# Advanced entropy methods for applied PDEs

## Project Summary and Overview

Many-particle systems are of great importance in a wide range of application fields – from gas flows (around airfoils, e.g.) in statistical physics and engineering to the electron transport in quantum systems (nano-semiconductor devices or lasers), from biology (chemotactic motion of cells, e.g.) to chemistry (coagulation and fragmentation phenomena of polymer chains). While the detailed models are clearly very different in all of these application fields, they still have important common features: The huge number of interacting individuals (being gas molecules, electrons, or cells) in such a system makes it impossible to track the time evolution of each individual. Instead one is typically interested in averaged macroscopic quantities like the particle density, average velocity, or temperature, using tools from statistical physics. On this macroscopic level such systems have the tendency to converge to an equilibrium configuration (if left alone). On the other hand, when such a large particle system is subjected to a continuous exterior stimulus (e.g. a force field) it exhibits an interplay between non-equilibrium and equilibrium regimes, which are of particular interest in computational sciences.

This proposal is concerned with the mathematical modeling of many-particle systems using non-linear partial differential equations and their mathematical analysis. In particular we are interested in qualitative properties of the solutions like convergence to equilibrium (with explicit decay rates, if possible). Detailed models for many-particle systems involved the mathematical analysis of high dimensional partial differential equations, called kinetic equations, since a statistical description is performed in "phase space", i.e. position+momentum for a electron cloud or position+size for polymerization. Approximative models are obtained as asymptotic limits of the former ones and they give rise to nonlinear diffusion-type equations/systems with genuinely derived new terms from the kinetic level description, force terms or reactive terms.

The main tool for our approach will be entropy functionals, or relative entropy functionals. By this we mean functionals which have an interpretation at the physical level, but could be more properly called free energies, or enthalpies, etc, depending on the context. We also refer to the methods developed in probability theory, although we have in mind functionals rather designed for nonlinear equations of, for instance, porous media type. "Relative" entropy refers to the case where some equilibrium is known, and the entropy is defined in such a way that the entropy is minimal for the equilibrium [6, 7]. Defining the relative entropy turns out to be an efficient way of taking constraints like mass normalization into account.

Considerable efforts have been done over the last years to take advantage of these ideas [2] and we have now in mind to apply them to less standard problems for which we expect that they can provide a real breakthrough. This is what we mean by "Advanced entropy methods..." which shows up in the title of the project. We shall focus on three questions:

1. Quantum entropies for open quantum systems, with applications in quantum Brownian motion, quantum semiconductors (Wigner-Fokker-Planck equation), and quantum optics (Dicke laser model, e.g.)

2. Entropy methods for reaction-diffusion and coagulation-fragmentation systems, arising in chemical reactions and in population dynamics.

3. Keller-Segel model for chemotaxis: blow-up and asymptotic behavior.

# Objectives

1. *Quantum entropies:* A generic formalism to describe mixed states of a quantum system is provided by density matrices, i.e. positive trace class operators on some Hilbert space. The time evolution of positivity preserving open quantum systems is typically modelled by a Von-Neumann master equation in Lindblad form [31]. Due to the dissipativity of such quantum models, one expects that the solution to many of these problems converges to its equilibrium as time goes to infinity. On finite dimensional Hilbert spaces sufficient conditions have been derived such that the *relative quantum entropy* (or von-Neumann entropy) is indeed a Lyapunov functional [33, 34]. In the infinite dimensional case similar results are only known for a few special models ([32] for the quantum Fokker-Planck equation in a harmonic external potential, e.g.).

   We aim at extending the entropy method for (linear) parabolic PDEs [4, 5, 3] to the non-commutative case of density matrices. To this end the following issues shall be addressed:

   – Identify the simplest dissipative quantum evolution model to serve as an analogue of the classical Fokker-Planck (or Ornstein-Uhlenbeck) equation.

   – Prove the existence of (possibly unique) quantum steady states for a wider class of linear quantum evolution equations (including the quantum Fokker-Planck equation from [32] as a special case). For some special models non-constructive proofs of that type were given in [26, 27].

   – Derive entropy-entropy dissipation estimates for the time evolution. In a Fock space setting related *fermion logarithmic Sobolev inequalities* were derived in [11, 28].

   – Identify the quantum analogue of the Bakry-Emery criterium (cf. [4]).

   – Analyse of the Boltzmann-Uehling-Uhlenbeck equation for quantum particles [21, 25].

   Once decay of the quantum entropy is established, a "quantum Csiszár-Kullback inequality" [30] yields convergence in the trace class norm. Lieb-Thirring type inequalities recently derived in [18] will be important in some aspects of the above discussion.

