1st Joint Conference of A3 Foresight Program

Mathematics of Fluid Dynamics and Material Science

November 21-23, 2014
International Convention Center
Jeju, Korea

Organized by

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

Sponsored by

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

Time Table

A3-FM

Nov. 21, Friday		Nov. 22, Saturday	
9:10-10:00	KSIAM Plenary Lecture Haesun Park ICC Samda Hall	9:10-10:00	KSIAM Plenary Lecture Irene Fonseca ICC Samda Hall
10:20-12:00	Session 1 ICC Room 302	10:20-12:00	Session 4 ICC Room 302
1:00-2:40	Session 2 ICC Room 302	1:50-2:40	KSIAM Plenary Lecture Zhiming Chen ICC Samda Hall
4:00-5:40	Session 3 ICC Room 302	3:00-4:40	Session 5 ICC Room 302
6:00	Banquet ICC Delizia (3rd Floor)	5:00-6:30	Short Presentations ICC Room 302

Nov. 23, Sunday, 10:00-12:00
Discussion Session CoreaCondo Conference Hall

Participants

China

Yongqiang Cai	Graduate Student	Peking U.
Hongtao Chen	Assistant Professor	Xiamen U.
Huangxin Chen	Assistant Professor	Xiamen U.
Sheng Chen	Graduate Student	Xiamen U.
Yana Di	Associate Professor	Chinese Academy of Sciences
Masao Doi	Professor	Beihang U.
Kui Du	Associate Professor	Xiamen U.
Yu-wei Fan	Graduate Student	Peking U.
Yucheng Hu	Assistant Professor	Tsinghua U.
Can Huang	Assistant Professor	Xiamen U.
Zhiping Mao	Graduate Student	Xiamen U.
Ruo Li	Professor	Peking U.
Sirui Li	Graduate Student	Peking U.
Tiejun Li	Professor	Peking U.
Wei-ming Li	Graduate Student	Peking U.
Shimin Lin	Graduate Student	Xiamen U.
Jie Shen	Professor	Xiamen U.
Changtao Sheng	Graduate Student	Xiamen U.
Congmin Wu	Associate Professor	Xiamen U.
Lei Wu	Graduate Student	Peking U.
Jiechao Xiong	Graduate Student	Peking U.
Chuanju Xu	Professor	Xiamen U.
Qinwu Xu	Postdoc	Peking U.
Xianmin Xu	Assistant Professor	Chinese Academy of Sciences
Tetsuya Yamamoto	Research Associate	Beihang U.
Yuan Yao	Professor	Peking U.
Jingru Zhang	Graduate Student	Peking U.
Lei Zhang	Associate Professor	Peking U.
Pingwen Zhang	Professor	Peking U.

Japan

Emerson Escolar	Graduate Student	Kyushu U.
Zhijun Gao	Graduate Student	Tohoku U.
Elliott Ginder	Assistant Professor	Hokkaido U.
Takeshi Gotoda	Graduate Student	Kyoto U.
Yasuaki Hiraoka	Associate Professor	Kyushu U.
Hiroshi Kokubu	Professor	Kyoto U.
Motoko Kotani	Professor	Tohoku U.
Jun Masamune	Associate Professor	Tohoku U.

Yasumasa Nishiura	Professor	Tohoku U.
Hirofumi Notsu	Lecturer	Waseda Insitute for Advanced Study
Ippei Obayashi	Postdoc	Kyoto U.
Kiori Obuse	Assistant Professor	Tohoku U.
Norikazu Saito	Associate Professor	U. of Tokyo
Takashi Sakajo	Professor	Kyoto U.
Koya Sakakibara	Graduate Student	U. of Tokyo
Takiko Sasaki	Graduate Student	U. of Tokyo
Yoshiki Sugitani	Graduate Student	U. of Tokyo
Hiroshi Suito	Professor	Okayama U.
Kazuyuki Suzuki	Graduate Student	Okayama U.
Karel Svadlenka	Associate Professor	Kanazawa U.
Daisuke Tagami	Associate Professor	Kyushu U.
Chen Tao	Graduate Student	Tohoku U.
Shinya Uchiumi	Graduate Student	Waseda U.
Tomoki Uda	Graduate Student	Kyoto U.
Natsuhiko Yoshinaga	Assistant Professor	Tohoku U.
Guanyu Zhou	Graduate Student	U. of Tokyo

