2015 A3 joint Workshop on Fluid Dynamics and Material Science
Peking University, Beijing, China
Feb. 11-13, 2015

Venue:
Room 77201 at JingChunYuan #78, Beijing International Center for Mathematical Research, Peking University, Beijing.

Organizing Committee:
Pingwen Zhang (Peking University)
Yasumasa Nishiura (Tohoku University)

Workshop Program

Duration of talks:
For faculties: 30-minutes talks + 15-minute discussions
For students: 20-minutes talks + 10-minute discussions

Wednesday Afternoon (Feb. 11)

Theme: Revisit the concept of structural stablility and its application.
Chair: Lan Wen
16:00 – 17:00, **Hiroshi Kokubu (Kyoto University)**
Various stability concepts for global dynamics in applications

17:30, Dinner at ZhongGuanYuan Global Village

Thursday (Feb. 12)

Morning Session - Theme: Modeling and computation of dissipative patterns, selforganization in nonlinear problems.
Chair: Pingwen Zhang
9:00 – 9:45, **Yasumasa Nishiura (Tohoku University)**
Mathematical challenge to complex phenomena
9:45 – 10:30, **Tiejun Li (Peking University)**
Stochastic dynamics and rare events for the chemical reaction kinetics
10:30 – 10:45 Tea Break
10:45 – 11:30, **Yucheng Hu (Tsinghua University)**
Defects of Liquid Crystals in Confined Volume
11:30 – 12:15, **Elliott Ginder (Hokkaido University)**
Threshold dynamical algorithms for curvature dependent interfacial motions

12:15 – 14:00, Lunch in Campus (ShaoYuan)

Afternoon Session - Theme: Free boundary problems.
Chair: Yasumasa Nishiura
14:00 – 14:45, **Karel Svadlenka (Kyoto University)**
Numerical and mathematical analysis of evolution problems related to wetting phenomena
14:45 – 15:30, **Xianmin Xu (Chinese Academy of Sciences)**
Wetting and some related mathematical problems
15:30 – 15:45, Tea Break

15:45 – 16:15, **Jie Xu (Peking University)**
Modeling of bent-core molecules from molecular theory: a tensor model for nematic phases
16:15 – 16:45, **Zhijun Gao (Tohoku University)**
Dynamics of traveling spots with oscillatory tails for the generalized three-component FitzHugh-Nagumo equations
16:45 – 17:30, Free Discussion

17:30, Dinner (outside of campus)

Friday (Feb. 13)

Morning Session - Theme: Numerical analysis in fluid dynamics.
Chair: Hisashi Okamoto

9:00 – 9:45, **Huazhong Tang (Peking University)**
High-order accurate physical-constraints-preserving finite difference WENO schemes for special relativistic hydrodynamics

9:45 – 10:30, **Hirofumi Notsu (Waseda Insitute for Advanced Study)**
Error estimates of stabilized Lagrange-Galerkin finite element schemes for flow problems

10:30 – 10:45 Tea break

10:45 – 11:30 **Daisuke Tagami (Kyushu University)**
Pressure-Stabilized Finite Element Methods for Viscoelastic Flow Problems

11:30 – 12:15 **Jun Hu (Peking University)**
Mixed Finite Element Methods for Linear Elasticity

12:15 – 14:00, Lunch in Campus (ShaoYuan)

Afternoon Session - Theme: Topology and Applied dynamical systems.
Chair: Lei Zhang

14:00 – 14:45, **Tomoo Yokoyama (Kyoto University of Education)**
Topological Methods to Analyze Hamiltonian Surface Flows and Their Applications

14:45 – 15:15, **Yusuke Imoto (Kyushu University)**
Error estimates of a generalized particle-based method for partial differential equations

15:15 – 15:30, Tea Break

15:30 – 16:00, **Weiming Li (Peking University)**
Tackling stiffness in radiative transfer coupled with background medium

16:00 – 16:30, **Guanyu Zhou (University of Tokyo)**
A penalty method for the stationary Navier-Stokes equations with the slip boundary condition.

16:30 – 17:30, Free Discussion & Wrap Up

17:30, Dinner at ZhongGuanYuan Global Village

Talk's title & abstract

Various stability concepts for global dynamics in applications

Hiroshi Kokubu

Graduate School of Science, Kyoto University

Structural stability is a fundamental notion for robustness of dynamics, and the bifurcation theory of dynamical systems is, in a sense, a classification theory of the changes of dynamics when the structural stability is lost. Recent progress of computational dynamics theory provides us with various results and methods for the analysis of robust dynamics by computation, such as computer- assisted verification of structural stability, methods for computing Morse decompositions of dynamics, and so on. I will give a brief survey of these methods and discuss potential applications to some problems in this A3 project.

