonance is closely related to the spectrum of the Neumann-Poincare (NP) operator defined on the surface. In this talk I will explain the connection of the plasmon resonance and the spectrum of the NP operator and review recent development in the spectral theory of the NP operator. The NP spectrum is also closely related to the anomalous localized resonance which attracts much attention in connection with the invisibility cloaking. I will explain this as well.

Reference

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Analysis of plasmonic resonance on smooth domains using the spectral properties of the Neumann-Poincaré operator

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We study plasmonic resonance on bounded simply connected domains with smooth boundary in two and three dimensions using the spectral properties of the Neumann-Poincaré (NP) operator. It has been known that plasmonic resonance is deeply related to the spectrum of NP operator. The resonance at the essential spectrum is known as anomalous localized resonance (ALR). Using the quasi-static approximation, we show that in a sense ALR is weaker than the resonance at the eigenvalues. It is quite difficult to compute the exact strength of ALR on general domains. We study two specific case: ellipses in two dimensions and balls in three dimensions. We show that ALR occurs for ellipses in two dimensions and compute the asymptotic behavior of the resonance, and that ALR does not occur for balls in three dimensions. Finally, we validate the quasi-static approximation for the plasmonic resonance at the eigenvalues.

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[1] K. Ando and H. Kang, "Analysis of plasmon resonance on smooth domains using spectral properties of the Neumann-Poincaré operator", *J. Math. Anal. Appl.*, **435**, 162-178 (2016).

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Mathematical challenges in tissue formation related to interface network dynamics

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In this survey talk we present several examples of problems in tissue morphogenesis and tissue formation that were solved or are thought to be approachable by mathematical theories and computational techniques.

Some examples are the role of morphogens in embryo evolution (scaling with the size of embryo), the formation of signaling centers such as shoots of plants (symmetry breaking), genetic clock in vertebrate segmentation (synchronization) or the possibility of diagnosis of various illnesses based on the images of the corresponding deformed tissues. Potential role of cell membranes in these processes will be considered and possible connections discussed to interfacial network dynamics studied by our group.

Reference

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[2] L.G. Morelli, K. Uriu, S. Ares, A.C. Oates, *Computational Approaches to Developmental Patterning*, Science Vol. 336, pp. 187-191, 2012.

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3D Thin-Layer Structure Only Models for Coronary Atherosclerotic Plaques

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Mechanical forces play an important role in vulnerable plaque rupture process which is often associated with drastic cardiovascular syndromes such as heart attack and stroke. MRI-based Fluid-structure interactions (FSI) models for atherosclerotic plaques have been developed to perform mechanical analysis to investigate the association of plaque wall stress (PWS) with coronary artery disease. However, the complex deformable plaque structure and high non-linear material properties increased the difficulty of the construction of FSI model significantly. What's more, it's very difficult to obtain convergence due to the complexity of the model.

In this study, a 3D thin-layer structure only (TLS) model was proposed to perform mechanical analysis for human atherosclerotic plaques. In this study, a 3D thin-layer structure only (TLS) plaque model was proposed as an approximation with much less computational cost to 3D FSI models for better clinical implementation potential. For each 2D slice, the neighbored slices were used to construct the corresponding TLS model. Both the artery wall and the plaque components were assumed to be hyperelastic, isotropic, incompressible, and homogeneous. Plaque wall stress was extracted from all nodal points on the lumen surface of each plaque for analysis. The maximum value of Plaque wall stress (MPWS) and average value of plaque wall stress (APWS) of each slice were used to compare with those from corresponding FSI models. The relative errors for MPWS and APWS were 9.76% and 9.89%, respectively. Both MPWS and APWS values obtained from TLS models showed very good correlation with those from 3D FSI models. Correlation results from TLS models were consistent with FSI models.

Our results indicated that the proposed 3D TLS plaque models may be used as a good approximation to 3D FSI models with much less computational cost. With further validation, 3D TLS models may be possibly used to replace FSI models to save time and perform mechanical analysis for atherosclerotic plaques for clinical implementation.

On Hyperbolic Moment Models for Kinetic Equation

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In this talk, I will introduce the theory of the moment model reduction of Boltzmann equation we developed in recent years, together with the latest progress. By our exploration, it was found that the hyperbolicity of the reduced moment model can always be achieved, and the method provides us a symmetric hyperbolic system that the local wellposedness of the reduced model is not a problem anymore.

An Introduction to Quiver Representation Theory
for Topological Data Analysis

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In this talk, we give an overview of the use of the representation theory of quivers in topological data analysis, particularly in persistent homology and its generalizations. We review classical persistence [1] and zigzag persistence [2], where persistence modules can be viewed as representations of an underlying A_n-type quiver. We then discuss persistence modules on commutative ladder quivers of finite type [3]. We show that the persistence diagrams can be generalized to this setting by using Auslander-Reiten quivers, and provide some motivating examples for their interpretation and applications.

