A3 Workshop on Soft Matter 2019
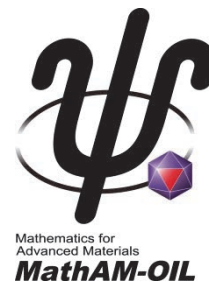

Date: 30 May-1 June 2019
Venue: WPI-AIMR, Tohoku University, Sendai
Organizer:
Masao Doi (Beihang University), Yasumasa Nishiura(Tohoku University), Jinhae Park (Chungnam National University), Yana Di (Chinese Academy of Sciences), Xianmin Xu (Chinese Academy of Sciences), Natsuhiko Yoshinaga (Tohoku University, AIST),

Program

30 May

11:30 Registration

11:45 – 13:15 Lunch at Hagi restaurant

13:20
"Opening"

13:30 - 14:30   Yoshinobu Kawahara (Kyushu University)
                Operator Theoretic Analysis of Dynamical Systems and Dynamic Mode Decomposition

                (Coffee Break)

14:45 - 15:45   Haijun Yu (CAS)
                Phase-field modeling, analysis and numerical simulation of multi-phase fluids with moving contact lines

                (Coffee Break)

16:00 – 17:00   Chihiro Urata　(AIST)
                Siloxane Based Inorganic-Organic Hybrid Materials for Liquid-Repellent Surfaces

31 May

9:30 – 10:30   Yana Di (CAS)
                An Energy Stable method for Q-tensor Hydrodynamic Model of Nematic Liquid Crystal Flows

                (Coffee Break)

10:45 – 11:45   Rhudaina Z. Mohammad (Kyoto University)
                Modeling cell-to-cell adhesion dynamics in multicellular organisms

11:45 – 13:15   Lunch at Hagi restaurant

13:15 – 14:15   Xianmin Xu (CAS)
                Numerical simulations and analysis for wetting on rough surfaces

                (Coffee Break)

14:30 – 15:30   Shinichi Ito (University of Tokyo)

Uncertainty quantification for massive simulation models based on a second-order adjoint method

(Coffee Break)

15:30 – 16:30   Hirofumu Notsu (Kanazawa University)
A mass-conservative Lagrange-Galerkin scheme of second-order in time with adaptive mesh refinement and its application

(Coffee Break)

16:45 – 17:45   Jinhae Park (Chungnam National University)
Mathematical Theory of Ferroelectirc Liquid Crystal

18:30 -   Banquet at Biwane
https://www.hotpepper.jp/strJ000705369/map/

1 June
9:30 – 10:30   Uyen Lieu (MathAM-OIL, AIST)
Numerical Simulation of Assembly of Patchy Particles Confined to Spherical Surface

(Coffee Break)

10:45 – 11:45   Xu Ye (Beihang University)
Imaging complex behaviors of dense particle suspension: packing, fracturing, and fluid transport

11:45 - 13:15   Lunch at Hagi restaurant

13:15 - 14:15   Narina Jung (UNIST)
Collective Behavior of Flocks in a Marginalized Ordering State

(Coffee Break)

14:30 - 15:30   Natsuhiko   Yoshinaga   (AIMR   Tohoku   University, MathAM-OIL AIST)