Mathematical challenge to complex phenomena

Yasumasa Nishiura Tohoku University WPI AIMR

I am interested in the following topics.
1. Dynamics of localized patterns in dissipative systems: Pulses and spots arising in reaction-diffusion systems, binary fluids, and biological systems
2. 3D morphologies of diblock copolymer (under constraint).
3. Amorphous structures in materials science: An application of computational homology to characterize the amorphous structures
4. Network Dynamics and the recovery properties: When the network has some damage, one of the interesting questions is how the network can spontaneously recover its function without external stimulus.

Stochastic dynamics and rare events for the chemical reaction kinetics

Tiejun Li, Peking University

I will first talk about the basic mathematical setup of the stochastic chemical reaction kinetics arising in systems biology. Then I introduce the basic numerical methods for the simulation such as the SSA, tau-leaping methods, etc. The main emphasis will be the analysis and improvement of tau-laping methods, and the rare event study for the chemical reaction kinetics, which is closely related to the energy landscape theory for the biological systems recently.

Defects of Liquid Crystals in Confined Volume

Yucheng Hu, Tsinghua University

Abstract: Defects in liquid crystals are of great practical importance and theoretical interest. Despite tremendous efforts, predicting the location and transition of defects under various topological constraint and external field remains to be a challenge. We investigate defect patterns of nematic liquid crystals confined in three-dimensional spherical droplet and two-dimensional disk under different boundary conditions, within the Landau-de Gennes model. From numerical results we found many interesting common features of defect patterns under the influence of boundary anchoring conditions.

Threshold dynamical algorithms for curvature dependent interfacial motions

Elliott Ginder, Hokkaido University

Mean curvature flow (MCF) refers to the motion of a hypersurface whose velocity, in the normal direction to the interface, is given by mean curvature and the method of BMO is a well-known threshold dynamical (TD) algorithm for approximating multiphase motion by MCF. TD-based methods enjoy the ability to formulate approximation methods that can be used in computations, as well as in the mathematical analysis of such motions.

We will discuss signed distance formulations of TD-based algorithms for multiphase MCF, as well as one for the so-called hyperbolic MCF. These methods allow one to compute mulitiphase volume preserving motions, as well as to control contact angles that interfaces make with obstacles.

Prospective joint research: Xianmin Xu (AMSS, Chinese Academy of Sciences), Karel Svadlenka (Kyoto University, Japan), Elliott Ginder (Hokkaido University, Japan)

Numerical and mathematical analysis of evolution problems related to wetting phenomena

Karel Svadlenka, Kyoto University

An evolutionary free boundary problem representing a simple model of non-stationary wetting phenomena will be presented. The parabolic version of this problem is related to a generalized notion of the gradient flow for a non-smooth and non- convex functional, called ‘curve of maximal slope’. The known facts about curves of maximal slope for the considered surface energy functional will be reviewed together with some new partial results on the hyperbolic version of the problem. Idea of numerical approximation by the method of time semi-discretization and results of computations will be addressed.

Prospective joint research: Xianmin Xu (AMSS, Chinese Academy of Sciences), Elliott Ginder (Hokkaido University, Japan), Karel Svadlenka (Kyoto University, Japan)

Topic: Mathematical analysis related to the dynamics of wetting (development of suitable mathematical model, mathematical analysis of the free-boundary model equation, classification of factors important in wetting dynamics and their modeling, numerical approximation).

Wetting and some related mathematical problems

Xianmin Xu
Academy of Mathematics and Systems Science, Chinese Academy of Sciences

The study of wetting phenomenon is of critical importance for many applications and has attracted much interest in physics and material sciences, stimulated by the development of surface engineering and the studies on the super-hydrophobicity property in a variety of nature and artificial objects. There are many interesting mathematical problems in this field, such as free interface, moving three-phase contact line, multi-scale phenomena induced by rough boundaries. In this talk, I will illustrate some of our recent studies in this field. Starting from a simplified model, which includes only interface effects, we analyze various homogenization limits of wetting on rough boundaries and chemically patterned surfaces, the well-posedness of a Cahn-Hilliard equation with relaxed boundary condition and its sharp-interface limit. By these analyses, we investigate some interesting physical properties of wetting, such as Wenzel's and Cassie's equations for macroscopic contact angles, contact angle hysteresis, and dynamics of the contact angle. The talk is based on the joint work with Xiaoping Wang and Xinfu Chen.

