COmputing & apprOximating KInetic Equations

I. Problem statement & general aims.

The present proposal is focused on the **numerical simulation** and **analysis** of **kinetic equations** and related models. These models arise in a wide spectrum of applications, ranging from plasma physics to gas dynamics and fluid mechanics. They describe **multi-scale** and **high dimensional** problems, which lead to exhausting computations and act as a significant bottleneck for advanced modeling and simulation in applied sciences. Our goal is to design efficient numerical schemes, capable to encompass both the multi-scale dynamics of kinetic models, as well as their high dimensional nature. This project will address two key categories of numerical methods:

- the first one is based on a **Lagrangian** point of view which is robust and well suited to treat an arbitrary geometry and high dimensional problems ;
- the second one is related to **Eulerian** methods for very accurate approximations in particular when the exact solution is close to thermal *equilibrium*.

I..1 Lagrangian point of view

The **particle** method is the basis of a variety of popular schemes to transport densities in computational plasma physics and fluid mechanics. It is conceptually simple and straightfoward to implement. However it suffers from weak convergence properties which in practice often result in "noisy", *i.e.* oscillating solutions. To improve the **accuracy** of the method several variants have been developed over the past decades, such as particle **remappings** [CRS09, CPC16, CPS17, D24], weight correction schemes [CKS96]. In this proposal we adopt the remapping approach and aim to design this essential step according to the particular **features of the physical flow**.

In the case of compressible flows, our methodology is based on moving Voronoï meshes for the numerical simulation of shocks and internal interfaces between different gases [D24]. To our knowledge, the mathematical foundations of moving Voronoï mesh techniques interpreted as particle methods are not discussed *per se* in the literature. We plan to develop numerical methods which on the one hand are based on rigorous **Lagrangian Voronoï meshes** and which, on the other hand, can be interpreted as particle methods which rigorously preserve mass, total impulse and total energy and for which an additional discrete entropy inequality can be proved. A first order in space and time numerical scheme has been analyzed and applied to basic test problems in [D24]. The method is based on the closed form formula of the partial derivative of the volume of Voronoï cells with respect to the generators. This preliminary work is the basis of more elaborated methods where all the arsenal of modern computational fluid dynamics techniques (high-order techniques, non linear limiters, various remeshing techniques) can be introduced to enhance the final quality of practical simulations.

For incompressible flows, we aim to design **particle-in-cells** [BL04, RC20] and **semi-Lagrangian** methods [SRB99] specifically oriented towards transport kinetic equations, thereby targeting the complexities inherent in **multi-scale** and **high-dimensional** problems. The main feature of this approach is concerned with the coupling of charged particles with a Poisson or a Maxwell solver. We may consider the **Vlasov-Poisson system** taking into account electrical interactions with a strong external magnetic field applied to confine the plasma. We have already developed a class of accurate and stable (implicit/explicit) time discretization methods to handle with the stiffness due to the intense magnetic field and to filter high frequencies [FR17, FR20, CCL20]. The key idea is to reformulate the model by leveraging the fast and slow scales of the solution. Our first focus is to extend our approach to derive numerical schemes that are able to preserve not only the **asymptotic limit**, but also the **structure** (Hamiltonian or Poisson structure, invariants preserving,...). One of the major difficulty in these problems lies in the fact that the Hamiltonian depends on (fast scale) time which makes difficult the use of standard methods (discrete gradient technique). We intend to recast the strategies proposed by some members of this proposal in such a way some schemes that are popular in computational physics literature (Boris, Crank-Nicolson) can be used to preserve some invariants. Moreover, strategies like Scalar Auxiliary Variables or Invariant Energy

Quadratization [SMB18, SXY23] will also be analyzed and combined to our framework. Furthermore, to reduce the inherent noise of particle methods [CPC16], we will develop **linearly transformed particles** for the remapping procedure and aim to carry out a complete convergence analysis for the uniform norm.

In addition to the aforementioned methods, we will also explore the implementation of **semi-Lagrangian** methods, which are often based on time splitting, permitting to reduce the computations to a sequence of one dimensional constant advection steps. However some situations require full multi-dimensional advection, which leads to a loss of mass conservation. If mass conservative versions exist [ZC22, EM24], they suffer from high computational cost, which is prohibitive in high dimension. Following [YF14], we plan here to elaborate efficient conservative semi-Lagrangian methods specifically adapted to cartesian grids, while being able to treat relevant **tokamak/stellerator geometries** and Vlasov models, ensuring that the numerical solutions satisfy the fundamental conservation laws.

Our commitment to these methods stems from their foundational ability to incorporate a priori information into the discretization process. This integration not only promotes accuracy but also conserves valuable computational ressources. Preliminary publications [D24, FR17, FRZ21] indicate that our scientific groundwork is robust enough to support concurrent advancements in both implementation and numerical analysis, enabling us to push the frontiers of kinetic theory computation effectively.

I..2 Eulerian point of view

The Eulerian approach consists in solving an equation by discretizing the phase space on which it is set. Our goal is to design Eulerian numerical methods which are **stable**, and which encompass **the long time behavior** of kinetic model as well as their **multi-scale behavior** in oscillating regimes. We aim for numerical methods which are both efficient and for which we can rigorously prove the aforementioned properties. Our methodology is based on **spectral discretization** in the velocity space, where the original kinetic equation is recast into a large hyperbolic system of balanced laws [BCF22, BCF23, DD24].