Model Selection of PDE for Targeted Crystalline Patterns
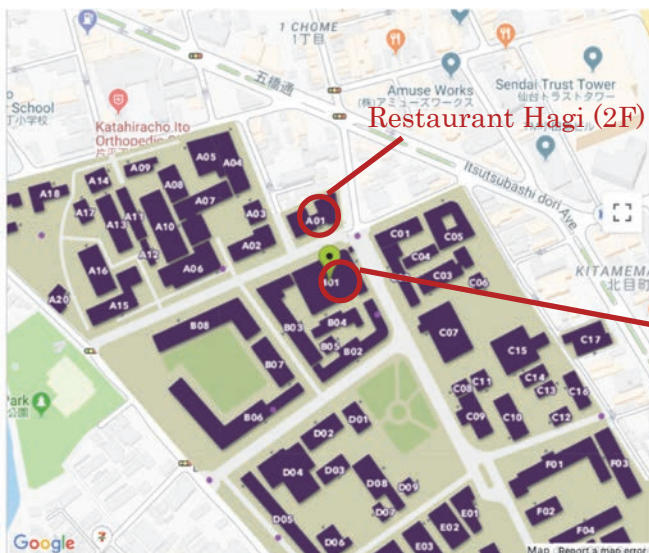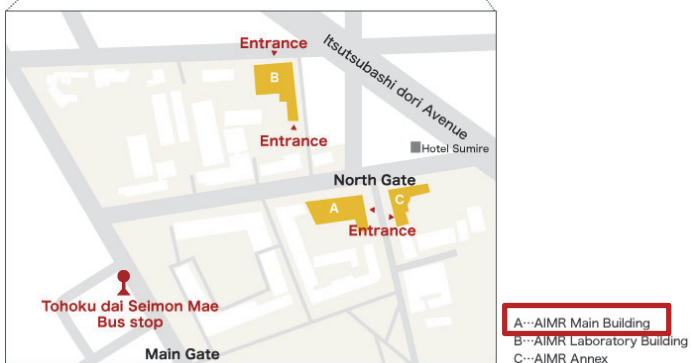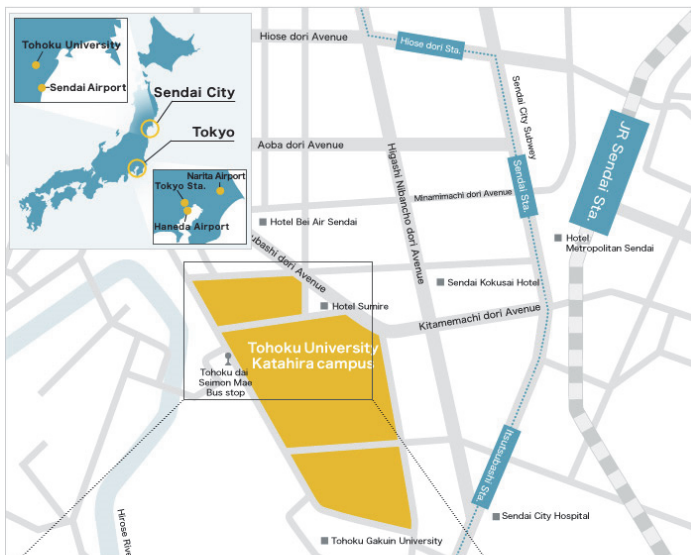
(Coffee Break)

15:30 – 16:30   Round   Table   Discussion   (session   organiser: Natsuhiko Yoshinaga)

Access

2F Meeting Room in AIMR Main Building, Katahira Campus, Tohoku University

Detailed information is available in:

https://www.wpi-aimr.tohoku.ac.jp/en/about/access/

A···AIMR Main Building
B···AIMR Laboratory Building
C···AIMR Annex

Restaurant Hagi (2F)

AIMR Main Building

Abstract

Operator Theoretic Analysis of Dynamical Systems and Dynamic Mode Decomposition

Yoshinobu Kawahara (Kyushu University)

Operator-theoretic methods provide a link to the large collections of mathematical tools related to geometrical properties of a dynamical system in its analysis, and data-driven algorithms for the analysis, such as dynamic mode decomposition (DMD), has attracted much attention in various scientific fields in a decade. In particular, Koopman operator plays an important role in the analysis because the spectral analysis of the operator directly gives physical interpretations of evolution equations. In this talk, I first overview the basic idea behind operator-theoretic analysis of dynamical systems, focusing on the one with transfer operators including Koopman operator, and then give brief reviews on DMD and its variants. Then, I describe some of our related works such as DMD using machine learning techniques and the application of DMD-type methods to analyses of collective motions.

Phase-field modeling, analysis and numerical simulation of multi-phase fluids with moving contact lines

Haijun Yu (Academy of Mathematics and Systems Science, Chinese Academy of Science)

Phase-field model is one of the major tools to deal with multi-phase fluids and the moving contact line problem. In this talk, we investigate the moving contact line problem in multi-phase fluids by using a phase-field model proposed by Qian et al in 2013, which consists of incompressible Navier-Stokes equations with a generalized Navier boundary condition and Cahn-Hilliard equation with a dynamic contact line condition. We design several energy stable first order and second order time discretization schemes for the coupled nonlinear PDE system with matched densities and non-matched densities. The developed schemes are used to verify the convergence of the sharp-interface limits of the phase-field model. We will

also discuss a phase-field model approach for moving contact line problem in multi-phase complex fluids.

Siloxane Based Inorganic-Organic Hybrid Materials for Liquid-Repellent Surfaces

Chihiro Urata (AIST)

Keywords: bio-inspired surfaces, organogel, secretion, anti-stick, omniphobicity

Functional coatings with exceptional surface properties, such as liquid-repellency and low-friction/adhesion, have been commonly prepared by combining textured surfaces with long-chain perfluori-nated compounds (LPFCs) [1]. However, unfortunately, the chemical and physical effects of the LPFCs on human health and environment have been viewed lately with concern [2]. In addition, perfluorinated com-pounds emit corrosive and toxic gasses when they are overheated (above ca. 260 °C). Thus, an alternative approach not requiring LPFCs has is strongly demanded.