Modeling of bent-core molecules from molecular theory: a tensor model for nematic phases

Jie Xu, Peking University

We describe a procedure to derive a tensor model for bent-core molecules from the second virial expansion. The terms in the model are determined by the C_2v symmetry of the molecule, and the coefficients are derived from molecular parameters. An extension of the Bingham closure is employed that is able to restrict the tensors in physical range. As a simple case, we examine a tensor model for nematic phases. We give a phase diagram about molecular parameters, and show some novel structures we find with artificial coefficients.

Dynamics of traveling spots with oscillatory tails for the generalized three-component FitzHugh-Nagumo equations

Zhijun Gao, Tohoku University Mathematical Institute, WPI Advanced Institute for Materials Research

The research is concerned with the dynamics of traveling spots with oscillatory tails arising in a three-component reaction diffusion systems called the generalized three-component FitzHugh-Nagumo equations. As is known by Yves Couder's oil droplet experiments on a liquid surface, particles (droplets) associated with waves (surface waves caused by bouncing of particles) show a macroscopic quantum-like behaviors similar to Young's slit experiments and tunnel's phenomena. The main aim is to show numerically that such traveling spots also display a similar wave-particle duality, and moreover by using center manifold reduction theory, we are able to show that the dynamics of single spot dynamics can be reduced to a 4D system of ODEs. Via the analysis of such ODEs, we can show at least partially the origin of such quantum-like behaviors that is never observed for monotone-tail spots. This is a joint work with Yasumasa Nishiura.

High-order accurate physical-constraints-preserving finite difference WENO schemes for special relativistic hydrodynamics

Kailiang Wu and Huazhong Tang*
LMAM, School of Mathematical Sciences, Peking University

We develop high-order accurate physical-constraints-preserving finite difference WENO schemes for special relativistic hydrodynamical (RHD) equations, built on the local Lax-Friedrich splitting, the WENO reconstruction, the physical-constraints-preserving flux limiter, and the high order strong stability preserving time discretization. They are formal extensions of the existing positivity-preserving finite difference WENO schemes for the non-relativistic Euler equations. However, developing physical-constraints-preserving methods for the RHD system becomes much more difficult than the non-relativistic case because of the strongly coupling between the RHD equations, no explicit expressions of the conservative vector for the primitive variables and the flux vectors, and one more physical constraint for the fluid velocity in addition to the positivity of the rest-mass density and the pressure. The key is to prove the convexity and other properties of the admissible state set and discover a concave function with respect to the conservative vector replacing the pressure which is an important ingredient to enforce the positivity-preserving property for the non-relativistic case. Several one- and two-dimensional numerical examples are used to demonstrate accuracy, robustness, and effectiveness of the proposed physical-constraints-preserving schemes in solving relativistic problems with large Lorentz factor.

Error estimates of stabilized Lagrange-Galerkin finite element schemes for flow problems

Hirofumi Notsu, Waseda Institute for Advanced Study, Waseda University

Stabilized Lagrange-Galerkin finite element schemes for the Oseen and the Navier- Stokes equations are mathematically analyzed. Stability and convergence results with optimal error estimates for both of the schemes are proved. They are combined fi- nite element schemes with a Lagrange-Galerkin (characteristics) method, cf. [1], and Brezzi-Pitka¨ranta's (pressure-)stabilization [2]. Both of the resulting matrices are sym- metric by virtue of the Lagrange-Galerkin method and Brezzi-Pitka¨ranta's stabilization is employed in order to reduce the numbers of degrees of freedom via a cheap P1/P1 element. The scheme for the Oseen equations is unconditionally stable and its error estimates are optimal, cf. [3]. On the other hand, the scheme for the Navier-Stokes equations is conditionally stable and its error estimates are optimal, cf. [4]. The con- vergence orders are recognized in two- and three-dimensional numerical results.

Our research interests are numerical methods for flow problems and their analysis.

References
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Pressure-Stabilized Finite Element Methods for Viscoelastic Flow Problems

Daisuke Tagami, Kyushu University

The viscoelastic flow is one of the important physical phenomena both from the theo- retical and from the practical points of view. Blood flows in the human body and plastic flows during the injection molding are typical examples of the viscoelastic flow; for more ex- amples and details, see Owens–Phillips [4], and its references. Therefore, there encounter many researches on the numerical analysis and simulation of viscoelastic flows; see, for example, Bonito–Clement–Picasso [1], Owens–Phillips [4], and their references.