Even if Eulerian methods have been successfully applied to high dimensional transport equations such as the **Vlasov-Poisson system** [EM24, PDM23, PMK23], there are, however, very few results concerning their stability [BCF22, BCF23, DD24]. Understanding the stability properties of numerical methods is key in order to achieve efficient simulations, especially in the context of kinetic equations, where the transport of particles may lead to stringent stability conditions and thus increase the computational cost. Our goal is to design Eulerian solvers for which we can prove conditional or unconditional stability properties in high dimensional frameworks and then, to subsequently implement these efficient numerical methods. Furthermore, we aim for a convergence theory in agreement with the structure of the underlying nonlinear kinetic models. Our methodology is to take advantage of the regularity theory of the continuous problem and to provide error estimates on the spectral method when the number of discrete modes is large enough.

Our second focus lies in the simulation of kinetic models over large periods of time. Our goal is to capture numerically the macroscopic relaxation induced by microscopic collisions, described thanks to physically relevant models such as **Landau operator** (resp. **Boltzmann operator**) in the context of plasma physics (resp. rarefied gas dynamics). More precisely, we will develop Eulerian numerical schemes for these models and rigorously analyze their long time behavior: we aim at proving quantitative estimates ensuring that our approximations enjoy the same relaxation properties as the solution to the continuous model. Our methodology is to develop numerical schemes which preserve the structure of the stationary states to the continuous model. Then, we will extend the spectral analysis of the underlying kinetic model to its discrete counterpart in order to prove that these *equilibria* are stable at the discrete level [BF24, BF24b]. More precisely, we will focus on discrete hypocoercive methods, which rely on a fine understanding of the linearized dynamics in kinetic theory [H06, AAC18, HR18] and dissipative hyperbolic systems [BZ11, CBD22]. To conclude, we emphasize that preserving the long time behavior at the discrete level is essential to design efficient solver. Indeed these solvers typically enjoy stability properties which allow to reduce computational costs.

Our last interest lies in the numerical simulation and analysis of multiscale regimes arising in plasma physics. We will focus separately on the quasi-neutral limit [CDV16, CPS17][a] and on the strongly magnetized regimes of the **Vlasov-Poisson system** [HK10][b]. These regimes are particularly relevant in applications such as nuclear fusion, as they describe some key features of plasma within a Tokamak reactor. The simulation of these regimes is particularly intricate, as they both generate fast oscillations in time. Our goal is therefore to design numerical schemes capable to filter these fast oscillations and thus accurately account for the underlying limiting dynamics. Our methodology consists in applying a spectral decomposition of the velocity variables. This approach has revealed to be particularly efficient in this context, as it allows to decompose the oscillating components of the solution [CDD23].

Central to our approach is the effective use of local and global information—specifically, the multi-scale data pertaining to local *equilibria*—that is inherent in the physical phenomena or the governing equations. By leveraging this information, we propose to design advanced approximation strategies and develop numerical codes that seek to maximize efficiency and accuracy while minimizing computational costs.

To uncover the practical implementation challenges—including CPU and memory requirements, linear algebra issues for implicit schemes, and compatibility with modern computing architectures—we will test our methods on demanding physical *scenarii*, specifically within both magnetized and non-magnetized plasma physics.

II. Consortium.

The team of the proposal involves **15 mathematicians** (juniors and seniors) with various competences in numerical analysis, modeling and PDE analysis, planning to devote in average about **half of their research time** to the project over the next **five years**. Most of them have collaborated with at least one other member of the project and together they do cover the wide spectrum of required technical skills : PDE analysis (Badsi, Crin-Barat, Herau), analysis of **numerical schemes** for hyperbolic systems (Després, Vignal) and kinetic equations (Bessemoulin-Chatard, Blaustein, Charles, Filbet, Mehrenberger) and scientific computing (Crestetto, Crouseilles, Martaud). We also anticipate that the realization of the project is likely to involve collaborations with some other experts external to the project but connected to some of its members.

The team is planned to be administratively split in **two partners**, based on geographical grounds:

- The **South** pole managed by the **scientific coordinator** from **Toulouse**

  F. Charles, T. Crin-Barat, F. Filbet, M. Mehrenberger, K.H. Trinh (PhD), M.H. Vignal
  Grenoble Toulouse Toulouse Aix-Marseille Toulouse Toulouse

- The **North** pole managed by **Marianne Bessemoulin-Chatard** in **Nantes**

  M. Badsi, M. Bessemoulin-Chatard, A. Blaustein, A. Crestetto, N. Crouseilles, B. Després,
  Nantes Nantes Lille Nantes Rennes Sorbonne
  B. Grosse (PhD), F. Hérau, L. Martaud.
  Nantes Nantes Rennes

Both **partner managers** will be **involved at a 75% rate**. **Two post-docs and PhD** researchers, supported by this ANR project, will study modeling and numerical analysis in Toulouse (one post-doc) and Nantes (one post-doc and half PhD).

Past contributions of the P.I. have already involved all the technical aspects of the project (scientific computing, numerical analysis, computational models for fluids and plasmas). He has already collaborated with several members of the project. In direct connection to the project, he has received a prize from the French Academy of Science in 2012, was selected as a junior member of the Institut Universitaire de France in 2015 and is in the editorial board of SIAM J. Sci. Computing since 2021.

The project team has several members with extensive experience in engaging with research institutions focused on addressing underlying physical challenges. Notably, they have collaborated with researchers from CEA (French Alternative Energies and Atomic Energy Commission) and the startup Renaissance Fusion.

[a] the Debye length goes to zero compared to the natural physical space scale, leading to a singular limit in the Poisson equation [b] the Larmor radius depending on the magnitude of the external magnetic field goes to zero compared to the Debye length, leading to a singular limit in the Lorentz force occuring in the Vlasov equation

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