References

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Recent Developments in Computational Modeling of Nucleation in Phase Transformations

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Nucleation is one of the most common physical phenomena in physical, chemical, biological and materials sciences. Due to the difficulties and challenges in making direct experimental observation, many computational methods have been developed to model and simulate various nucleation events. In my talk, I will provide a sampler of some newly developed numerical algorithms that are widely applicable to many nucleation and phase transformation problems. I first describe some recent progress on the design of efficient numerical methods for computing saddle points and minimum energy paths, and then illustrate their applications to the study of nucleation events associated with several different physical systems. Nucleation is a complex multiscale problem. Development of efficient numerical algorithms and modeling approaches is bringing new light to this challenging subject.

Killing of escaped living modified organisms: Integrating a suicidal circuit into bacteria.

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Abstract

Living modified organisms (LMOs) generated from various biological experiments and biotechnology industries pose potential risks to biological diversity in our ecosystem. International efforts, such as the Cartagena Protocol on Biosafety, have been made to prevent possible harm from LMOs. However, practical solutions for blocking LMO leakage remain elusive. To this end, we developed a suicidal genetic circuit to kill modified bacteria when they escape a preset condition such as a laboratory. We designed the circuit to contain two separable modules called the 'sensing module' and 'killing module'. The sensing module detects the existence of a 'synthetic survival factor (SSF)' that is only provided in a preset condition and serves as a repressive signal to the killing module. When SSF is absent, the killing module produces a toxic protein to kill the bacteria. To prove this concept, IPTG inducible promoter and cI repressor from λ phage were used to construct a sensing module. In the killing module, cI unbound promoter activates the production of a toxic protein, T4 endolysin. The suicidal genetic circuit with exchangeable modules enables customized applications to various organisms.

Linearized Bregman Path Algorithms — Statistical Consistency and New Applications

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Estimate or recovery of sparse parameters from their noisy measurements is a fundamental problem in high dimensional statistics and compressed sensing, etc. In the past two decades, convex regularization approach such as LASSO or BPDN has been made popular for its algorithmic tractability. However, a well-known shortcoming of LASSO and any convex regularizations lies in the bias of estimators, which motivates further investigation of nonconvex regularization yet suffering the computational hurdle. Here we bring an idea based on some dynamics developed in applied mathematics to address this challenge in statistics. Such dynamics can be shown to traverse a path passing through the oracle estimator, an unbiased estimate of the true parameter whose entries have the same signs as those of the true signs, while the LASSO regularization path always deviates from that due to its bias. A discretization of the dynamics leads to the Linearized Bregman iteration algorithm, which is a simple iterative thresholding rule and easy to parallelize in favor of big data analysis. This approach adapts to various sparse regularizations, including logistic regression, fused lasso, matrix regression, and graphical models etc. In particular, equipped with variable splitting for structural sparsity, it leads to improved model selection consistency than generalized LASSO in both theory and applications. New application examples will be demonstrated in statistical ranking, social networks, and computational biology etc., together with a new R package — Libra.

Some applications of very accurate numerical methods in fluid mechanics

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There are a variety of numerical problems in fluid mechanics. Some involve singular (discontinuous) or nearly singular functions, and some involve highly oscillatory functions. In this talk I will show some examples in which I encountered serious difficulty. Here stress is placed on accuracy and not speed of computation. Keywords are: double exponential transform, numerical verification, and FFT.

Reference

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Fluid-structure interactions and vortex dynamics

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In this talk, I present the modelling of fluid-structure interactions by the vortex dynamics. First, I discuss on the recent development of vortex shedding models. The vortex separated from a solid is one of the most important problems in fluid dynamics. However, an unsteady vortex shedding model was presented only recently [1]. A key issue here is the modeling of the unsteady Kutta condition, which regularizes the point of velocity infinity. Applications to aerodynamics and biofluids, and the limitation of the vortex shedding model are also discussed.

Secondly, I discuss on the vortex dynamics on a rotating sphere, which is a joint work through A3 program. There have been research attempts to explain atmospheric phenomena by the vortex dynamics [2]. We consider a barotropic vortex patch and strips on a rotating sphere, in order to investigate the stability of the cold region in the north pole and the jet stream. We discuss briefly on the linear stability and results of numerical computations for the two problems.

