# Quantum & Kinetic Problems: Modeling, Analysis, Numerics & Applications

Partially supported by Centre for Advanced 2D Materials (CA2DM)

## Workshop 3: Emergent Phenomena – from Kinetic Models to Social Hydrodynamics (16 - 20 December 2019)

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Venue: IMS Auditorium

Institute

**Admission is free** 

3 Prince George's Park Singapore 118402 ims.nus.edu.sg

# Quantum and Kinetic Problems: Modeling, Analysis, Numerics and Applications

## Workshop 3: Emergent Phenomena – from Kinetic Models to Social Hydrodynamics (16 - 20 December 2019)

Venue: IMS Auditorium, 3 Prince George's Park Singapore 118402

Monday, 16 Dec 2019		
Time	Title	Speaker
0900 - 0910	Registration	
0910 - 0915	Welcome by local organizer	
0915	Chair: Weizhu Bao, National University of Singapore, Singapore	
0915 - 1000	Emergent behaviors of Lohe tensor flocks	Seung-Yeal Ha Seoul National University, Korea
1000 - 1045	A hydrodynamic model for synchronization phenomena	Young-Pil Choi Yonsei University, Korea
1045 - 1115	Group Photo & Coffee Break	
1115 - 1200	Kinetic approximation of optimal control problems for collective dynamics	Giacomo Albi Università degli Studi di Verona, Italy
1200 - 1400	Lunch reception at IMS	
1400	Chair: Lorenzo Pareschi, University of Ferrara, Italy	
1400 - 1500	<i>Distinguished Visitor Lecture Series:</i> Emergent behavior in collective dynamics	Eitan Tadmor University of Maryland, USA
1500 - 1530	Coffee Break	
1530 - 1615	Diffusion of new products in social networks	Gadi Fibich Tel Aviv University, Israel
1615 - 1700	Collective dynamics of quantized vortices in superfluidity and superconductivity	Weizhu Bao National University of Singapore, Singapore
Tuesday, 17 Dec 2019		
Time	Title	Speaker
0900 - 0915	Registration	
0015		

0915	Chair: Seung-Yeal Ha, Seoul National University, Korea	
0915 - 1000	Multifidelity Monte Carlo methods for kinetic equations with uncertainties	Lorenzo Pareschi University of Ferrara, Italy
1000 - 1045	Uncertainty quantification and control for collective phenomena	Mattia Zanella University of Pavia, Italy

Tuesday, 17 Dec 2019		
Time	Title	Speaker
1045 - 1115	Coffee Break	
1115 - 1200	A stable scheme for a 2D dynamic Q-tensor model of nematic liquid crystals	Yongyong Cai Beijing Computational Science Research Center, China
1200 - 1330	Lunch Break	
1330	Chair: Eitan Tadmor, University of Maryland, USA	
1330 - 1415	Swarming models with local alignment effects: phase transitions & hydrodynamics	José Antonio Carrillo Imperial College London, UK
1415 - 1500	Bacterial swarming: experiments and modelling	Gil Ariel Bar Ilan University, Israel
1500 - 1530	Coffee Break	
1530 - 1615	Boltzmann and Fokker-Planck equations modelling the Elo rating system with learning effects	Marie-Therese Wolfram University of Warwick, UK
1615 - 1700	The Aw-Rascle traffic model: Enskog-type kinetic derivation and generalisations	Giacomo Dimarco University of Ferrara, Italy

Wednesday, 18 Dec 2019		
Time	Title	Speaker
0900 - 0915	Registration	
0915	Chair: Tong Yang, City University of Hong Kong, Hong Kong	
0915 - 1000	Rigorous continuum limit for the discrete network formation problem	Jan Haskovec King Abdullah University of Science and Technology, Saudi Arabia
1000 - 1045	Models for data propagation in large-scale computer systems	Michael Herty RWTH Aachen University, Germany
1045 - 1115	Coffee Break	
1115 - 1200	Symbolic computations in PDE	Diogo Gomes King Abdullah University of Science and Technology, Saudi Arabia
1200 - 1330	Lunch Break	
1330	Free Afternoon	