2. *Entropy methods for reaction-diffusion and coagulation-fragmentation systems:* In the classical theory of reaction-diffusion systems, rates for convergence to equilibrium have been a matter of dominating diffusion, see e.g. [14]. Recently, explicit asymptotic rates of convergence were obtained for reaction-diffusion systems appearing in chemical reactions and population dynamics, where a-priori $L^\infty$ bounds are known, which grow no faster than polynomially in time [15, 17, 16]. These results are based on (system type of) entropy-entropy dissipation inequalities, which combine the entropy dissipation produced by both diffusion and reaction,

but they typically depend on very particular structures of the reactive terms. In this project, we will discuss the following issues:

- Obtain more general results for reaction-diffusion systems and include nonlinear diffusion. To achieve this objective the question of blow-up of solutions and *a priori* $L^\infty$ bounds becomes essential. We expect decomposition of $L^\infty$ bounds into $L^1$ and $L^\infty$ parts will provide room for improvements.

- To understand asymptotic rates towards equilibrium in spatially inhomogeneous coagulation-fragmentation models. No asymptotic rates of convergence towards equilibrium are known so far. For a spatially inhomogeneous Aizenman-Bak model [1] of coagulation and fragmentation polymerization with non-degenerate size-dependent diffusion coefficients, there is work in progress [13] to show explicit exponential decay towards equilibrium as well as uniform in time smoothing-estimates. Refinements of some of these techniques will surely allow to understand more general models.

- Coagulation-Fragmentation models show a unique qualitative feature with respect to other kinetic models, namely, the gelation phenomena [22, 23, 24]. This phenomena is related to the decay of solutions for large sizes since the total mass of monomers might not be conserved. Further understanding of this interesting issue [20] will be addressed.

3. *Keller-Segel model: blow-up and asymptotic behavior:* For Keller-Segel type models, we would like to better understand the effect of nonlinearities on the diffusion coefficient and the chemosensitivity. Such nonlinearities account for the volume effect of cells or can be justified by more elaborate drift-diffusion limit asymptotics. Here the starting point will be the recent note [19], expanding on [8], on finding the best constant for distinguishing the global existence range from the blow-up regime. Preliminary results have been obtained in [12, 9]. The question of behavior of the solutions past the blow-up in the linear diffusion Keller-Segel model is relevant from the rich mathematical structure and new ideas that have to be developed. Different regularizations of the Keller-Segel model can be proposed leading to different approximations for solutions of the equation past the blow-up time. We plan to attack the following items:

   - Models with saturated mobilities will be further analysed. These models are relevant in biological modelling and they provide a natural regularization for the Keller-Segel model.

   - Contraction of suitable distances related to mass-transportation problems for these models could lead to new analytical results in case nonlocal drift terms in the equation are considered. Typically nonlocal term in these biological models lead to non displacement convex functionals. The competition between diffusion and nonlocality determines the asymptotic behavior or these models, either their blow-up or their equilibration [10].

   - Numerical simulation of some the above issues will be conducted to get intuition on some of the results that could be analytically addressed.

## Methodology and Work Plan

The working plan will be based on the complementary expertise of all teams. Below we simply list people from each side that will eventually work in some of the research lines and specific topics between parentheses.

1. *Quantum entropies:* Neumann-Dolbeault-Vega (Steady States), Arnold-Escobedo, Sparber-Aguirre (Time decay), Arnold-Dolbeault-Gentil (Bakry-Emery criterion).

2. *Reaction-Diffusion, Coagulation-Fragmentation systems:* Fellner-Desvillettes-Carrillo (inhomogeneous Aizemann-Bak model), Mischler-Escobedo (gelation).

3. *Keller-Segel model, blow-up and asymptotic behavior:* Dolbeault-Blanchet-Carrillo (saturation), Schmeiser-Dolak-Cáceres (numerical simulation), Carrillo-Rosado-Dolak (Wasserstein approach to saturated diffusion models).

There are 3 different kinds of interaction, we plan to establish:

(i) The interaction between senior researchers by means of short visits to establish the basic ideas, models and methods and to devise novel strategies.
(ii) Longer visits by the young members of the group for maturating ideas and developing the results.
(iii) The organisation of a small event (series of short courses) on the topics of the proposal will be considered during the duration of the project with external funding to this project.

The topics of this research project are openings to new and challenging questions. If the research on these subjects turns out to be successful, it will definitely be one of the components of future european projects in which all participants will be involved.

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