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Continuum modeling of nonlinear deformation and aggregation of red blood cells

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For precise prediction of rheology of an isolated red blood cell (RBC) and a group of multiple RBCs, continuum mathematical models for describing nonlinear mechanical properties of cellular structures of an RBC and inter-cellular interactions among multiple RBCs are developed [1]. The viscoelastic behavior of an RBC membrane is determined using a generalized Maxwell model for loading and unloading conditions. The present viscoelasticity model is capable of predicting both of stress relaxation and stress–strain hysteresis, of which prediction is not possible using the commonly used Kelvin–Voigt model [2, 3]. Nonlinear elasticity of an RBC is determined using the Yeoh hyperelastic material model using finite-element approximation. Based on the physical models of electrostatic and depletion energy [4], a novel method to model inter-cellular interactions among multiple adjacent RBCs is also developed. Simulations for elongation and recovery deformation of an RBC and for aggregation of multiple RBCs are conducted to evaluate the efficacy of the present continuum modeling methods. Recently, Yoon et al. [5] and Puig-de-Morales-Marinkovi et al. [6] found that viscoelastic properties of an RBC membrane under periodic loading conditions follow a fractional power-order, which behavior cannot be modeled with the classical linear elements in time and frequency domains. Craiem and Magin [7] shows possibility of the fractional derivative to model the power-law behaviors of an RBC in time and frequency domains mathematically. The fractional derivative is a non-local operation which is computationally intensive due to inclusion of the accumulated contribution of function values. In order to reduce the computational load while maintaining the accuracy of the fractional derivative, a novel numerical method for the Caputo fractional derivative is developed. The present adaptive memory method significantly reduces the requirement for the computational memory for storing function values at the previous times and also significantly improves the accuracy by calculating convolution weights to function values at the previous time steps which can be non-uniform. The superior accuracy of the present method to the previously reported methods [8, 9] is revealed by deriving numerical errors analytically.

Reference

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Variational Principle in Dynamics

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Many equations describing the dynamics of soft matter are derived from a variational principle proposed by Onsager in his celebrated paper on the reciprocal relation[1,2, 3]. This includes Stokes equation for hydrodynamics, Smoluchowskii equation for Brownian motion, Cahn-Hilliard equation for phase separation (model H), elasto-diffusion equation for gels, Leslie-Ericksen equation for liquid crystals etc. Here I discuss how this principle is useful in solving practical problems and the implication of this principle.

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8. A Principle in Dynamic Coarse Graining - Onsager Principle and its Applications -, Masao Doi,   DOI 10.1140/epjst/e2016-60128-5, EPJE (2016)

Collective synchronization of classical and quantum oscillators

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Synchronization of weakly coupled oscillators is ubiquitous in biological, chemical and physical complex systems. Recently, research on collective dynamics of many-body systems has been received much attention due to their possible applications in engineering. In this survey talk, we mainly focus on the large-time dynamics of several synchronization models and review state-of-art results on the collective behaviors for synchronization models. Following a chronological order, we begin our discussion with two classical phase models (Winfree and Kuramoto models), and two quantum synchronization models (Lohe and Schrodinger-Lohe models). For these models, we present several sufficient conditions for the emergence of synchronization using mathematical tools from dynamical systems theory, kinetic theory and partial differential equations in a unified framework.

Reference

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Mathematical problems in soft matter like hydrogel

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Hydrogel is a kind of polymeric materials, have attracted some theoretical and experimental studies. The new hydrogel predominately consists of MMS (macromolecular microsphere), chains and water molecules, which shapes its well-defined structure and high mechanical strength. But, how is it phase transition and forming these well-defined micro-structure? Why the hydrogels have such high mechanical strengths?

what is the structure-property relationship? How do the structural factors affect, such as nanoparticle size, grafting density, polymer chain length, entanglement, and so on? Here we will review some mathematical progress to partly answer them, including phase transition, micro-structure, macro-property and related numerical methods. Meanwhile, we also present some mathematical problems to be solved.

# Carbon structures and trivalent discrete surfaces

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We discuss geometries of trivalent discrete surfaces. In particular, a definition of Gauss and mean curvatures and subdivision of given trivalent discrete surface. A trivalent discrete surface is a mathematical model of sp2 carbon structures (C60, single wall carbon nanotubes, negatively curved fullerens).

In this talk, we illuminate negatively curved fullerens (Mackay type crystals). First we introduce constructions of new Mackay type crystals [1]. Next we talk about a definition of curvatures for trivalent discrete surfaces [2].
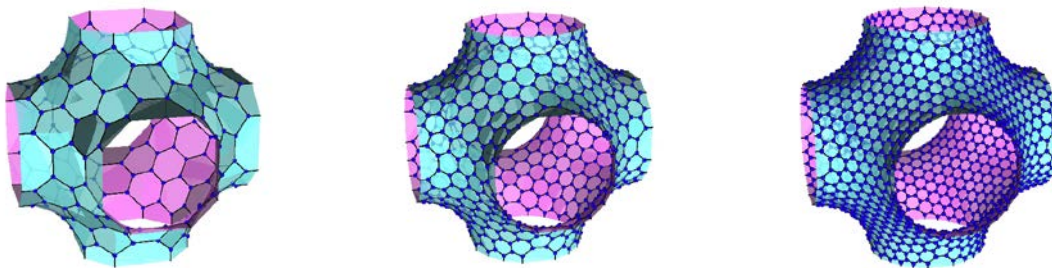
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A study of ferroelectric liquid crystals in a thin film

