Autumn School

From Interacting Particle Systems to Kinetic Equations

modelling, control and numerical methods

26–30 November 2018

Università di Verona
Dipartimento di Informatica

INdAM
GNCS
Gruppo Nazionale per il Calcolo Scientifico

School program

Schedule, Verona 26-30 2018 ***From interacting particle systems to kinetic equations***					
Day	Monday 26	Tuesday 27	Wednesday 28	Thursday 29	Friday 30
Location	Ca' Vignal	Polo S. Marta (Veronetta)			Ca' Vignal
9:00-9:30	Registration	M2: Fornasier SMT02	M1: Carrillo SMT02	M2: Fornasier SPC	
9:30-10:00	M1: Carrillo Sala Verde				F3: Zanella Aula Alfa
10:00-10:30					
10:30-11:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00-11:30	Coffee Break	M1: Carrillo SMT02	M2: Fornasier SMT02	M3: Wang SPC	F1: Kalise Aula Alfa
11:30-12:00	M3: Wang Sala Verde				
12:00-12:30					Conclusion
12:30-13:00		Lunch Break	Lunch Break	Lunch Break	
13:00-13:30	Lunch Break				
13:30-14:00					
14:00-14:30		M3: Wang SMT02	F3: Zanella SMT02	F1: Kalise SPC	* = TBC
14:30-15:00	F2: Totzeck Aula B				
15:00-15:30			F2: Totzeck SMT02	Break	
15:30-16:00		Break		Junior Researcher Meeting	
16:00-17:20		Junior Researcher Meeting	Social activity*		
20:00-23:00		Social Dinner			

Minicourses

M1: Agent Models of 1st and 2nd order: From micro to macro

José A. Carrillo (Imperial College London)

During this course I will discuss microscopic models of collective behavior and consensus of first and second order, their rich dynamical structure and the stability properties of particular solutions such as flocks and mills. I will also discuss how to coarse grain these models into kinetic and macroscopic PDEs and how to connect and analyse the different type of models.

M2: Mean-field optimal control and other types of games

Massimo Fornasier (Techniche Universität München)

In the first part of the course we introduce the concept of mean-field optimal control, which is the rigorous limit process connecting finite dimensional optimal control problems with ODE constraints modeling multi-agent interactions to an infinite dimensional optimal control problem with a constraint given by a PDE of Vlasov-type, governing the dynamics of the probability distribution of interacting agents. In the second part of the course we introduce and study a mean-field model for a system of spatially distributed players interacting through an evolutionary game driven by a replicator dynamics. Strategies evolve by a replicator dynamics influenced by the position and the interaction between different players and return a feedback on the velocity field guiding their motion.

M3: Numerical methods for kinetic and macroscopic equations

Li Wang (University of Minnesota)

In this short course, I will first discuss numerical aspects related to kinetic equations, including the development of asymptotic preserving methods with multiple scales, and stability analysis in both forward and inverse setting in the presence of uncertainty. Then I will discuss the numerical methods for macroscopic equations that come from the coarse-graining of the microscopic system, with emphasis on their connection to free boundary dynamics and variational formulation.

Focused Seminars

F1: Numerical Methods for Control and Games over Multiscale Agent-Based Models

Dante Kalise (Imperial College London)

We will discuss different approximation techniques for the solution of optimal control problems and games where the governing dynamics are give by multiscale models. We will start by reviewing some classical results concerning the solution of nonlinear optimal control problems, illustrating some of the difficulties which arise when the number of agents increases. This will lead us to mean-field and multiscale models, for which we will study their approximation within the framework provided by PDE-constrained optimization. Finally, starting from mean-field type control problems, we will move towards the numerical solution of mean field games.

F2: Herding Sheep - a mathematical approach

Claudia Totzeck (Technische Universität Kaiserslautern)

In this seminar we discuss a model for the application of herding sheep. The starting point is the interaction of the sheep crowd itself and then the interaction of the sheep with the guides. Then the question of well-posedness is discussed before we can implement optimisation strategies to obtain simulation results.

