Numerical analysis of lattice Boltzmann schemes through Green's functions

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Context

Partial Differential Equations (PDEs) are a universal tool in the mathematical modelization of complex phenomena. As finding explicit formulae of the solution of such PDEs is generally out of reach, numerical methods (Finite Difference, Finite Volume, Finite Elements, etc.) to approximate those solutions play an essential role in today's science. Although numerical methods conveniently provide approximations, they bring new challenges, such as reduce their cost and complexity vs. accuracy, and devise tools to analyse their properties, which can be far from those of the approximated model. Kinetic methods, and in particular lattice Boltzmann methods (LBM) introduced at the end of the 80s, revolutionized simulations within (among other fields) computational fluid dynamics, both for incompressible and compressible flows featuring one or several phases. These methods achieve impressive speed and parallelization capabilities, and feature a very simple structure, owing to their derivation inspired from the Boltzmann equation and uniform Cartesian meshes. Despite these advantages, a significant challenge concerns a strongly lacunary rigorous mathematical understanding, the core of numerical analysis, due to the lack of relevant tools—contrarily to traditional numerical methods.

Results on rigorous numerical analysis for LBM schemes are extremely rare and scattered. This is probably due to the extreme polarization towards applications and the fact that these schemes are intrinsically challenging to study due to the presence of merely numerical unknowns, which do not correspond to unknowns in the PDEs, thus bring no "easy" numerical property. During his PhD, Thomas Bellotti started looking at this issue by bridging with traditional **Finite Difference** methods [Bellotti et al., 2022], to re-use theoretical tools germane to this framework [Bellotti, 2023c, Bellotti, 2023a], which are nowadays classical [Strikwerda, 2004, Brenner et al., 2006], on LBM schemes. Then, the natural question is whether LBM schemes can be studied, for instance concerning guarantees on their convergence, without turning them into something else, and fostered a research path built on the relation to kinetic/relaxation schemes [Aregba-Driollet, 2024, Aregba-Driollet and Bellotti, 2025]. The present post-doctoral research project shall conveniently navigate between both standpoints, considering that—roughly speaking—the first one is more suitable for linear problems, whereas the second one handles non-linearities more easily.

Objectives and research paths for the candidate

Monotonicity, invariant compact sets, and L^{∞} stability are essential features of numerical schemes in order to prove their convergence to weak-solutions in non-linear contexts [Godlewski and Raviart, 1991]. These themes shall be explored concerning LBM schemes, where the difficulty to be taken into account is the fact that—to achieve computational efficiency—these methods feature a large number of unknowns, whence some freedom on their **initialization**. In particular

- T. Bellotti [Bellotti, 2023b, Chapter 11] has investigated monotonicity, invariant compact sets, and L^{∞} for a simple two-unknowns scheme (known as D1Q2) using its multi-step Finite Difference counterpart, adapting the classical framework of [Godlewski and Raviart, 1991]. However, this procedure—even in the linear setting—does not provide the whole set of parameters where these properties can be obtained. This is due to the presence of negative coefficients, which however play no role when the initialization is taken into account. This has been partly understood through the use of Green's functions: the first path in the post-doc will be to fully understand this fact (some gaps are still to be filled) and embed in a larger proof of convergence for this numerical method, making the adaptation to the non-linear setting.
- Further developments [Aregba-Driollet, 2024] have shown how to analyze these properties directly on LBM schemes. Although it was believed that this would secure the whole space of parameters where invariant compact sets determined by the initial datum are expected, this is far from being true for more involved schemes (e.g., D1Q3). A second big step in the post-doc will be to understand why—thanks to **specific initializations**, which roughly speaking put the numerical solution on the "right manifold", invariant compact sets are preserved even in presence of negative weights, where the definition of monotonicity is violated. It is quite impressive that if E is the scheme matrix and I the initialization matrix, one can have $\sup_n \|E^n\|_{\infty} \gg 1$ but, thanks to the initialization, $\sup_n \|E^nI\|_{\infty} = 1$.

Again, this study shall be achieved by the study of Green's functions for the multi-step Finite Difference scheme and/or those (which are still to be envisioned and defined) for the raw LBM scheme. This study involves a precise understanding of the **spectrum** of the schemes analogously to [Godillon, 2003, Coeuret, 2024, Coeuret, 2025], from which a great deal of inspiration could be taken. From a larger perspective, if the post-doctoral researcher is interested on this topic, it will be very stimulating to provide a more general characterization of the **spectrum of block banded Toeplitz matrices** (or operators) involved in LBM scheme, which has only been shallowly and non-rigorously described in [Bellotti, 2025] for the simple D1Q2.

- Something which is tightly linked to the previous discussion—and which comes from no longer requesting that the scheme's solution lies in an invariant compact set—is **plain** L^{∞} **stability**. Indeed, the compact set can grow for a finite number of iterations and then stabilize, i.e. $\sup_n \|E^n\|_{\infty} < +\infty$. Another objective of the post-doc will be to extend the results of [Thomée, 1965] (see also [Coulombel, 2022]), to multi-step Finite Difference schemes (and thus to LBM schemes): characterize L^{∞} stability **only by means of Taylor expansions of the eigenvalues of the scheme's matrix near tangency points** to the unit circle. Preliminary observations seem to show that LBM schemes possess these properties most of the time, except when they are **time-reversible**. The post-doc shall try to make this guess more rigorous.
- Finally, the description of Green's functions, which is a staple between all previous items, also allows the study of **discrete shock profiles** [Godillon, 2003, Coeuret, 2024], sustained by numerical schemes. To the best of T. Bellotti's knowledge, this has never been investigated concerning LBM schemes. If time permits, it will be very interesting to dig into this issue during the post-doctoral program.

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