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In this talk, we consider a system of liquid crystals occupying a thin domain. A system of ferroelectric liquid crystals possesses the spontaneous polarization which gives fast rotation of molecules with respect to applied electric fields. Using the Landau-de Gennes theory, we discuss periodic structures and a homogenization problem for such a system.

Exotic ordered structures of a spatially confined chiral liquid crystal

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Because of the absence of mirror symmetry, chiral liquid crystals spontaneously adopt twisted local orientational order, and as a result exhibit various orientationally and/or positionally ordered structures [1]. The simplest non-trivial structure is a cholesteric phase with twisted order along a certain direction (helical axis) and uniform order along directions perpendicular to the helical axis. Cholesteric blue phases [1,2], far more complex than a cholesteric phase, comprise topological line defects of orientational order (disclinations) and so-called "double-twist" cylinders in which local orientational order is twisted along all the directions perpendicular to the cylinder axis. The complex structures of cholesteric blue phases arise from frustrations between the local energetic preference of double-twist ordering over a single twist of the cholesteric phase, and the inability of the double-twist ordering to fill the whole space retaining the energetic preference. Cholesteric blue phases have thus intrigued physicists as interesting examples of frustration-induced order of soft matter. Cholesteric blue phases are also regarded as promising photonic materials because typical periodicity of ordering is a few hundred nanometers, on the order of the wavelength of visible light.

Here we present our theoretical study on the structures of a chiral liquid crystal exhibiting cholesteric blue phases in the bulk when it is confined spatially between two parallel plates with small distance (Here "small" means that the spacing is of the order of or smaller than the periodicity of the orientational ordering in the bulk, typically a few hundred nanometers). Our study is based on a continuum theory describing the orientational order of the liquid crystal by a second-rank tensor. Numerical calculations reveal that various exotic ordered structures different from those in the bulk can form as thermodynamically stable structures, depending on the interaction between the liquid crystal and the confining surface (surface anchoring), distance between the two confining plates, and temperature. Such ordered structures include a parallel array of disclinations of double-helix form [3], a regular array of ring defects [4] , and a hexagonal lattice of Skyrmion-like excitations, swirl-like vectorial order without singularity at the center [5]. Our thin system of a chiral liquid crystal thus offers an interesting platform for the investigation of exotic ordering and excitations such as Skyrmions.

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Poster Presentations

P-1.   Yongqiang Cai (Peking University)
"Liquid Crystalline Phases of Self-Assembled Bilayers from Rod-Coil Diblock Copolymers"

P-2.   Gao Zhijun(Tohoku University)
"Dynamics of traveling pulse with oscillatory tails in heterogeneous media"

P-3.   Takeshi Gotoda (Kyoto University)
"Enstrophy dissipation in incompressible flow via singular vortex dynamics"

P-4.   Yucen Han (Peking University)
"Finding transition pathways of 2D nematic liquid crystal disk"

P-5.   Yong-Gwan Ji (Inha University)
"Spectral properties of the Neumann-Poincaré operator and cloaking by anomalous localized resonance for the elasto-static system"

P-6.   Soyoung Kim (Konkuk University)
"Mathematical model of transmission dynamics and optimal control strategies for 2009 A/H1N1 influenza in the Republic of Korea"

P-7   Koya Sakakibara (The University of Tokyo)
"Numerical conformal mappings by the dipole simulation method"

P-8   Yuuki Shimizu (Kyoto University)
"Vortex dynamics on a toroidal surface"

P-9   Joon-hyun Song (Handong Global University)
"Bacteria Programming: Developing Suicidal Circuit to Prevent LMO Leakage"

P-10   Yoshiki Sugitani (The University of Tokyo)
"Analysis of the immersed-boundary nite-element method for the Stokes problem"

P-11   Kuan Tao (Peking University)
"Exploring the inhibition effect of membrane tension on cell polarization"

P-12   Keiichi Ueda(University of Toyama)
"Differentiation of behavioral type induced by environmental variations in an amoeba"

P-13   Yiwei Wang (Peking University)
"Defect structures around spherical particles in a nematic liquid crystal"

P-14   Daegeun Yoon (POSTEC)
"Nonlinear modeling of viscoelasticity and aggregation energy of red blood cells"

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