In order to enhance the mathematical justification of numerical methods for viscoelastic flows, we establish error estimates of a pressure-stablized finite element method for ones. Moreover, we show some numerical examples of

contraction flows, and compare numerical results with experimental ones among some viscoelastic models; the Oldroyd-B model [3], the Giesekus model [2], and the PTT model [5].

Recently, viscoelastic flows are regarded as one of examples of the complex fluids, which have self-structuring systems composed by molecules, particles, and monomers; for exam- ple, polymeric fluid, surfactant micellar solution, colloidal particle dispersion, and liquid crystal. Because the complex fluids show interesting peculiar phenomena, we want to un- derstand their behavior, and apply their peculiarity into engineering facilities. In order to understand, numerical simulations play important role, and their mathematical justifica- tions are required.

Therefore, understanding the behavior of complex fluids and mathematical justification of numerical methods for ones may be considered as themes of our joint works.

References

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Mixed Finite Element Methods for Linear Elasticity

Jun Hu, Peking University

How to design stable mixed finite elements for linear elasticity is a challenging, surprisingly hard problem. This problem has been open for more than fifties years and has been studied by most of prestigious Mathematician, including D. N. Arnold, Jim Douglas Jr., and F. Brezzi the founder of mixed finite element theories since last sixties, in the finite element field. In 2002, Arnold and Winther designed the first family of mixed finite element methods in 2D, based on polynomial shape function spaces, which was extended to 3D in 2008. The key ingredient for the analysis there was the elasticity complexes in 2D and 3D. The two dimensional results were taken as a main part of Arnold’s plenary lecture in the International Congress of Mathematician 2002.

By achieving two basic algebraic results and one intrinsic structure of H(div) piecewise polynomial spaces, we proposed a direct method to design mixed finite elements of linear elasticity. The main differences between these new mixed elements and those within Arnold–Winther's framework are summarized as follows:

(1) Our method is a direct method, which does not apply any other tool like the elasticity complexes.
(2) The mixed elements in any space dimension by our method can be designed and analyzed in a unified fashion; since the elasticity complexes in two and three di- mensions are completely different, their two and three dimensional mixed elements have to be analyzed separately, in addition, mathematically, their method can not be generalized to any space dimension at moment.
(3) Above all, on simplex grids, we were able to match the discontinuous piecewise P_{k-1} displacement space by a suitable H(div, Ω, S)-P_k stress space, which leads to an optimal k-th order convergence; while they had to match the same displacement space by a H(div, Ω, S)-P_{k+1} stress space and a H(div, Ω, S)-P_{k+2} stress space in two and three dimensions, respectively. Similar phenomena happen for product grids.
(4) For cuboid grids, we were able to design a family of stable and optimal mixed elements of any order; while only a first order mixed element was proposed based on their method so far.

As a summary, our method is a direct and intrinsic method. Consequently, the discrete stress spaces have a simple structure and a surprisingly simple basis which consists of essential matrix–valued Lagrange basis functions of order k. Our mixed elements are based on the Hellinger–Reissner variational principle, completely new, and very difficult to simplify.

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TOPOLOGICAL METHODS TO ANALYZE HAMILTONIAN SURFACE FLOWS AND THEIR APPLICATIONS

Tomoo Yokoyama (Kyoto University of Education)

We introduce new topological methods, which are word representations and graph representations, to analyze Hamiltonian flows on surfaces. In particular, a graph representation is an injection from generic Hamiltonian surface flows. Using these representations, we can estimate the intermediate flow structures for two flow structures at different times for a time-dependent Hamiltonian surface flow. Moreover, in the case of the numerical simulation, although a word or graph rep- resentation is a simplified data of the original numerical data, we can obtain a new information which is hard to obtain directly from the original data. Since a topolog- ical method is more adapted for qualitative problems than analytical or geometric one, we discuss possibility of applications to fluid dynamics and relative issues.

Research collaboration possibilities between Japan and China: At the aspect of dynamical systems, we'd like to collaborate on several kinds of stabilities, the associated bifurcations, and their applications. For instance, we'd like to generalize word or graph representations for general (e.g. non-wandering) flows on surfaces or 3-manifolds, and construct quantities, which measure global properties of time-dependent (Hamiltonian) flows, from sequences of representations.

At the aspect of applications, we'd like to approach several kinds of problems from topological point of view, using rough (e.g. topological, discrete) stabilities and their bifurcations. In fact, we'd like to classify certain structures (e.g. hydrodynamic phenomena (blood stream, current of the sea or air)) by rough stabilities, analyze their bifurcations, distill essence of the structures, and control the structures.

