International Workshop on Interacting Particle Systems

Sunday March 29, Shanghai Jiao Tong University, China
Organizer: **Shi Jin**

Sponsors: Institute of Natural Sciences
School of Mathematical Sciences
Ministry of Education Key Lab in Scientific and Engineering Computing
Shanghai Center for Applied Mathematics (SJTU)
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山川异域，风月同天
青山一道同云雨，明月何曾是两乡
千里同好，坚于金石

Unis nous vaincrons

Siamo onde dello stesso mare, foglie dello stesso albero, fiori dellow stesso giardino

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Zoom APP:

Session 1: 9:20 am-12 noon, Beijing Time
Conference ID: 375-800-267
PIN Code: 490207

Session 2: 6:50 pm-10:30 pm, Beijing Time
Conference ID: 971-593-732
PIN Code: 938470

Schedule (all Beijing time)

Session 1

09:25-09:30 Opening remarks by the organizer

09:30-10:00 **Jian-Guo Liu**, Duke University, USA
Data-driven efficient solvers and predictions of conformational transitions for Langevin dynamics on manifold in high dimensions

10:05-10:35 **Seung-Yeal Ha**, Seoul National University, Korea
Emergent behaviors of thermomechanical Kuramoto ensemble on a ring lattice

10:40-11:10 **Jingwei Hu**, Purdue University, USA
A deterministic particle method for the homogeneous Landau equation

11:15-11:45 **Zhenfu Wang**, University of Pennsylvania, USA
Quantitative Methods for the Mean Field Limit Problem

Session 2

18:50-18:55 Opening remarks by the organizer

19:00-19:20 **Francois Golse**, Ecole Polytechnique, France
Convergence of time splitting methods for quantum dynamics in the semiclassical regime

19:25-19:45 **Thierry Paul**, Sorbonne University, France
Quantum transport is cheaper

19:50-20:10 **Jose Carrillo**, Imperial College, UK
Consensus Based Models and Applications to Global Optimization

20:15-20:35 **Lorenzo Pareschi**, University of Ferrara, Italy
Monte Carlo Stochastic Galerkin methods for the Boltzmann equation

20:40-21:00 **Sergio Simonella,** Ecole Normale Superieure Lyons, France
Dynamical connectivity of hard spheres

21:05-21:25 **Franca Hoffman**, California Institute of Technology, USA
Kalman-Wasserstein Gradient Flows

21:30-22:50 **Ruiwen Shu**, University of Maryland, USA
Equilibration of aggregation-diffusion equations with weak interaction forces

21:55-22:15 **Peter Pickl**, University of Munich, Germany
Derivation of the Vlasov equation for short range interactions

Abstracts

Jose Carrillo, Imperial College, UK
Consensus Based Models and Applications to Global Optimization

We will review the state of the art in Consensus Based Optimization models both from the theoretical and practical viewpoint. Ideas on the proof of the convergence of the algorithm will be given together with a discussion about its performance in the challenging problem of global optimization. The talk is based on recent works with Y.-P. Choi, O. Tse, C. Totzeck, L. Li, S. Jin, and Y. Zhu.

Francois Golse, Ecole Polytechnique, Paris, France
Convergence of time splitting methods for quantum dynamics in the semiclassical regime

The purpose of this talk is to give quantitative convergence estimates proving that time splitting methods for quantum dynamics converge uniformly in the semiclassical regime. (Joint work with Shi Jin and Thierry Paul).

Seung Yeal Ha, Seoul National University, Korea
Emergent behaviors of thermomechanical Kuramoto ensemble on a ring lattice

The temporal evolution of thermomechanical Kuramoto oscillators often appears in biological oscillator ensemble. In this talk, we propose a new generalized thermomechanical Kuramoto model on a ring lattice. Our proposed model is derived from the thermodynamic Cucker-Smale model for flocking on the 2D free space under the assumption that the ration between velocity field and temperature field at each lattice point has a uniform magnitude. The proposed model satisfies an entropy principle and exhibits emergent dynamics under some sufficient frameworks formulated in terms of initial data and system parameters. Moreover, the phase field tends to the Kuramoto phase field time-asymptotically.

Franca Hoffman, California Institute of Technology, USA
Kalman-Wasserstein Gradient Flows

Abstract: We study a class of interacting particle systems that may be used for optimization. By considering the mean-field limit one obtains a nonlinear Fokker-Planck equation. This

equation exhibits a gradient structure in probability space, based on a modified Wasserstein distance which reflects particle correlations: the Kalman-Wasserstein metric. This setting gives rise to a methodology for calibrating and quantifying uncertainty for parameters appearing in complex computer models which are expensive to run, and cannot readily be differentiated. This is achieved by connecting the interacting particle system to ensemble Kalman methods for inverse problems. This is joint work with Alfredo Garbuno-Inigo (Caltech), Wuchen Li (UCLA) and Andrew Stuart (Caltech).

Jingwei Hu, Purdue University, USA
A deterministic particle method for the homogeneous Landau equation

We propose a novel deterministic particle method to numerically approximate the Landau equation for plasmas. Based on a new variational formulation in terms of gradient flows of the Landau equation, we regularize the collision operator to make sense of the particle solutions. These particle solutions solve a large coupled ODE system that retains all the important properties of the Landau operator, namely the conservation of mass, momentum and energy, and the decay of entropy. We illustrate our new method by showing its performance in several test cases including the physically relevant case of the Coulomb interaction. The comparison to the exact solution and the spectral method is strikingly good maintaining 2nd order accuracy. Moreover, an efficient implementation of the method via the treecode is explored. This gives a proof of concept for the practical use of our method when coupled with the classical PIC method for the Vlasov equation. This is joint work with J. A. Carrillo, L. Wang, and J. Wu.