Korea

Kazunori Ando	Postdoc	Inha U.
Jaehoon Cha	Graduate Student	Chungnam National U.
Durga Challa	Postdoc	Inha U.
Tingting Feng	Graduate Student	Inha U.
Juwon Jang	Graduate Student	Yonsei U.
Younghoon Jung	Graduate Student	KAIST
Hyeonbae Kang	Professor	Inha U.
Myeongseok Kang	Graduate Student	POSTECH
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Nary Kim	Graduate Student	Ajou U.
Samu Kim	Graduate Student	Chung-Ang U
Sun-Chul Kim	Professor	Chung-Ang U
Yunji Kim	Graduate Student	Ajou U.
Changhoon Lee	Professor	Yonsei U.
Hojun Lee	Graduate Student	Yonsei U.
Hyung-Chun Lee	Professor	Ajou U.
Mikyoung Lim	Professor	KAIST
Jinhae Park	Professor	Chungnam National U.
Jeongbo James Shim	Graduate Student	POSTECH
Sung-Ik Sohn	Professor	Gangneung-Wonju National U.
Donghyun You	Professor	POSTECH
Sung Sic You	Graduate Student	Inha U.
Sanghyeon You	Graduate Student	KAIST

Program

Session 1. Nov. 21, Friday, 10:20-12:00 ICC Room 302

Chair. Hiroshi Suito

10:20-10:45, Ruo Li (Peking University)
Finding 13-Moment System Beyond Grad

10:45-11:10, Hyung-Chun Lee (Ajou University)
An Efficient Sparse grid stochastic collocation method for stochastic Burgers equation

11:10-11:35, Norikazu Saito (University of Tokyo)
Mathematical and numerical analysis for flows and related problems

11:35-12:00, Chuanju Xu (Xiamen University)
Numerical investigation of complex flows with abnormal diffusion

Session 2. Nov. 21, Friday, 1:00-2:40 ICC Room 302

Chair. Jie Shen

1:00-1:25, Yasumasa Nishiura (Tohoku University)
Mathematical topics in materials science and life science

1:25-1:50, Lei Zhang (Peking University)
Phase Field Approach to Finding Critical Nuclei in Solid State Phase Transformations

1:50-2:15, Donghyun You (POSTECH)
Integrated simulations of turbulent flow and multimode heat transfer during a manufacturing process of CIGS solar cells

2:15-2:40, Hiroshi Suito (Okayama University)
Topics in Computing for flow problems and applications

Session 3. Nov. 21, Friday, 4:00-5:40 ICC Room 302

Chair. Sung-Ik Sohn

4:00-4:25, Changhoon Lee (Yonsei University)
Direct Simulation of Sedimenting Droplets in the Air

4:25-4:50, Jie Shen (Xiamen University and Purdue University)
Decoupled, linear and energy stable schemes for phase-field models for multi-phase complex fluids

4:50-5:15, Takashi Sakajo (Kyoto University)
Topics in mathematical and theoretical fluid dynamics

5:15-5:40, Sun-Chul Kim (Chung-Ang University)
Vortex sheet motion on the spheroid

Session 4. Nov. 22, Saturday, 10:20-12:00 ICC Room 302

Chair. Ruo Li

10:20-10:45, Masao Doi (Beihang University)
Onsager Principle as a Tool of Approximation

10:45-11:10, Jinhae Park (Chungnam National University)
Variational Problems in Smectic Liquid Crystals

11:10-11:35, Natsuhiko Yoshinaga (Tohoku University)
Active Soft Materials

11:35-12:00, Pingwen Zhang (Peking University)
Computable Modeling

Session 5. Nov. 22, Saturday, 3:00-4:40 ICC Room 302

Chair. Yasumasa Nishiura

3:00-3:25, Hiroshi Kokubu (Kyoto University)
Topological-computation methods for global dynamics in multiparameter systems

3:25-3:50, Yuan Yao (Peking University)
Applied Hodge Theory

3:50-4:15, Yasuaki Hiraoka (Kyusyu University)
Topological Data Analysis and Materials Science