Thursday, 19 Dec 2019		
Time	Title	Speaker
0900 - 0915	Registration	
0915	Chair: José Antonio Carrillo, Imperial College London, UK	
0915 - 1000	A well-posedness theory for the Vlasov- Nordstrom-Fokker-Planck system	Tong Yang City University of Hong Kong, Hong Kong
1000 - 1045	Uniqueness and non-uniqueness of steady states of aggregation-diffusion equation	Yao Yao Georgia Institute of Technology, USA
1045 - 1115	Coffee Break	
1115 - 1200	Eulerian dynamics in multi-dimensions with radial symmetry	Changhui Tan University of South Carolina, USA
1200 - 1330	Lunch break	
1330	Chair: Gadi Fibich, Tel Aviv University, Israel	
1330 - 1415	Regularized 13-moment equations for inverse power law models	Zhenning Cai National University of Singapore, Singapore
1415 - 1445	Numerical simulations of vortex interactions in the nonlinear Schrödinger equation with periodic boundary conditions	Teng Zhang National University of Singapore, Singapore
1445 - 1515	Computing committor functions for the study of rare events using deep learning	Bo Lin National University of Singapore, Singapore
1515 - 1545	Coffee Break	
1545 - 1700	Round table discussion: Opportunities and Challenges in Kinetic Modeling and Simulation	
1800 - 2100	Conference dinner (Volunteer and self-paid)	

Friday, 20 Dec 2019		
Time	Title	Speaker
0900 - 0915	Registration	
0915	Chair: Jan Haskovec, King Abdullah University of Science and Technology, Saudi Arabia	
0915 - 1000	Analysis on the model hierarchy for mean field interacting particle system via non Lipschitz and velocity dependent force	Li Chen Universität Mannheim, Germany
1000 - 1045	Evolution of initial discontinuity for the defocusing complex modified KdV equation	Dengshan Wang Beijing Information Science and Technology University, China
1045 - 1115	Coffee Break	
1115- 1200	Phase field approach for simulating solid-state dewetting problems	Wei Jiang Wuhan University, China
1200 - 1205	Closing Remarks	

Quantum and Kinetic Problems: Modeling, Analysis, Numerics and Applications Workshop 3: Emergent Phenomena – from Kinetic Models to Social Hydrodynamics (16–20 Dec 2019)

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# Kinetic approximation of optimal control problems for collective dynamics

## GIACOMO ALBI

University of Verona, Italy

#### ABSTRACT

Kinetic models arising in the mathematical description of collective behavior have been studied in a wide spectrum of applications such as animal behaviour, cellular aggregation, opinion dynamics and human crowd motion. Our research addresses the design of external control actions which are able to steer a large system of interacting agents towards prescribed stable patterns. We address this challenge by means of optimal control techniques, thus minimizing an energy measure of both the control and the state of the system. In order to circumvent the solution of a large scale non-linear optimization problem arising at the microscopic level we derive a consistent mean-field optimal control problem, where agent dynamics evolve according to a nonlocal PDE model. In order to solve numerically the mean-field optimal control problem we propose a stochastic based on the efficient simulation of a Boltzmann-like model. Hence we derive the solution of the optimal control problem at the level of binary interactions, generating a hierarchy of feedback control for the original dynamics. Furthermore, we will also show that tackling directly the control of such Boltzmann-like model gives a consistent approximation of the meanfield optimal control. Finally we will show that the associated stochastic algorithms are extremely efficient to cope with the solution of the mean-field control problem. Different numerical examples will be presented in the context of consensus dynamics, and swarming models.

# Bacterial swarming: experiments and modelling

## GIL ARIEL

Bar-Ilan University, Israel

#### ABSTRACT

Bacterial swarming is a collective mode of motion in which cells migrate rapidly over surfaces, forming dynamic patterns of whirls and jets. The basic physical principles underlying the swarm and their relation to models of collective motion (both agent-based and continuous) will be reviewed and discussed in the context of the biological properties of swarming cells.