Here, we introduce our recent developments for the preparation of eco-friendly liquid-repellent coat-ings using several type of siloxane sources through a monolayer formation of polydimethylsiloxane[3,4], a simple sol-gel reaction using organosilanes[5-7], crosslinking reaction of modified silicones[8-10].

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An Energy Stable method for Q-tensor Hydrodynamic Model of Nematic Liquid Crystal Flows

Yana Di (Chinese Academy of Sciences)

Nematic liquid crystals are complex fluids that exhibit an orientational order on average in their molecular orientation, but do not normally possess any

positional order. The most popular mathematical model for flows of low molecular weight nematic liquid crystals is the Ericksen–Leslie model. This theory describes uniaxial symmetry in all flow geometries including the shear flow and at defects, neglecting any potential biaxiality. However, the Q-tensor, a second order tensor of trace zero, can be traced back to the deviatoric part of the second moment of a probability distribution function for the nematic liquid crystal system. The reflective symmetry of the system as well as biaxiality are naturally built in the tensor-based theories. And the Q-tensor nematic liquid crystal model obeys an energy dissipation law. In this talk, we develop an energy stable numerical scheme for a Q-tensor based hydrodynamic model of nematic liquid crystal flows. Then we study defect dynamics in flows of nematic liquid crystals in a channel. The numerical schemes are shown to be efficient in solving the Q-tensor based liquid crystal model.

Modeling cell-to-cell adhesion dynamics in multicellular organisms
Rhudaina Z. Mohammad (Graduate School of Science, Kyoto University)

We study the dynamics of multicellular aggregate formation driven by cell-to-cell adhesion as a surface energy gradient flow constrained by the preservation of cell volumes. Under this motion, an aggregate of a single cell type forms a hexagonal tessellation satisfying the symmetric Herring angle condition at triple cell junctions. Moreover, an aggregate of two cell types - as observed in sensory epithelial tissues consisting of sensory and supporting cells - expressing different types of cellular adhesion molecules (nectin and/or cadherin) form either a checkerboard-like, segregated, or football-like pattern. To realize this interface evolution problem, we consider a variation of the Merriman-Bence-Osher (MBO) algorithm in two folds: a vector-type variational approach to diffusion-thresholding scheme with volume penalization technique; and a convolution-redistribution scheme with localized auction dynamics considering topological constraint of preserving cell connnectivity. We present some preliminary numerical results on cellular pattern formation and simulation of developmental stages of an olfactory epithelial tissue.

Numerical simulations and analysis for wetting on rough surfaces

Xianmin Xu (Institute of Computational Mathematics, Chinese Academy of Sciences)

Wetting on rough surface is common in nature and industry applications. Mathematically, it is a free interface problem proposed in a domain with rough boundaries. Due to the complicated boundary conditions, numerical simulation for wetting problems is quite difficult. We introduce a volume preserving threshold dynamics method for wetting on rough surfaces, which is based on minimization of the weighted surface area functional over an extended domain that includes the solid phase. The method is simple, stable and quite efficient. It is not sensitive to the inhomogeneity or roughness of the solid boundary. The method is also improved to fulfill the local contact angle condition. We also show some mathematical analysis for the method. Finally, we also discuss the possibility to use the Onsager principle to approximate the dynamic wetting problem.

Uncertainty quantification for massive simulation models based on a second-order adjoint method

Shinichi Ito (University of Tokyo)

Data assimilation (DA) is a fundamental computational technique that integrates numerical simulation models and observational data based on the Bayesian statistics. Although the DA is now an accepted technique in various scientific fields, one key issue is the construction of DA algorithms in massive simulation models under the constraints of limited computational time and resource. In this study, we propose an adjoint-based DA algorithm for massive simulation models that produces optimum estimates and their uncertainties within reasonable computational time and resource constraints. The uncertainties are given as several elements of an inverse Hessian matrix, which is the covariance matrix of a normal distribution that approximates the target posterior probability density function in the neighborhood of the optimum. The proposed method based on a second-order adjoint method allows us to

directly evaluate the elements of the inverse Hessian matrix without computing all of its elements. Some numerical tests assuming a massive simulation model confirm that the proposed method works well and enables us to evaluate the uncertainties of the parameters involved in the assumed model faster than the conventional DA approaches.

A mass-conservative Lagrange-Galerkin scheme of second-order in time with adaptive mesh refinement and its application

Hirofumu Notsu
Kanazawa University, Faculty of Mathematics and Physics, Institute of Science and Engineering

We present a mass-conservative Lagrange-Galerkin scheme of second-order in time with adaptive mesh refinement (AMR) and apply it to two-fluid flow problems. For convection-diffusion problems, error estimates of second-order in time and the mass-conservation property have been proved. Numerical experiments are shown to see the theoretical results and the effectiveness of AMR.