4:15-4:40, Mikyoung Lim (KAIST)
Electric field enhancement in between two nearly touching perfect conductors

Short Presentations. Nov. 22, Saturday, 5:00-6:30 ICC Room 302

Chair. Pingwen Zhang

Sheng Chen (Xiamen University)
Generalized Jacobi Polynomial and their application to the fractional PDE

Emerson Escolar (Kyushu University)
Computing Persistence Modules of Quiver Complexes

Tingting Feng (Inha University)
Free boundary problem for GPT-vanishing structure

Zhijun Gao (Tohoku University)
Wave-particle duality in dissipative systems

Sung Sic Yoo (Inha University)
Numerical simulation of particle movement by immersed finite element method

Zhiping Mao (Xiamen University)
Fast algorithm for fractional partial differential equation

Guanyu Zhou (University of Tokyo)
Finite element method with various types of penalty on domain/boundary

Sanghyeon Yu (KAIST)
Stress concentration in between two nearly touching elastic holes

Yuwei Fan (Peking University)
On the model reduction for kinetic theory

Tomoki Uda (Kyoto University)
Numerical Verification for Elliptic Boundary Value Problem with Nonconforming P1 Finite Elements

Tetsuya Yamamoto (Beihang University)
Stability of water that is captured by Chinese brushes

Discussion Session. Nov. 23, Sunday, 10:00-11:40 CoreaCondo Convention Hall

Chair. Hyeonbae Kang

10:00-10:20, Motoko Kotani (Tohoku University)
A test case at AIMR –Collaboration between mathematics and materials science

10:30-12:00, discussion on future cooperation and collaboration

Abstracts

Session 1. Nov. 21, Friday, 10:20-12:00

Finding 13-Moment System Beyond Grad

Ruo Li (Peking University)

We point out that the thermodynamic equilibrium is not an interior point of the hyperbolicity region of Grad's 13-moment system. With a compact expansion of the phase density, which is compacter than Grad's expansion, we derived a modified 13-moment system. The new 13-moment system admits the thermodynamic equilibrium as an interior point of its hyperbolicity region. We deduce a concise criterion to ensure the hyperbolicity, thus the hyperbolicity region can be quantitatively depicted.

An Efficient Sparse grid stochastic collocation method for stochastic Burgers equation

Hyung-Chun Lee* (Ajou University)
Yun Nam (Ajou University)

We describe an efficient approximation of solution to stochastic Burgers equation driven by an additive space-time noise. We discuss existence and uniqueness of a solution through the Orstein-Uhlenbeck (OU) process. To approximate the OU process, we introduce the Karhunen-Loève expansion, and sparse grid stochastic collocation method. About spatial discretization of Burgers equation, two separate finite element approximations are presented: the conventional Galerkin method and Galerkin-conservation method. Numerical experiments are provided to demonstrate the efficacy of schemes mentioned above.

Mathematical and numerical analysis for flows and related problems

Norikazu Saito (University of Tokyo)

The aim of the second area's group is to develop novel numerical methods for solving various flow problems and related nonlinear problems. I will first explain FEM and FVM for a nonlinear convection-diffusion problem appearing in mathematical biology (Keller-Segel system modelling chemotaxis) by myself. The schemes possess the conservation of the L^1 norm and the free energy, which are salient properties of the original PDE. Then, I am going to briefly mention the other members' work; high accuracy FEM for non-stationary 3D Navier-Stokes equations by Dr. Notsu (Waseda) and some variational methods for free boundary problems by Dr. Svadlenka (Kanazawa) and Dr. Ginder (Hokkaido).

Numerical investigation of complex flows with abnormal diffusion
Chuanju Xu (Xiamen University)

In this talk, we will present efficient methods for numerical simulations of complex flows with abnormal diffusion. The main ingredients of the talk include:

1) Spectral methods for space fractional elliptic equations;

2) A stable direction splitting schema for the fractional diffusion equation in high dimension;

3) Applications of the above methods, and numerical simulation of some two-phase flows governed by the fractional Allen-Cahn equation.

Mathematical topics in materials science and life science

Yasumasa Nishiura (WPI-AIMR, Tohoku University)

I will give a short overview of relevant topics to A3 foresight program, which might enhance the collaborations among three countries. This may include several geometric methods, topological approaches, phase field methods and pattern dynamics arising in materials science and life science. If time permitted, I will also touch on self-recovery phenomena for network dynamics where each node is of excitable type with post-inhibitory rebound property.