F3: Uncertainty quantification for kinetic equations of collective behavior

Mattia Zanella (Politecnico di Torino)

In this seminar we concentrate on collocation and stochastic Galerkin methods for the uncertainty quantification of Vlasov–Fokker–Planck (VFP) equations with nonlocal flux. In particular, we develop methods that preserve their structural properties and that are spectrally accurate in the random space. In contrast to a direct application of classical uncertainty quantification methods, which are typically lead to the loss of positivity and of entropy properties, the proposed schemes are capable to achieve high accuracy in the random space without losing non-negativity of the solution, which dissipates the entropy under suitable assumptions. Applications of the developed methods will be presented in the context of social and traffic dynamics.

Junior Researcher Meeting			
Tue 27, SMT02		Thu 29, SPC	
16:00-16:20	Bonafini	15:30-15:50	Bailo
16:20-16:40	Estrada	15:50-16:10	Thomann
16:40-17:00	Loy	16:10-16:30	Zoppello
17:00-17:20	Segala		

Abstracts

Fully discrete positivity-preserving and energy-decaying schemes for aggregation-diffusion equations with a gradient flow structure

Rafael Bailo (Imperial College London)

We propose fully discrete, implicit in time finite volume schemes for general nonlinear nonlocal Fokker-Planck type equations with a gradient flow structure, usually referred to as aggregation-diffusion equations, in any dimension. The schemes enjoy the positivity-preserving and energy-decaying properties, essential for their practical use. The first order in time and space scheme unconditionally verifies these properties for general nonlinear diffusion and interaction potentials while the second order scheme does so provided a CFL condition holds. Dimensional splitting allow us to construct these schemes with the same properties and a reduced computational cost in higher dimensions. Numerical experiments validate the schemes and show their ability to handle complicated phenomena in aggregation-diffusion equations such as free boundaries, metastability, merging, and phase transitions.

A convex approach to the Steiner problem

Mauro Bonafini (University of Trento)

The Steiner Tree Problem (STP) can be described as follows: given N points $P_1, \dots, P_N$ in $\mathbb{R}^d$ find a connected graph $F \subset \mathbb{R}^d$ containing the points P_i and having minimal length. From a theoretical point of view the situation is well understood: an optimal graph F always exists and can be described as a union of segments connecting the endpoints, possibly meeting at 120° in at most $N-2$ further branch points, called *Steiner points*. Any optimal graph turns out to be a tree and is thus called a *Steiner Minimal Tree* (SMT).

The question has been widely studied through combinatoric optimization techniques and finding a Steiner Minimal Tree is known to be a NP hard problem (and even NP complete in certain cases). Nonetheless, the problem has recently attracted a lot of attention in the Calculus of Variations community and several authors have proposed different approximations of it, mainly in the planar case and using a phase field based approach together with some coercive regularization.

In this communication we present a convex framework for STP which is based on a reformulation of the problem in terms of an optimization over a suitable family of tensor valued measures. The resulting convex problem maintains its validity in any dimension and, with the appropriate modifications, also on manifolds. In many cases sharpness of the formulation can be proved via calibration type arguments.

From a numerical point of view we end up with a conic problem involving a set of 2^{N-1} quadratic constraints which can then be solved either via a conic solver or via primal–dual proximal schemes. A localization procedure is also implemented so to focus the computational effort only around the optimal 1d structure. Examples in $\mathbb{R}^2$, $\mathbb{R}^3$ and in the surface case are presented.

[1] Mauro Bonafini, Giandomenico Orlandi, and Édouard Oudet. Variational approximation of functionals defined on 1-dimensional connected sets: the planar case. SIAM J. Math. Anal., 2018.

[2] Mauro Bonafini and Édouard Oudet. A convex approach to the Gilbert–Steiner problem. arXiv:1810.05417, 2018.

[3] Andrea Marchese and Annalisa Massaccesi. The Steiner tree problem revisited through rectifiable G-currents. Adv. Calc. Var., 9(1):1939, 2016.