# Collective dynamics of quantized vortices in superfluidity and superconductivity

## Weizhu Bao

National University of Singapore, Singapore

#### ABSTRACT

Quantized vortices have been experimentally observed in type-II superconductors, superfluids, nonlinear optics, etc. In this talk, I will review different mathematical equations for modeling quantized vortices in superfluidity and superconductivity, including the nonlinear Schrodinger/Gross-Pitaevskii equation, Ginzburg-Landau equation, nonlinear wave equation, etc. Asymptotic approximations on single quantized vortex state and the reduced dynamic laws for quantized vortex interaction are reviewed and solved approximately in several cases. Collective dynamics of quantized vortex interaction based on the reduced dynamic laws are presented. Extension to bounded domains with different boundary conditions are discussed.

# A stable scheme for a 2D dynamic Q-tensor model of nematic liquid crystals

## YONGYONG CAI

Beijing Computational Science Research Center, China

#### ABSTRACT

We propose a stable numerical scheme for a 2D dynamic Q-tensor model of nematic liquid crystals. This dynamic Q-tensor model is a  $L^2$  gradient flow generated by the liquid crystal free energy that contains a cubic term, which makes the free energy unbounded from below, and has been avoided in other numerical studies. The unboundedness of the energy brings significant difficulty in analyzing the model and designing numerical schemes. By using a stabilizing technique, we construct an unconditionally stable scheme, and establish its unique solvability and convergence. Our convergence analysis also leads to, as a byproduct, the well-posedness of the original PDE system for the 2D Q-tensor model. Several numerical examples are presented to validate and demonstrate the effectiveness of the scheme.

# Regularized 13-moment equations for inverse power law models

## Zhenning Cai

National University of Singapore, Singapore

#### ABSTRACT

For rarefied gases, classical hydrodynamic equations such as Euler equations and Navier-Stokes equations cannot accurately describe the gas dynamics. The kinetic models such as the Boltzmann equation and the Enskog equation are usually too expensive to solve numerically.

This inspires people to search for models between the hydrodynamic models and kinetic models. We developed a systematic methodology to derive a class of intermediate models called "regularized 13-moment models", which is suitable for slip and transitional flows. The method is implemented for general inverse power law models, which has never been considered before. In our implementation, the derivation of the models are automated by computer codes, and the numerical solver is also automatically generated by programs. The resulting models are tested for shock structure problems, and the results show its capability to capture the correct flow structure in strong nonequilibirum.

# Swarming models with local alignment effects: phase transitions & hydrodynamics

## JOSÉ ANTONIO CARRILLO

Imperial College London, UK

#### ABSTRACT

We will discuss a collective behavior model in which individuals try to imitate each others'velocity and have a preferred asymptotic speed. It is a variant of the wellknown Cucker-Smale model in which the alignment term is localized. We showed that a phase change phenomenon takes place as diffusion decreases, bringing the system from a 'disordered" to an "ordered" state. This effect is related to recently noticed phenomena for the diffusive Vicsek model. We analysed the expansion of the large friction limitaround the limiting Vicsek model on the sphere leading to the so-called Self-Organized Hydrodynamics (SOH). This talk is based on papers in collaboration with Aceves-Sanchez, Barbaro, Bostan, Cañizo and Degond.

# Analysis on the model hierarchy for mean field interacting particle system via non Lipschitz and velocity dependent force

## LI CHEN

Universität Mannheim, Germany

#### ABSTRACT

In this talk, I will briefly present the model hierarchy from interacting particle system to the corresponding hydrodynamic system, where the interaction contains the velocity alignment effect. It has been used to model pedestrian flow and convey band transport. The hierarchy includes the mean field limit from microscopic particle model to mesoscropic Vlasov type equation, and the macroscopic fluiddynamical system after reasonable closure Ansatz. For i.i.d. initial data, we prove the convergence in measure of the N-particle system to the solution of the Vlasov equation with properly chosen cut-off. Results on the propagation of chaos will be also deduced as a byproduct. Furthermore, the existence of weak solution of the Vlasov equation with velocity allignment effect are investigated, which is needed in obtaining the mean field limit. The corresponding hydrodynamic system is an Euler system with nonlocal force and damping, where the influence matrix of velocity alignment is not positive defi nit. Sound speed is used to reformulate the system into symmetric hyperbolic type. The global existence and uniqueness of smooth solution for small initial data is provided.