Mathematical Theory of Ferroelectirc Liquid Crystal

Jinhae Park
Chungnam National University

Liquid crystal is a self-assembled media which is composed of anisotropic molecules. It has been used widely in a large variety of applications because it contains outstanding physical properties and is susceptible to electric fields. In particular, ferroelectric liquid crystals exhibit a spontaneous polarization which plays an important role in the system. In order to study such a phenomena, we consider the governing energy functional for smectic liquid crystals which include the classical Oseen Frank energy and the Chen-Lubensky energy. In this talk, we take a simplied energy functional and and investigate some properties of the direction field in the application of electric fields.

Numerical Simulation of Assembly of Patchy Particles Confined to Spherical Surface

Uyen Lieu (MathAM-OIL, AIST) and Natsuhiko Yoshinaga (Tohoku University and MathAM-OIL AIST)

Patchy colloidal particles are particles having patches on specific sites. Their interaction depends on not only the distance but also the mutual orientation of the particles. Such particles are capable of organising themselves into complex structures with novel properties, which are essential ingredients for materials design. On the other hand, controlling and predicting of defects are important because defects are inevitable in disordered-ordered transition, and often govern the function of materials. Curvature is considered as an external driving force to control defects and microstructure of the ordered state. However the relation of the curvature and the ordered structure is not fully understood.

The aim of this study is to understand the interplay between particle's degree of freedom and geometry/topology of the embedded space. The simulation is conducted by Brownian Dynamics. A general model for estimating the interaction of spherical patchy particles is developed based on spherical harmonics and irreducible tensors. We investigate the dynamics of defects and crystallisation of the dipole-like particles on spherical surface, then compare with the case that the particles are confined to planar geometry.

Imaging complex behaviors of dense particle suspension: packing, fracturing, and fluid transport

Xu Ye (School of Mechanical Engineering and Automation, Center of Soft Matter Physics and its Applications, Beihang University)

Dense particle suspension in commonly seen many industrial applications including paints, personal care products, and oil production. However, the behaviors of those dense particle suspension, particularly under flow, are rather complex and therefore difficult to model. In this talk, I will use two examples to show our experimental efforts to probe some of their complex

behaviors. The first one is the fracture in drying colloidal coatings. Combining in situ fluorescent imaging and a technique called Traction Force Microscopy, we reveal the underlying mechanism of the drying-induced fracture in colloidal coatings, as well as the effect of fluid transport in the deformation of packed particle networks. In the second example, we use a shear flow to prepare silver nanowire networks with various degree of alignment. We established a relation among shear rates, degree of alignment, and electrical and optical anisotropy in silver nanowire networks. Those experimental results will shed light in better understanding and modeling of complex behaviors of dense particle suspension under flow.

Collective Behavior of Flocks in a Marginalized Ordering State
Narina Jung (UNIST)

We develop a model for the rich dynamics of a flock in a marginalized ordering state. The aim is to present an inter-individual coordination mechanism that keeps a flock constantly ready to respond to perturbations naturally present in biological systems. We extend the generalized Cucker-Smale model with the coupling of acceleration, and introduce adaptive reaction times of each bird. We regard two key factors in the reaction times: (1) the local ordering state of each bird and (2) reaction sensitivity of a flock to the neighbor's momentum change with 1/kappa. We show that our model displays innate fluctuations that lead to rich dynamics as a reminiscent of natural flocks due to the adaptive reaction delay. This happens without relying on stochastic variables. We compute the correlation lengths of the fluctuations and find that the correlation of velocity and speed is scale-free, indicating some criticality of a flock. Surprisingly, at a large value of 1/kappa (i.e., reaction sensitivity is high), the transition occurs from the standard diffusion to the super-diffusive Levy flights as we increase the strength of the velocity alignment. Our results indicate that the emergence of long-term behaviors such as Levy flights can also be explained in terms of the inter-individual interaction that makes the system in a marginalized ordering state.

Model Selection of PDE for Targeted Crystalline Patterns

Natsuhiko Yoshinaga (AIMR Tohoku University, MathAM-OIL AIST)

Partial differential equations (PDE) have been widely used to reproduce patterns in nature, and to give an insight on the mechanism underlying pattern formation. Although enormous number of PDE models have been proposed, they rely on pre-request knowledge of physical laws and symmetries, and one has difficulties to develop a model to reproduce a given desired pattern. Here we show the order parameters extracting symmetries of a pattern together with Bayesian model selection successfully estimate parameters in a model as well as the best model to make the target pattern. We apply our method two-dimensional and three-dimensional nontrivial patterns, namely quasi-crystal with twelve-fold symmetry and double gyroid structure reproduced by using a family of generalised Swift-Hohenberg equations. Our method not only estimates the parameters to reproduce these patterns, but gives an insight on the appropriate number of length scales hidden in the patterns.