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Postdoctoral Research Project Proposal

Numerical Analysis of the Lattice Boltzmann Method for Transport-Reaction-Diffusion Equations

1- Location, Duration, and Supervision

The postdoctoral research project will be carried out over a two-year period starting in September 2027 at the *Laboratoire de Mathématiques d'Orsay* (LMO), Paris-Saclay University, under the supervision of Benjamin Graille (Paris-Saclay University, LMO) and Thomas Bellotti (CNRS, CentraleSupélec, EM2C).

The postdoctoral fellow will join a research group consisting of Thomas Bellotti, Filipa Caetano (Paris-Saclay University, LMO), François Dubois (CNAM), and Benjamin Graille. The project will also involve interactions with the CMAP at École polytechnique, in particular around `pylbm`, a research code dedicated to the lattice Boltzmann method.

2- Scientific Context and Challenges

The lattice Boltzmann method is a numerical method for simulating a wide range of systems of partial differential equations (PDEs). It was introduced in the late 1980s by the fluid mechanics community [2, 3] and subsequently gained widespread popularity due to its simplicity of implementation and high computational efficiency. It is now widely used to simulate a variety of problems in fluid mechanics [6, 10], solid mechanics [11], quantum mechanics [8], and other areas.

The lattice Boltzmann method consists in evolving a vector of quantities (often referred to as *particles*) on a regular space-time grid according to a two-step algorithm: a so-called collision step, which relaxes the vector towards an equilibrium state, followed by a transport step, during which the quantities move along the lattice from one grid point to another. The analogy with a discretization of the Boltzmann equation provides a formal argument showing that certain quantities arising from this algorithm converge towards solutions of PDEs. The main challenge is to establish a rigorous mathematical framework that justifies this connection.

Mathematicians have only recently started to investigate these schemes, and the mathematical tools required for their analysis are still under development. Work initiated during Thomas Bellotti's PhD thesis has led to a significant change in the understanding of these schemes: it is now possible to rewrite a lattice Boltzmann scheme as a multistep scheme involving only the conserved moment(s), i.e., the quantity (or quantities) that converge towards the solution of the underlying PDE [18]. This purely algebraic formulation makes it possible to study the method

using the same tools as for more standard numerical schemes, with particular attention to the initialization phase, which requires special treatment due to the multistep nature of the scheme [20].

Approaches based on tools from finite volume methods have also led to convergence results for several simple lattice Boltzmann schemes [19, 21, 22, 23]. More recently, initial studies of stability suggest that Lax-type theorems may be within reach, with consistency and stability potentially providing sufficient conditions for convergence [26]. These results are currently restricted to hyperbolic problems.

An open-source Python module has been developed over the past few years jointly by LMO and CMAP (the `pylbm` package[1]), dedicated to lattice Boltzmann schemes. Its modularity and efficiency make it a powerful tool for developing and analyzing such schemes. It already makes it possible to construct schemes in one, two, and three spatial dimensions on complex domains, and provides tools for studying equivalent equations (*i.e.*, the approximated PDEs and the associated error terms) [9] as well as stability properties. At present, however, it is limited to hyperbolic scalings, although a parabolic scaling can be artificially enforced.

Despite these advances, a rigorous and systematic analysis of lattice Boltzmann schemes for parabolic problems remains largely open, particularly when consistency, stability, convergence, and boundary conditions are considered within a unified framework.

3- Objectives

The objective of this project is to extend the analysis of lattice Boltzmann schemes to systems of parabolic equations. The model problem will initially be the constant-coefficient advection-diffusion equation before considering reaction terms, which will serve as the first object of study. We will build upon previous work by Michael Junk and co-authors [7, 13], which we will revisit using the new tools developed within our research group. The work may be organized around the following four research axes.

1. The first direction will be the study of the consistency of several classical schemes that could be promising candidates for the simulation of transport-reaction-diffusion equations in d spatial dimensions, with $d \in \{1, 2, 3\}$.
2. This will naturally be followed by a stability analysis of the *best-performing* schemes selected in the previous stage, where "best" may refer to accuracy, simplicity, or other criteria that may emerge during the study.
3. A third direction, which can and should be pursued in parallel with the two previous ones, will be the implementation of the schemes in `pylbm`, in order to compare the theoretical results with standard test cases from the literature. This development work is expected to be substantial and may require a major redesign of the current scheme-description framework in `pylbm`. A particular objective will be to introduce new functionalities allowing users to define their own elementary operators and combine them freely, thus providing a flexible and extensible framework for designing, implementing, and analyzing new lattice Boltzmann schemes.

[1] https://pylbm.readthedocs.io/en/latest/

4. The final direction we wish to explore concerns the efficient, accurate, and stable enforcement of Dirichlet and Robin boundary conditions for the heat equation at the numerical scheme level. Traditionally, boundary conditions for lattice Boltzmann methods are imposed during the transport step on the populations entering the computational domain. This does not directly correspond to the boundary conditions that need to be imposed on the limiting PDE. The first step will therefore be to determine the most effective way of imposing such conditions in order to achieve the desired level of accuracy at the boundary. We will then focus on the stability of these boundary conditions, building on the notion of *strong stability* [1], which has recently been revisited and adapted to lattice Boltzmann schemes [24, 25].

4- References

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