Error estimates of a generalized particle-based method for partial differential equations

Yusuke IMOTO* and Daisuke TAGAMI, Kyushu University

Abstract: Numerical analysis of a generalized particle-based method for partial differential equations, Poisson equations and heat equations, is considered. Particle-based methods, especially Smoothed Particle Hydrodynamics (SPH) and Moving Particle Simulation (MPS) [1], are widely used as numerical methods

for flow problems with moving boundaries like Tsunami. Our generalized method describes the interpolants and the approximate differential operators in case of not only SPH or MPS but also other methods, where it is possible to choose various weight functions not considered in the conventional ones.

Error estimates are established by introducing regularity and connectivity conditions of particle distributions and influence radius. Their convergence orders are optimal in the sense that its have the same ones of interpolations with respect to the influence radius. Moreover, numerical convergence orders agree well with theoretical ones.

Possibility of joint works: Our final goal is to establish error estimates of particle-based methods for flow problems with moving boundary. Therefore, the following facts are to be justified mathematically:

(1) Fractional step methods such as MAC method [2] are used as the time integration. Does the fractional step method well approximate the original flow problem?
(2) The material derivative is used for approximating the inertial terms [3]. Therefore, particle distributions become ununiform as time steps progress. On the other hand, it is required that particles are uniformly distributed to obtain approximate solutions precisely. How are particles uniformly redistributed?
(3) To apply the methods into practical problems such as the fluid-structure interactions when Tsunami hits artificial structures, it is required to compute flow force. How are flow force computed more precisely?

References
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Tackling stiffness in radiative transfer coupled with background medium

Weiming Li, Peking University

We consider radiative transfer coupled with electrons. This process is described using a radiative transfer equation coupled with an ordinary differential equation for describing electron temperature. The radiative transfer equation is approximated using the Pn model.Coupling between the two equations (as in cases with high temperatures) can introduce stiffness into the problem.
By giving an accurate ansatz for electron temperature, combined with direct integration for energy intensity in radiative transfer, stringent restrictions on the time step can be avoided. Numerical results show the effectiveness of our

approach.

A penalty method for the stationary Navier-Stokes equations with the slip boundary condition.

Guanyu Zhou, University of Tokyo

We consider the stationary Navier-Stokes equations with the slip boundary condition in a smooth domain $\Omega \in R^d$ (d=2,3), with $\partial\Omega = D \cup \Gamma$. Let (u,p) be the velocity and pressure of solution. We impose the Dirichlet boundary condition u = 0 on D, and the slip boundary condition $u_n = 0$ on Γ, where $u_n = u \cdot n$, and n is the unit outer normal vector to Γ. The idea of the penalty method is to approximate $u_n|_\Gamma = 0$ by a Robin type boundary condition $\tau(u_\varepsilon,p_\varepsilon)+\varepsilon^{-1}u_{\varepsilon n}n = 0$ on Γ, where $(u_\varepsilon,p_\varepsilon)$ is the approximate solution, $\tau(u_\varepsilon,p_\varepsilon)$ is the stress tensor, ε is the penalty parameter ($0 < \varepsilon \ll 1$), and $u_{\varepsilon n} = u_\varepsilon \cdot n$. The penalty method has several advantages in numerical computation, for example, avoiding the variational crime and easy implementation. We prove the error estimates of penalty method $\|u-u_\varepsilon\|_{H^k(\Omega)} \leq C\varepsilon$, for any $k \in N$. We also investigate the finite element method with P1b/P1 element to the penalty problem. Two implementation methods for the penalty term is considered, and the error estimates are obtained.

Some topics for collaboration: We have some future work for the penalty method for slip boundary condition, especially for the non-stationary Naver-Stokes equations. Besides of that, we, the Numerical Analysis Group of the University of Tokyo, would like to promote joint works concerning other topics, which is briefly presented in the following.

(1) Nonstandard boundary conditions for the Navier-Stokes equations. So far we have developed analytical and numerical study for nonstandard boundary conditions such as leak/slip conditions of friction type and a unilateral condition of Signorini's type. We are interested in real world applications.
(2) The conservative finite volume/finite element scheme for the Keller-Segel system. We have worked on this topics for simplified and the classical model problems. But there are various types of model problem for chemotaxis with different types of nonlinear term, the solution of which has different properties. We are inter- ested in the numerical method which preserves those properties in a discrete version.