Phase Field Approach to Finding Critical Nuclei in Solid State Phase Transformations

Lei Zhang (Beijing International Center for Mathematical Research, Peking University)

Predicting the shape of a critical nucleus in solids has been a long-standing problem in solid-state phase transformations. In this talk, we present a phase field model combined with efficient numerical algorithms for saddle-point search to predict the morphologies of critical nuclei in solids. Mathematically, finding an unstable critical nucleus is equivalent to solving a saddle point on an energy surface. By taking the advantage of the phase filed model, we are able to apply the shrinking dimer dynamics to find critical nuclei in both non-conserved and conserved solid fields. Optimization methods can be naturally implemented to further improve the performance of the shrinking dimer dynamics. Numerical simulations on heterogeneous nucleation reveal some fascinating findings of critical nuclei.

Integrated simulations of turbulent flow and multimode heat transfer during a manufacturing process of CIGS solar cells

Donghyun You* (Department of Mechanical Engineering, POSTECH)
Deageun Yoon (POSTECH)

CIGS solar cells are composed of layers of copper, indium, gallium, and selenium on a glass substrate. One of the thin film solar cells, CIGS solar cells have high photon absorption coefficients and absorb effectively the sunlight with a small thickness. To build the layer, selenide components are coated on the glass inside a chemical reactor chamber. The reactor chamber heats up selenide gas to induce reaction on the glass through thermal conduction, convection, and radiation. Uniformity in the CIGS layer is important because the layer thickness determines the energy conversion efficiency. Physical phenomena in the reactor, which determine the layer uniformity, include coupled turbulent convection of the selenide gas and conduction and radiation through the reactor and glass structures. In the present work, an effective methodology for integrated simulations of the coupled fluid dynamics and multimode heat transfer is presented. Turbulent convection of the selenide gas is predicted using a large-eddy simulation (LES) technique, while conduction and radiation of thermal energy through the associated structures are predicted using a finite-element method. The newly developed integrated simulation technique is utilized to predict the multiphysics during a CIGS selenization process.

Topics in Computing for flow problems and applications

Hiroshi Suito (Okayama University)

In the third area, various flow problems are considered from the practical points of view in computations and real-world applications. The researchers group of this area consists of Dr. Ishihara (Nagoya), Dr. Tagami (Kyushu), Dr. Obuse (Tohoku) and myself. I will briefly introduce their research topics including high-performance computing, particles dynamics in turbulent or laminar flows related to material sciences, etc. Then, I will present my current topics on collaborations with medical doctors mainly for cardiovascular problems, funded by Japan Science and Technology Agency.

Direct Simulation of Sedimenting Droplets in the Air

Changhoon Lee* (Dept. of Computational Science and Engineering, Yonsei University)
Yongnam Park (Yonsei University)
Itzhak Fouxon (Weizmann Institute of Science)

Many attempts to model sedimenting droplet particles in cloud have been made to understand fundamental mechanism of droplet collision or coalescence in warm cloud rain formation. Among many possible modelings, we consider the most basic numerical approach, i.e., direct simulation of particle-laden turbulence. Although the domain is very small (1m X 1m X 1m), accurate description of dynamics of turbulence and of particles is possible in this direct simulation. Since the range of the droplet size varies from submicron to 100 microns, two approaches are considered simultaneously: point-particle approach and finite-size particle simulation. In the point-particle approach, due to the simple nature of the governing equation of a particle, many theoretical investigations are possible. We show that the preferential concentration, usually observed in gravity-free turbulence laden with moderate-size particles, takes a different form when gravity is taken into account. This new clustering was explained by the property of the skewness of the velocity gradient of fluid. In the finite-size particle approach, we successfully implement an immersed boundary method in our spectral simulations. When gravity settles these finite-size particles, strong dissipation is observed near the particles while the kinetic energy is hardly modified, suggesting that excess energy due to gravitational settling is instantaneously dissipated by vorticity or shear generated by the particles. In conclusion, direct simulation of particle-laden turbulence can provide detailed physical mechanism of behavior of particles, and thus contribute much to better understanding of droplet dynamics in cloud.