Nonlocal macroscopic limits of kinetic equations in biological and robotic systems

Gissell Estrada-Rodriguez (Maxwell Institute and Heriot-Watt University)

In this talk I will clarify the form of biologically relevant PDE descriptions when the movement of organisms is governed by long distance runs, according to an approximate Lévy distribution as has been observed in the case of bacteria *E. coli* [2] and T cells [3]. We consider a microscopic velocity-jump model in which an individual performs occasional long jumps and derive the appropriate kinetic-transport equations, where the collision term describes the nonlocal motion. Under a perturbation argument and an appropriate hyperbolic scaling in space and time, we derive fractional Patlak-Keller-Segel [1] and space-time fractional diffusion equations [4].

Motivated by these biological examples we combine superdiffusive random movement with emergent collective behaviour from local communications to describe efficient search strategies in swarm robotic systems. Starting from a kinetic equation which describes the movement of robots based on alignment, collisions and occasional long distance runs, we obtain a system of evolution equations for the fractional diffusion for long times. We show that the system allows efficient parameter studies for a search problem, addressing basic questions like the optimal number of robots needed to cover an area in a certain time.

[1] G. Estrada, H. Gimperlein, K. J. Painter. *Fractional Patlak-Keller-Segel equations for chemotactic superdiffusion*, SIAM Journal on Applied Mathematics, 78 (2018), pp. 1155-1173.

[2] E. Korobkova, T. Emonet, J.M.G Vilar, T.S. Shimizu, P. Cluzel. (2004). *From molecular noise to behavioural variability in a single bacterium*, Nature 428, 574–578.

[3] T. Harris et al. (2012). *Generalized Lévy walks and the role of chemokines in migration of effector CD8+ T cells*, Nature 486, 545–548.

[4] G. Estrada, H. Gimperlein, K. J. Painter, J. Stocek. *Space-time fractional diffusion in immune cell models with delay*, M3AS to appear (2018), arXiv: 1802.08675.

Cell migration: velocity-jump process or microscopic algorithms?

Nadia Loy (Politecnico of Torino and University of Torino)

Cell migration is the process that is at the basis of the formation and the maintenance of multicellular organisms. Cells move by run and tumble, that is a kind of dynamics in which the cell alternates runs over straight lines and re-orientations. During this erratic motion, cells may interact with each other and with the external environment in which there may be chemical signals, nutrients or fibers of the extra-cellular matrix. Such factors may bias the choice of the velocity after a re-orientation. In mathematical biology the run and tumble has been successfully described by velocity jump processes implemented in kinetic equations: in this framework, the transition probability of assuming a certain post-tumbling velocity is the key element of the model.
It is widely known that kinetic models also allow to describe the dynamics of particles through microscopic rules. Such dynamics can be included in an evolution equation for density function $f(v,t)$ that is a collision-like weak Boltzmann equation. We want to establish a parallelism between velocity jump processes and collision-like models and to see which analytical and numerical techniques may be used in the two approaches.

[1] Nadia Loy, Andrea Tosin, *Kinetic models for cell migration: a parallelism between velocity jump processes and binary interaction algorithms*, in preparation.

[2] Nadia Loy, Mattia Zanella, *Structure preserving schemes for nonlinear Fokker-Planck equations with anisotropic diffusion*, in preparation.

Tracking and filtering on SE(2)

Chiara Segala (University of Trento)

Attitude estimation is a core problem in many robotic systems, such as unmanned aerial and ground vehicles. The configuration space of these systems is properly modelled exploiting the theory of Lie groups. In this talk we propose a second-order-optimal minimum-energy filter on the matrix Lie group SE(2). The mathematics behind it is quite challenging and is not a simple generalization of previous results on Lie groups.

In the last decades many linear and nonlinear, deterministic and stochastic, observers have been proposed in the literature, some of them exploiting the theory of Lie groups to provide the proper mathematical structure for the attitude of a mechanical system [1].

We propose a *second order optimal minimum energy filter*. The filter is based on the results of Mortensen [2] where a methodology of generating progressive realizable approximations of a minimum-energy functional was proposed. The solution is obtained by differentiating the boundary conditions of the associated optimal control problem. It is called *second order* optimal in the sense that it is a truncation of the exact solution that would be an infinite dimensional system. The filter takes the form of a gradient observer coupled with a kind of Riccati differential equation that updates its gain (similarly to the standard Kalman filter).