The talk is based on the join works with Simone Göttlich, Lining Tong, Shu Wang, and Qitao Yin.

# A hydrodynamic model for synchronization phenomena

## Young-Pil Choi

Yonsei University, Korea

#### ABSTRACT

In this talk, I will present a new hydrodynamic model for synchronization phenomena which is a type of pressureless Euler system with nonlocal interaction forces. For the proposed system, we first establish local-in-time existence and uniqueness of classical solutions. For the case of identical natural frequencies, we provide synchronization estimates under suitable assumptions on the initial configurations. We also analyze critical thresholds leading to finite-time blow-up or global-in-time existence of classical solutions. Finally, we numerically investigate synchronization, finite-time blow-up, phase transitions, and hysteresis phenomena.

# The Aw-Rascle traffic model: Enskog-type kinetic derivation and generalisations

## GIACOMO DIMARCO

University of Ferrara, Italy

#### ABSTRACT

In this talk, we discuss the derivation of second order macroscopic traffic models from kinetic descriptions. In particular, we recover the celebrated Aw-Rascle model as the hydrodynamic limit of an Enskog-type kinetic equation out of a precise characterisation of the microscopic binary interactions among the vehicles. In a second part, we discuss optimal control strategies related to the kinetic model under consideration.

# Diffusion of new products in social networks

### Gadi Fibich

Tel Aviv University, Israel

#### ABSTRACT

Diffusion of new products that mainly spread through word-of-mouth is a classical problem in Marketing. This problem falls under the category of spreading on a graph, but it has unique characteristics that set it apart from e.g., spreading of diseases. In this talk, I will discuss how the diffusion is affected by the network structure, physical boundaries, temporal effects, and consumers' heterogeneity.

# Symbolic computations in PDE

### DIOGO GOMES

King Abdullah University of Science and Technology, Saudi Arabia

#### ABSTRACT

Proofs in partial differential equations often require the analysis of integral expressions and through integration by parts obtain equivalent expressions with a definite sign. While these computations are in many cases elementary, they are usually performed using ad-hod methods and may seem more art than science. However, these procedures can be systematized, as pointed out by Ansgar Jungel and his collaborators and in some cases provide identities that would be extremely hard to foresee. In this talk, we discuss a number of algorithms, heuristics, and rigorous results that make it possible to simplify complex integral expressions that arise in the study of partial differential equations. Moreover, we present a software package implementing these methods and discuss some applications in the theory of mean-field games.

# Emergent behaviors of Lohe tensor flocks

### SEUNG-YEAL HA

Seoul National University, Korea

#### ABSTRACT

In this talk, we present a new aggregation model on the space of rank-m tensors with the same size, and study emergent dynamics. Our proposed new model encompass Lohe type models such as the Kuramoto model, the Lohe sphere model and the Lohe matrix models for the ensemble of real rank-0, rank-1 and rank-2 tensors, respectively. In this regard, we call our proposed model as the Lohe tensor model for rank-m tensors with the same size. For emergent dynamics of the proposed model, we employ the ensemble diameter as a Lyapunov functional to derive a Riccati type differential inequality. As a direct application of these differential inequalities, we provide two sufficient frameworks leading to the emergent dynamics for homogeneous and heterogeneous ensembles in terms of system parameters and initial data. This is a joint work with Hansol Park (SNU).

# Rigorous continuum limit for the discrete network formation problem

## JAN HASKOVEC

King Abdullah University of Science and Technology, Saudi Arabia

#### ABSTRACT

Motivated by recent papers describing the formation of biological transport networks we study a discrete model proposed by Hu and Cai consisting of an energy consumption function constrained by a linear system on a graph. For the spatially two-dimensional rectangular setting we prove the rigorous continuum limit of the constrained energy functional as the number of nodes of the underlying graph tends to infinity and the edge lengths shrink to zero uniformly. The proof is based on reformulating the discrete energy functional as a sequence of integral functionals and proving their  $\Gamma$ -convergence towards a continuum energy functional.