Decoupled, linear and energy stable schemes for phase-field models for multiphase complex fluids

Jie Shen (Xiamen University and Purdue University)

I shall discuss how to construct decoupled, linear and energy stable schemes for a phase-field model of multiphase complex fluids, and present numerical results which not only demonstrate the effectiveness of the numerical schemes, but also validate the flexibility and robustness of the phase-field model.

Topics in mathematical and theoretical fluid dynamics

Takashi Sakajo (Kyoto University)

The group of the first area consists of Prof. Kaneda (Aichi-Tech), Prof. Okamoto (Kyoto), Prof. Kimura (Nagoya) and Prof. Sakajo (Kyoto), whose research activities mainly aim to understand fundamental fluid phenomena mathematically as well as numerically. In the present talk, on behalf of this group, I am going to introduce their research topics including vortex dynamics, mathematical and numerical analysis of the Navier-Stokes equations and theory of fluid turbulence, which are followed by a brief description of my current research project on 2D incompressible fluids in multiply connected domains funded by Japan Science and Technology Agency.

Vortex sheet motion on the spheroid

Samu Kim (Chung-Ang University)
Sun-Chul Kim* (Chung-Ang University)

Vortex sheet is an interface of discontinuity between two different velocity fluid flow. The dynamics of vortex sheet has been studied a lot for the plane and also for the sphere. In this talk, we study the motion of vortex sheet on the speroid numerically. More precisely, we asymptotically calculate the linear stability and compute the time evolution of roll ups.The effect of eccentricity is also considered.

Onsager Principle as a Tool of Approximation

Masao Doi (Center of Soft Matter Physics and its Applications, Beihang University)

In the celebrated paper on the reciprocal relation for the kinetic coefficients in irreversible processes, Onsager extended Rayleigh's principle of the least energy dissipation to general irreversible processes. The principle has been shown to be useful in deriving basic equations which describe non-linear and non-equilibrium phenomena in soft matter [1, 2]. Here I want to show that the principle is useful in getting an approximation solution using the examples of diffusion and gel dynamics [3].

References

[1] Masao Doi, Soft Matter Physics, Oxford University Press, 1-257 (2013).

[2] Masao Doi, Onsager's variational principle in soft matter dynamics, in Non-Equilibrium Soft Matter Physics ed S. Komura and T. Ohta, World Scientific, 1-35 (2012).

[3] Masao Doi, Gel Dynamics, J. Phys. Soc. Jpn 78, 052001, 1-19 (2009).

Variational Problems in Smectic Liquid Crystals

Jinhae Park (Chungnam National University)

We introduce mathematical modeling describing nematic/smectic liquid crystals with physically realistic boundary conditions. In particular, we discuss the Chen-Lubensky energy which explains stable states of liquid crystals from smectic phases to coexisting nematic/smectic states. After that, we investigate minimum energy configurations of the direction field with Dirichlet or Neumann boundary conditions.

Active Soft Materials

Natsuhiko Yoshinaga (WPI-AIMR, Tohoku University)

In this talk, I will discuss recent theoretical developments of active soft materials. One of the striking phenomena in biology is the ability of a cell to move without external force. This is distinct from passive systems. Active matters are assemblages of moving soft materials individually fueled by energy source. The studies in this field fall into two categories; one is mechanism of self-propulsion of an individual object, and the second is the collective motion of actively moving objects. The central question of the former studies is how spontaneous motion appears under nonequilibrium states. The example includes cell motility, and moving droplet.

Spontaneous motion is not driven by external force, but is sustained under a force-free condition. This requires breaking translational invariance in space. The broken symmetry is either extrinsic that is imposed externally by boundary conditions or by material properties or intrinsic namely nonlinear coupling makes an isotropic state unstable. The latter mechanism makes the system going to lower symmetry. When there is relative distance between a propelled object and another component, the translational symmetry is broken and a steady velocity emerges.

Computable Modeling

Pingwen Zhang (Peking University)

Computable modeling is to construct or simplify models using the related information through the precision of problems, the goal of which is to reduce the computational cost and increase the efficiency, such that the model could be computable using the computer nowadays. The computable modeling is an important component of scientific computing. This talk is to introduce the concept of computable modeling by the modeling of liquid crystals based on the molecular structures, including the model reduction.