The theoretical result in [3] is our starting point [4]. We apply the theorem for a general Lie group to the case of a system modelled on the Lie group SE(2). Such group is very important to model vehicles moving on a plane and so, coupled with the dynamical part, to estimate their pose. However it is worth highlighting that this work is not just a 'straightforward' extension of the result in [3]. The SE(2) case turns out to be particularly complicated since we don't have the Lie algebra isomorphism between $\mathfrak{se}(2)$ and $\mathbb{R}^3$. Contrary to the SO(3) case, we can't identify the bracket operation of the Lie algebra $\mathfrak{se}(2)$ with the classical cross product in $\mathbb{R}^3$.

Our main contribution is then to derive a second order optimal minimum energy filter for SE(2) and to provide all the mathematics for the many technical operations needed to compute it.

We formulate the problem and we recall the explicit formula for the second-order-optimal minimum-energy filter on a general Lie group as stated in [3]. We described the SE(2) case, where we provide the main contribution in a Proposition with proof and all the mathematical details.

[1] F. Bullo and A.D. Lewis, “Geometric Control of Mechanical Systems”, *Springer*, New York, 2005.

[2] R.E. Mortensen, “Maximum-likelihood recursive nonlinear filtering”, *Journal of Optimization Theory and Applications*, vol. 2, no. 6, 1968, pp 386394.

[3] A. Saccon, J. Trumpf, R. Mahony and A.P. Aguiar, “Second-Order-Optimal Minimum-Energy Filters on Lie Groups”, *IEEE Transactions on Automatic Control*, vol. 61, no. 10, 2016, pp 29062919.

[4] C. Segala, N. Sansonetto and R. Muradore, Second-Order-Optimal Filter on TSE(2) and Applications. Under submission.

A second order positivity preserving well-balanced finite volume scheme for Euler equations with gravity

Andrea Thomann (Università degli Studi dell'Insubria)

We present a well-balanced finite volume scheme for the compressible Euler equations with gravity where the approximate Riemann solver is derived using a Suliciu relaxation approach. Besides the well-balanced property, the scheme is robust with respect to the physical admissible states. General hydrostatic solutions are captured up to machine precision by deriving for a given initial value problem suitable time-independent functions and use them in the discretization of the source term. The first order scheme is extended to second order by reconstructing in equilibrium variables while preserving the well-balanced and robustness properties.

[1] Vivien Desveaux, Markus Zenk, Christophe Berthon, and Christian Klingenberg. *A well-balanced scheme to capture nonexplicit steady states in the Euler equations with gravity*, International Journal for Numerical Methods in Fluids, 81(2):104–127, 2016.

[2] Debojyoti Ghosh and Emil M. Constantinescu, *Well-Balanced Formulation of Gravitational Source Terms for Conservative Finite-Difference Atmospheric Flow Solvers*, American Institute of Aeronautics and Astronautics, jun 2015.

Game Theoretic Decentralized Feedback Controls in Markov Jump Processes

Marta Zoppello (University of Padova) In recent years, dynamics on networks have sparked

interest in different application domains such as data transmission, security, traffic flows and consensus. We study a decentralized routing problem over a network, using the paradigm of mean-field games with large number of players. Building on a state-space extension technique, we turn the problem into an optimal control one for each single player. The main contribution is an explicit expression of the optimal decentralized control which guarantees the convergence both to local and to global equilibrium points.

[1] F. Bagagiolo, D. Bauso, R. Maggistro, M. Zoppello.
Game Theoretic Decentralized Feedback Controls in Markov Jump Processes *Journal of Optimization Theory and Applications* 173(2): 704-726 (2017) DOI 10.1007/s10957-017-1078-3

Social Dinner
Tuesday 27, 8 PM

Antica Trattoria al Bersagliere
Via Dietro Pallone, 1 37121 Verona

Please confirm your participation at the registration desk.

https://unimathverona.wixsite.com/optke

Local Organizers: G. Albi, A. Marigonda, G. Orlandi
Scientific Committee: G. Albi, M. Caliari, G. Dimarco, L. Pareschi