COST Action 18232 - Mathematical models for interacting dynamics on networks

Joint WG2&WG5 Workshop

Modelling, analysis and numerical methods of complex dynamics

June 21-23, 2023

CIRM, Luminy, France

Abstracts of lectures

Learning stable cross-diffusion with reaction systems

Silvia Barbeiro
University of Coimbra, Portugal
silvia@mat.uc.pt

After the pioneering work of Keler and Segel in the 1970s cross-diffusion models became very popular in biology, chemistry and physics to emulate systems with multiple species. From a mathematical point of view, cross-diffusion models are described by time-dependent partial differential equations (PDE) of diffusion or reaction-diffusion type, where the diffusive part involves a general nonlinear non-diagonal diffusion matrix. This leads to a strongly coupled system where the evolution of each dependent variable depends on itself and on the others in a way governed by the diffusion matrix. The selection of the optimal coefficients and influence functions that rule the associated PDE system is always a critical question when modeling real phenomena. In this talk we will focus on nonlinear cross-diffusion systems for image filtering. We will start with a concise introduction about complex diffusion and cross-diffusion models for image restoration. Some attention will be given to the numerical discretization of the models and to the qualitative properties of the corresponding computed solutions. Then, we will discuss a flexible learning framework in order to optimize the parameters of the models improving the quality of the denoising process. In particular, we use a back propagation technique in order to minimize a cost function related to the quality of the denoising process while we ensure stability during the learning procedure.

References

[1] S. Barbeiro, D. Lobo. Learning Stable Nonlinear Cross-Diffusion Models for Image Restoration. *Journal of Mathematical Imaging and Vision* 62 (2020), 223–237.

[2] A. Araújo, S. Barbeiro, E. Cuesta, A. Durán, Cross-diffusion systems for image processing: II. The nonlinear case, *Journal of Mathematical Imaging and Vision*, 58 (3) (2017), pp. 447–467.

[3] A. Araújo, S. Barbeiro, P. Serranho, Convergence of finite difference schemes for nonlinear complex reaction-diffusion processes, *SIAM Journal on Numerical Analysis* 53 (1) (2015), 228– 250.

[4] A. Araújo, S. Barbeiro, P. Serranho, Stability of finite difference schemes for nonlinear complex reaction-diffusion processes, *IMA Journal of Numerical Analysis*, 35 (3) (2015), 1381–1401.

From collisional kinetic models to sprays: internal energy exchanges

Frédérique Charles
Sorbonne Université, France
frederique.charles@sorbonne-universite.fr

In this presentation we are interested in models describing the evolution of particles (such as solid dust particles or droplets) in a rarefied gas. We present here a derivation of a fluid-kinetic system in which the gas and the disperse phase are coupled not only by the drag force, but also by the exchange of temperature between the gas and the droplets/dust specks. We start from a kinetic collisional model, based on the hypothesis that collisions between dust particles and gas molecules are inelastic and are given by a diffuse reflexion mechanism on the surface of dust particles. We propose a model which preserves the total energy by introducing a new variable in the density function of macroscopic particles. We then derive an asymptotics to a Vlasov-Euler equation of compressible fluid when two small parameters tend to zero, namely the ratio of masses between gas molecules and dust particles on the one hand, and the Knudsen number of the gas on the other hand. We thus obtain an explicit expression of the transfer of energy between the phases. This work is a collaboration with Laurent Desvillettes.

Asymptotic-preseving discretization and state estimation for barotropic gas transport on networks

Teresa Kunkel
TU Darmstadt, Germany
tkunkel@mathematik.tu-darmstadt.de

We consider the transport of gas through gas pipe networks modeled by the one-dimensional barotropic Euler equations complemented with energy-conserving coupling conditions at the pipe junctions. In the first part of the talk we propose a structure-preserving discretization of the system using mixed finite elements in space and the implicit Euler method in time and show that the solution of the discrete system converges to the exact solution provided that there exists a smooth, subsonic solution that is bounded away from vacuum [1]. We can show that the convergence is uniformly in the friction parameter, i.e., the result also holds in the case of the parabolic limit problem. In the second part of the talk we consider the problem of state estimation, i.e., we want to reconstruct the system state in gas pipes from distributed measurements of one state variable [2]. Therefore we set up an observer-system of Luenberger type that contains additional source terms depending on the measurements and show that the state of the observer system converges exponentially in the long time limit towards the original system state. In both cases the proof is based on a Hamiltonian reformulation of the system, which allows to apply relative energy techniques in order to show the convergence, and due to the energy- conserving coupling conditions the results can be transferred to (star-shaped) networks.

