Sujet de stage M2 et de thèse

Responsable du stage et de la thèse:
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Title: *Mathematical and numerical study of multiscale problems arising in quantum or plasma physics.*

1 Context

Multiscale problems arise very often in nature. When we say that a problem is multiscale, we broadly mean that it involves phenomena at disparate spatial and/or temporal scales, spanning over several orders of magnitude. More importantly, these phenomena all play key roles in the problem, so that we cannot correctly model the problem under study without explicitly accounting for all these different scales. The theoretical and numerical treatment of problems with multiple scales has always been an interesting, very useful and challenging task.

In this M2-internship and the following PhD thesis we shall be concerned with two specific multiscale PDEs, namely

- the (non-linear) Schrödinger equation, arising in quantum mechanics

$$\mathbf{i}\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + V\,\psi + \gamma\,|\psi|^2\,\psi\,, \qquad (t,x)\in\mathbb{R}^+\times\mathbb{R}^3\,, \quad \gamma\in\mathbb{R}\,;$$

- the (non-linear) Fokker-Planck equation, arising in thermonuclear fusion plasma physics

$$\partial_t f + v\cdot\nabla_x f + \frac{e}{m}(E+v\times B)\cdot\nabla_v f = \nu\,\nabla_v\cdot\left[(v-u)\,f + \frac{k_B\,T}{m}\,\nabla_v f\right], \quad \forall (t,x,v)\in\mathbb{R}^+\times\mathbb{R}^3\times\mathbb{R}^3\,.$$

Both equations permit to describe the evolution of a system of N charged particles (electrons, ions) in a given or self-consistently computed electric (or electromagnetic) field. Here $\psi(t,x)$ denotes the wave-function, where $|\psi(t,x)|^2\,dx$ represents the probability of finding the particle at time t in the space-volume dx around x; and equally $f(t,x,v)$ stands for the particle distribution function, with $f(t,x,v)\,dv\,dx$ representing the number of particles to be found at time t in the infinitesimal phase-space volume $dv\,dx$ around (x,v).

One of the goals of a numerical scientist is to develop efficient as well as precise numerical schemes (accurate, not time- and not memory-consuming) for the discretization of a given mathematical problem, arising from the modeling of a physical/ biological/chemical phenomenon. It is usually a big challenge to develop numerical schemes which balance well the two rather contradictory requirements of ”efficiency” and ”precision”. Usually one has to make a compromise between these two quantities, meaning that one has to avoid unnecessary computations in order to be performant, however trying at the same time to attain the required accuracy. The main goal of multiscale techniques (which are the main subject of this PhD) is to design microscopic-macroscopic numerical methods, which are more efficient than solving the full microscopic model and at the same time furnish the desired accuracy.

The typical numerical difficulties one encounters when dealing with the numerical resolution of the (non-linear) Schödinger equation or the (non-linear) Fokker-Planck equation are for example:

- the high dimensionality of the problems (many-body problems); $6D$ phase-space;
- the balance or competition between dispersive effects and non-linearity (soliton solutions) in the Schrödinger equation;
- the balance or competition between the transport term and the dissipative collision operator in the Fokker-Planck equation;
- the occurrence of highly oscillating wave-functions (semi-classical limit of the Schrödinger equation); filamentation in the kinetic (Vlasov) equation;
- the numerical preservation of various properties (mass/energy conservation; entropy decay).

2 M2 internship

To start, we shall first review during the internship the basic features of the Schrödinger equation as well as of the Fokker-Planck equation, in particular of the corresponding eigenvalue problems. The aim is then to construct a first spectral method for an efficient resolution of both equations (in a simplified framework), and analyse then this numerical scheme. This shall put the basis of the subsequent PhD thesis.

3 Required knowledge

To cope with this thematic, the PhD student needs some basic knowledge of physics, functional analysis, PDEs, numerical methods, simulation languages (python for example).