# Models for data propagation in large-scale computer systems

## MICHAEL HERTY

RWTH Aachen University, Germany

#### ABSTRACT

In this talk, we present a recent model for the processing of data in largescale computer systems. In the many processor limit a macroscopic equation is obtained. Properties of analytical solutions to the model are discussed and typical structures are identified. A numerical method for efficient simulation is introduced and computational results will be presented. This is joint work with C. Hauck and G. Visconti.

# Phase field approach for simulating solid-state dewetting problems

## Wei Jiang

Wuhan University, China

#### ABSTRACT

We propose a phase field approach for simulating solid-state dewetting and the morphological evolution of patterned islands on a substrate. The evolution is governed by the Cahn–Hilliard equation with degenerate mobilities coupled with contact line boundary conditions. The proposed approach can include the surface energy anisotropy effect into the models. Several important features observed in experiments can be reproduced by numerically solving the proposed models.

# Computing committor functions for the study of rare events using deep learning

## Bo Lin

National University of Singapore, Singapore

#### ABSTRACT

The committor function is a central object of study in understanding transitions between metastable states in complex systems. However, computing the committor function for realistic systems at low temperatures is a challenging task, due to the curse of dimensionality and the scarcity of transition data. In this paper, we introduce a computational approach that overcomes these issues and achieves good performance on complex benchmark problems with rough energy landscapes. The new approach combines deep learning, data sampling and feature engineering techniques. This establishes an alternative practical method for studying rare transition events between metastable states in complex, high dimensional systems.

# Multifidelity Monte Carlo methods for kinetic equations with uncertainties

### LORENZO PARESCHI

University of Ferrara, Italy

#### ABSTRACT

The development of efficient numerical methods for kinetic equations with stochastic parameters is a challenge due to the high dimensionality of the problem. A tried and true approach for approximating statistics of quantities of interest is Monte Carlo sampling, in which, for each Monte Carlo realization, the random outputs are obtained by solving the resulting deterministic equation. While simple and robust, Monte Carlo sampling is plagued by slow convergence, a deficiency that may render it unusable when the underlying deterministic model is computationally expensive like the case of kinetic equations. Multifidelity control variate strategies based on surrogate models are capable to accelerate considerably the slow convergence of standard Monte Carlo methods for uncertainty quantification. In this talk we survey some recent results on this class of methods with a particular emphasis to the case of the Boltzmann equation and related models with uncertainties.

# Emergent behavior in collective dynamics

### EITAN TADMOR

University of Maryland, USA

#### ABSTRACT

A fascinating aspect of collective dynamics is the self-organization of small-scales and their emergence as higher-order patterns – clusters, flocks, tissues, parties. The emergence of different patterns can be described in terms of few fundamental "rules of interactions". I will discuss recent results of the large-time, large-crowd dynamics, driven by anticipation that tend to align the crowd, while other pairwise interactions keep the crowd together and prevent over-crowding.

In particular, I address the question how short-range interactions lead to the emergence of long-range patterns, comparing geometric vs. topological interactions.

# Eulerian dynamics in multi-dimensions with radial symmetry

## Changhui Tan

University of South Carolina, USA

#### ABSTRACT

The Eulerian dynamics describes many interesting phenomena in fluid mechanics. In this talk, I will discuss several equations that lie in this category, including the damped Burgers equation, the Euler-Poisson equation and the Euler alignment equation. Though a lot of work has been done for the problems in one-dimension, much less is known in multi-dimensions, due to the effect of the "spectral gap". I will explain the main difficulty of controlling the spectral gap, and introduce a new way to handle the term in the case when the solution is radially symmetric.

# Evolution of initial discontinuity for the defocusing complex modified KdV equation

DENGSHAN WANG

Beijing Information Science and Technology University, China

#### ABSTRACT

The complete classification of solutions to the defocusing complex modified Korteweg-de Vries (cmKdV) equation with the step-like initial condition is given by Whitham theory. The process of studying the solution of cmKdV equation can be reduced to explore four quasi-linear equations, which predicts the evolution of dispersive shock wave. The results obtained here are quite different from the defocusing nonlinear Schrödinger equation: the bidirectionality of defocusing nonlinear Schrödinger equation determines that there are two basic rarefaction and shock structures while in the cmKdV case three basic rarefaction structures and four basic dispersive shock structures are constructed which lead to more complicated classification of step-like initial condition, and wave patterns even consisted of six different regions while each of wave patterns is consisted of five regions in the defocusing nonlinear Schrödinger equation. Direct numerical simulations of cmKdV equation are agreed well with the solutions corresponding to Whitham theory.