Topological-computation methods for global dynamics in multiparameter systems

Hiroshi Kokubu (Kyoto University)

It is well established that multiparameter nonlinear dynamical systems exhibit extremely complex behaviors in their phase space and parameter space. For many applications, especially in settings in which precise measurements are difficult, an understanding of coarse but robust structures that exist over large ranges of parameter values is of greater importance than a detailed understanding of the fine structure. With this in mind, we discuss a new mathematical and computational framework for the analysis of the global dynamics of multiparameter nonlinear systems.

Our approach is based on a finite combinatorial approximation of the phase space, the parameter space, and the nonlinear dynamics. This is used to obtain a description of the global dynamics in terms of acyclic directed graphs called Morse graphs. A rigorous understanding of the dynamics is obtained using the Conley index, an algebraic topological invariant. The resulting information is finite and presented in the form of graphs and algebraic invariants and thus can be easily queried. For this reason, we view our procedure as producing a database for the global nonlinear dynamics for a parameterized nonlinear system. We give brief ideas of these methods along with some simple illustrative examples. If time permits, we also discuss how these ideas can also be applied to time-series data obtained from dynamical systems and generate Morse graphs representing underlying dynamics.

Applied Hodge Theory

Yuan Yao (Peking University)

Hodge Theory is a milestone bridging differential geometry and algebraic topology. It studies certain functions (called forms) on data rather than data points themselves, and brings an optimization perspective to decompose such functions adaptive to the underlying topology. Recently Hodge Theory inspires rising applications in computer vision, multimedia, statistical ranking, and game theory, in addition to traditional applications in mechanics etc. In this talk we give an introduction to Hodge Theory with examples in these applications.

Topological Data Analysis and Materials Science

Yasuaki Hiraoka (Kyusyu University)

In this talk, I will survey topological data analysis (TDA) and its applications to materials science. TDA is a new mathematical concept that allows us to study topological features in data. One of the representative methods in TDA is the so-called persistent homology. This algebraic tool describes not only topological features but also scales and their hierarchical relationships. From this characteristic property, it plays a significant role to investigate multi-scale phenomena appearing in a wide variety of science. After brief introduction of

TDA, I will explain applications of TDA to study characterizations of amorphous structures, and show that persistent homology elucidates new medium-range structures of silica glasses and properly encodes mechanical properties.

Electric field enhancement in between two nearly touching perfect conductors
Mikyoung Lim (KAIST)

Two nearly touching metallic spheres cause the enhancement of the electric field. In an external electric field of long wavelength compared to the size of spheres, the presence of nearly touching metallic spheres induces a very large electric field confined in the narrow gap region between the spheres. In this talk, we analyze this field enhancement based on the quasi-static approximation and the related conductivity equation for the electric scalar potential. The generic blow-up rate of the electric field, which is the gradient of the solution to the conductivity problem, is $|\epsilon \ln \epsilon|^{-1}$ in three dimensions and $\epsilon^{-1/2}$ in two dimensions, where ϵ is the distance between the two spheres. I present asymptotic formulas for the solution to the conductivity problem, which characterize the gradient blow-up of the solution. The analysis is based on the bipolar coordinates and the bispherical coordinates in two dimensions and three dimensions, respectively.

A test case at AIMR –Collaboration between mathematics and materials science
Motoko Kotani (Tohoku University)

A big experiment has been taken place at AIMR; How mathematics catalyzes interactions over disciplines and makes breakthroughs. There are interesting phenomena discovered in Materials science by advanced observation tools and technics which are waiting for mathematical descriptions of structures hidden behind. These newly discovered phenomena on the other hands inspire mathematician to develop concepts and theories. I will present outline of our mutually beneficial activities. I would also like to explain trends to promote mathematics in Japan. From 2006,the MEXT has encouraged interactions between mathematics and other scientific fields, and several actions were/are taken such as Nishiura CREST, Tanaka-CREST, Kitsuregawa-sakigake, Tsuboi-CREST and , Kokubu-sakigake. Through those actions we have proved importance of mathematics. Now Japanese government started organizing a basic plan for Science, Technology and Innovation Policy toward a digital society. I would like to discuss with you how math can contribute in the direction.