Jian-Guo Liu, Duke University, USA
Data-driven efficient solvers and predictions of conformational transitions for Langevin dynamics on manifold in high dimensions

We work on dynamic problems with collected data $\{\mx_i\}$ that well-distributed on manifold $\mm\subset\bR^p$, $p\gg 1$. Using the diffusion map, we first learn the reaction coordinates $\my$ such that dataset $\{\my_i\}\subset\nn$ is isometric embedded into a low dimensional Euclidean space $\bR^\ell$. This enables us to obtain an efficient approximation for the dynamics, described on a Fokker-Plank equation on manifold $\nn$. Thanks to this, we proposed an implementable data-driven upwind scheme which automatically incorporates the manifold structure and give the convergence analysis to the Fokker-Plank equation on $\nn$. The proposed upwind scheme also gives a Markov chain with transition probability between the nearest neighbor points, which enables us to conduct manifold-related computations directly such as finding optimal coarse-grained network and minimal energy path representing chemical reactions or conformational changes. As a byproduct, we also give the algorithms for generating equilibrium potential for new physical system with new parameters. Using the proposed upwind scheme, we calculate the trajectory of the Fokker-Plank equation on $\nn$ with new equilibrium and then pullback to the original high dimensional space as an effective generative data for the new physical system.

Lorenzo Pareschi, University of Ferrara, Italy
Monte Carlo Stochastic Galerkin methods for the Boltzmann equation

We propose a novel numerical approach for the Boltzmann equation with uncertainties. The method combines the efficiency of classical direct simulation Monte Carlo (DSMC) schemes in the phase space together with the accuracy of stochastic Galerkin (sG) methods in the random space. This hybrid formulation makes it possible to construct methods that preserve the main physical properties of the solution along with spectral accuracy in the random space. The schemes are developed and analyzed in the case of space homogeneous problems as these contain the main numerical difficulties. Several test cases are reported, both in the Maxwell and in the variable hard sphere (VHS) framework, and confirm the properties and performance of the new methods.

Thierry Paul, Sorbonne University, France
Quantum transport is cheaper

Bipartite (Euclidean) matching problems in classical and quantum mechanics are compared. The quantum case is treated in terms of a quantum version of the Wasserstein distance. We show that the optimal quantum cost can be cheaper than the classical one. We treat in detail the case of two particles: the equal mass case leads to equal quantum and classical costs. Moreover, we show examples with different masses for which the quantum cost is strictly cheaper than the classical cost.

Peter Pickl, University of Munich, Germany
Derivation of the Vlasov equation for short range interactions

The derivation of the Vlasov equation from Newtonian mechanics is an old problem in mathematical physics. But while the most interesting interactions in nature have singularities, one typically assumes some Lipschitz condition on the interaction force for its microscopic derivation. Recent developments have given results, where the interaction force gets singular when the particle number N tends to infinity. Usually by mollifying or cutting the singularity with a N-dependent mollifier or cut-off parameter.

In the talk I will present a recent result for short range interaction
which also get singular as N tends to infinity.

Ruiwen Shu, University of Maryland, USA
Equilibration of aggregation-diffusion equations with weak interaction forces

This paper studies the large time behavior of aggregation-diffusion equations. For one spatial dimension with certain assumptions on the interaction potential, the diffusion index m, and the initial data, we prove the convergence to the unique steady state as time goes to infinity (equilibration), with an explicit algebraic rate. The proof is based on a uniform-in-time bound on the first moment of the density distribution, combined with an energy dissipation rate

estimate. This is the first result on the equilibration of aggregation-diffusion equations for a general class of weakly confining potentials $W(r)$: those satisfying $\lim_{r\rightarrow\infty}W(r)<\infty$.

Sergio Simonella, Ecole Normale Superieure Lyons, France

Dynamical connectivity of hard spheres.

ABSTRACT. Vaguely inspired by some numerical simulations that recently populated the web, I will talk about collisional clusters of interacting particles, focusing on elementary hard sphere dynamics. Different notions of clusters may be typically bounded, or not, depending on their behaviour under time-reversal. Cluster dynamics is a tendency of self-organising in small groups (clusters), which behave independently for random intervals of time. This breaks with the sudden appearance of a giant cluster. Based on a kinetic limit, one can provide analytic formulations.

Zhenfu Wang, University of Pennsylvania, USA

Quantitative Methods for the Mean Field Limit Problem

We study the mean field limit of large systems of interacting particles. Classical mean field limit results require that the interaction kernels be essentially Lipschitz. To handle more singular interaction kernels is a longstanding and challenging question but which now has some successes. Joint with P.-E. Jabin, we use the relative entropy between the joint law of all particles and the tensorized law at the limit to quantify the convergence from the particle systems towards the macroscopic PDEs. This method requires to prove large deviations estimates for non-continuous potentials modified by the limiting law. But it leads to explicit convergence rates for all marginals. This in particular can be applied to the Biot-Savart law for 2D Navier-Stokes. To treat more general and singular kernels, joint with D. Bresch and P.-E. Jabin, we introduce the modulated free energy, combination of the relative entropy that we had previously developed and of the modulated energy introduced by S. Serfaty. This modulated free energy may be understood as introducing appropriate weights in the relative entropy to cancel the most singular terms involving the divergence of the kernels. Our modulated free energy allows to treat gradient flows with singular potentials which combine large smooth part, small attractive singular part and large repulsive singular part. As an example, a full rigorous derivation (with quantitative estimates) of some chemotaxis models, such as the Patlak-Keller-Segel system in the subcritical regimes, is obtained.