# Boltzmann and Fokker-Planck equations modelling the Elo rating system with learning effects

MARIE-THERESE WOLFRAM

University of Warwick, UK

#### ABSTRACT

In this talk we discuss kinetic rating models for a large number of players, which are motivated by the well-known Elo rating system used in chess, soccer and football. In the kinetic setting each player is characterised by a non-observable intrinsic strength and an observable rating. After each game, the rating and possibly the strength are updated. One wishes that the ratings converge to the intrinsic strength and thus reproduce the correct ranking. We state and analyse the respective Boltzmann type models and derive the corresponding nonlinear, nonlocal Fokker-Planck equation. We investigate the existence of solutions to the Fokker-Planck equation and discuss their behaviour in the long time limit. Furthermore, we illustrate the dynamics of the Boltzmann and Fokker-Planck equation with various numerical experiments.

# A well-posedness theory for the Vlasov-Nordstrom-Fokker-Planck system

## TONG YANG

City University of Hong Kong, Hong Kong

#### ABSTRACT

The Vlasov-Nordstrom-Fokker-Planck system that is a relativistic generalization of the well-known Vlasov-Poisson-Fokker-Planck system in the gravitational case, describes the ensemble motion of collision particles interacting by means of their own self-generated gravitational forces. In this talk, we will present a result on the global existence and large-time decay rates of the classical perturbative solution to its Cauchy problem. This is a joint work with Renjun Duan and Shuangqian Liu.

# Uniqueness and non-uniqueness of steady states of aggregation-diffusion equation

## ΥΑΟ ΥΑΟ

Georgia Institute of Technology, USA

#### ABSTRACT

In this talk, I will discuss a nonlocal aggregation equation with degenerate diffusion, which describes the mean-field limit of interacting particles driven by nonlocal interactions and localized repulsion. When the interaction potential is attractive, it is previously known that all steady states must be radially decreasing up to a translation, but uniqueness (for a given mass) within this class was open, except for some special interaction potentials. For general attractive potentials, we show that the uniqueness/non-uniqueness criteria are determined by the power of the degenerate diffusion, with the critical power being m=2. Namely, for m $i_c=2$ , we show the steady state for any given mass is unique for any attractive potential, by tracking the associated energy functional along a novel interpolation curve. And for 1<sub>1</sub>m<sub>1</sub>2, we construct examples of smooth attractive potentials, such that there are infinitely many radially decreasing steady states of the same mass. This is a joint work with Matias Delgadino and Xukai Yan.

# Uncertainty quantification and control for collective phenomena

## MATTIA ZANELLA

University of Pavia, Italy

#### ABSTRACT

We develop a hierarchical description of controlled multiagent systems in the presence of uncertain quantities by means of kinetic-type control strategies with applications to social and traffic models. Binary feedback controls are designed at the level of agent-to-agent interactions and then upscaled to the global flow via a kinetic approach based on the Boltzmann equation. The passage to hydrodynamic equations for constrained kinetic models of collective behavior is possible taking into account several closure methods. The action of the control is capable to dampen structural uncertainties naturally embedded in realistic dynamics and to promote effective decision-making tasks.

# Numerical simulations of vortex interactions in the nonlinear Schrödinger equation with periodic boundary conditions

TENG ZHANG

National University of Singapore, Singapore

#### ABSTRACT

In this talk, I will show the numerical simulations on quantized vortices under the 2D nonlinear Schrödinger equations with periodic boundary conditions. An efficient method for initial setups is proposed and the numerical simulation results coincide well with the reduced dynamical laws under the vanishing momentum assumption on squared domains. The simulations on non-vanishing momentum cases as well as general rectangle domain cases provide some extension guesses to the reduced dynamical laws. Vortex merging, phase in-painting, periodic vortex trajectories and some other interesting phenomena are also shown.