References

[1] H. Egger, J. Giesselmann, T. Kunkel, and N. Philippi. An asymptotic-preserving discretization scheme for gas transport in pipe networks. *IMA Journal of Numerical Analysis*, 2022.

[2] J. Giesselmann, M. Gugat, T. Kunkel. Observer-based data assimilation for barotropic gas transport using distributed measurements. *arXiv*, 2023.

Finite volumes for a generalized Poisson-Nernst-Planck system with cross-diffusion and size exclusion

Annamaria Massimini
TU Wien, Austria
annamaria.massimini@asc.tuwien.ac.at

In this talk I will present two finite volume approaches to modelling the diffusion of charged particles, in particular ions, in constrained geometries, using a degenerate Poisson-Nernst-Planck system with cross-diffusion and volume filling. Both methods use a two-point flow approximation and fall within the framework of exponential fitting schemes. The only difference between the two is the choice of a Stolarsky mean for the drift term that results from a self-consistent electric potential. The first version of the scheme, called (SQRA), uses a geometric mean and is an extension of the square root approximation scheme. The second scheme, (SG), uses an inverse logarithmic mean to create a generalised version of the Scharfetter-Gummel scheme. Both approaches guarantee the decay of a certain discrete free energy. Classical numerical analysis results, as well as some numerical simulations, will be discussed. The latter show that both schemes are effective for moderately small Debye lengths, with scheme (SG) demonstrating greater robustness in the regime of small Debye lengths.

Long-time behavior of scalar conservation laws: old and new

Nicola de Nitti
Friedrich-Alexander-University of Erlangen-Nürnberg, Germany
nicola.de.nitti@fau.de

The main aim of this presentation is to discuss the long-time behavior of scalar conservation laws and its viscous, non-local and numerical variants. Our focus will be on two primary examples: scalar convection-diffusion equations and a nonlocal regularization of the inviscid Burgers' equation.

In the first part of the talk, we will study the asymptotic behavior of the solutions to scalar convection-diffusion equations set in $\mathbb{R}^N$. When the initial datum is integrable, the mass of the solution is conserved along the evolution, leading to the long-time behavior being governed by the source-type solution of a limit equation. The form of this limit equation depends on the relative strength of convection and diffusion.

In the second part, we will consider a nonlocal regularization of the (one-dimensional) inviscid Burgers' equation, where the velocity is approximated by a one-sided convolution with an exponential kernel. We will assume that the initial datum is positive, bounded, and integrable. The asymptotic profile is given by the source-type entropy solution of the Burgers' equation, commonly referred to as the "N-wave".

The key components of our proofs involve suitable scaling arguments and Oleinik-type inequalities.

Finally, we will explore possible extensions of these results to the context of numerical approximation schemes and star-shaped graphs.

References

[1] G. M. Coclite, N. De Nitti, A. Keimer, L. Pflug, and E. Zuazua. Long-time convergence of a nonlocal Burgers' equation towards the local N-wave. *Preprint*, 2023.

[2] M. Escobedo, J. L. Vazquez, and E. Zuazua. Asymptotic behaviour and source-type solutions for a diffusion-convection equation. *Arch. Rational Mech. Anal.*, 124(1):43–65, 1993.

[3] M. Escobedo and E. Zuazua. Large time behavior for convection-diffusion equations in $\mathbb{R}^N$, *J. Funct. Anal.*, 100(1):119–161, 1991.

[4] J. Friedrich, S. Göttlich, and M. Osztfalk. Network models for nonlocal traffic flow, *ESAIM Math. Model. Numer. Anal.*, 56(1):213–235, 2022.

[5] E. Zuazua. Asymptotic behavior of scalar convection-diffusion equations. *Lecture Notes (arXiv:2003.11834)*, 2020.

Extended Models of Diffusion

Srboljub Simić
University of Novi Sad, Serbia
srboljub.simic@dmi.uns.ac.rs

Diffusion is a ubiquitous phenomenon which can modelled from different standpoints. It may be studied by means of statistical methods, within the framework of kinetic theory, or from the macroscopic point of view. Aim of this lecture is twofold. First, it will give an overview of different approaches to diffusion and their basic features. Second, an emphasis will be given on the Maxwell-Stefan model of diffusion and its generalizations. New results concerned with extended/higher-order models of diffusion will be presented, which include dissipation mechanisms other than diffusion.