Numerical analysis of characteristic discretizations of hyperbolic PDEs with and without boundaries: lattice Boltzmann methods

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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. The algorithm is made up of two simple steps: a local relaxation phase on each site of the grid, followed by a linear transport phase where quantities are exactly shifted from one site to the neighboring ones, according to some discrete velocities.

In spite of the advantages mentioned above, 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. One difficulty comes from the characteristic nature of these discretizations: some matrices appearing in the numerical scheme are singular.

Results on rigorous numerical analysis for LBM schemes are fairly rare and scattered. This is probably due to the extreme polarization towards applications and the intrinsic challenges in their 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, the advisor started looking at this issue by bridging

with traditional *Finite Difference* methods [7] only on the "physical" unknowns, to re-use theoretical tools germane to this framework [4, 3], which are nowadays classical [21, 8], 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 [1, 2]. This is especially interesting for problems with boundary conditions [6], where the elimination of the numerical unknowns is not easy to achieve (when possible). The present post-doctoral research project shall conveniently navigate between both standpoints.

Objectives and research paths for the candidate

The post-doc project aims at pushing the understanding of *LBM schemes for hyperbolic problems* forward by investigating, also according to the candidate's taste, two important points.

The first one is the *existence and stability of discrete shock profiles*, which are germane to a non-linear setting but in the case of an unbounded domain. The second one concerns the *stability and convergence* for linear schemes in presence of *boundary conditions*.

Discrete shock profiles and their stability

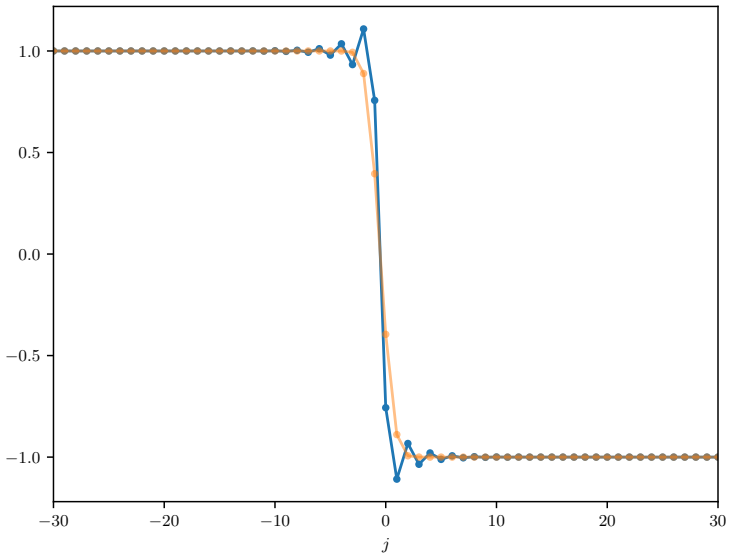

Figure 1: Two examples of (quite different) stationary discrete shock profiles.

Discrete shock profiles, see Figure 1, are *particular solutions* of the numerical scheme and analogous to, for example, regularized shock profiles for viscous regularizations of hyperbolic conservation laws:

$$\partial_t u + \partial_x(f(u)) = \epsilon \partial_{xx} u \qquad (\epsilon > 0).$$

They somehow arise as solutions where there is a perfect compensation between the sharpening effect of non-linearities and the regularizing force due to (numerical) dissipation.

We envision to consider both the case where the target equation is a scalar one and when one tackles a system of equations (e.g., the Euler system), treated with several classical LBM schemes. The study of discrete shock profiles generally separates the study of their *existence* and the one of their *stability*. The latter point investigates, roughly speaking, whether one can actually observe a given discrete shock profile (whose existence can be either proved or conjectured) when conducting numerical simulations.

Note that part of the candidate's work shall also focus on the implementation of schemes and on conducting numerical experiments to check theoretical findings on discrete shock profiles.

- *Existence.* Concerning this point, most of the available techniques apply to a scalar setting and are based on the seminal work of [14] for strictly monotone Finite Difference schemes. For schemes which are non-monotone and even of higher-order (and some well-designed LBM schemes that we are interested in are such), other approaches such as [20] must be envisioned. We plan to navigate between these two streams according to the setting: low-order schemes vs. high-order ones.
- *Stability.* There are many directions to investigate this aspect, according, for example, to the norm that one utilizes. Thus, we envision the following paths for the candidate.
  - One based on monotonicity and very much in the spirit of [1, 2], which measures stability in the L^1 norm, following the works of [18, 19]. One of the main advantages of this way of proceeding is that it does not assume that the perturbation of the discrete shock—which one would like to "return" to the shock—be small. This approach essentially deals with profiles that look like the yellow one in Figure 1.
  - Another approach builds on the L^2 norm and on finding precise energy estimates for the LBM scheme at hand, which can be quite technical to achieve. Roughly speaking, the perturbed solution around the shock profile converges to it due to dissipation. This path is inspired by previous works [17] on Finite Difference schemes and discretizations of relaxation systems [16], which share certain similarities with the LBM approach.
  - A third path, especially interesting when the target problem is a system of hyperbolic equations, concerns the spectral stability that is investigated by linearizing the scheme around the shock profile. This involves the precise understanding of the Green functions and the the spectrum of the scheme analogously to [13, 9, 10], from which a great deal of inspiration can 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 schemes, which has only been shallowly and non-rigorously described in [5] for the simple D1Q2 scheme.

Stability and convergence with boundary conditions

This second part of the proposal introduces the difficulty of dealing with *boundary conditions* but considers *linear equations*. Generally, boundary conditions are enforced on the incoming information linked to the discrete velocities of the scheme, and thus almost never correspond to boundary conditions needed by the target PDEs.

A previous contribution [6] has focused on the stability of schemes with boundaries with respect to boundary data. Here, the difficulties and subtleties linked to the *characteristic* nature of the schemes have been emphasized. However, important gaps to fill to reach actual proofs of convergence with boundaries, which we aim at tackling with the candidate, are as follows.

- Introduce *internal source terms* within the setting of strong stability (roughly speaking, using the $L^2_t L^2_x$–topology). Of particular interest is understanding how the characteristic character of the schemes seems to be harmless in this context compared to the case of boundary source terms. This is likely due to "good properties" of specific spectral projectors on part of the spectrum of the operators involved in the numerical schemes.
- A second theme is considering *more natural topologies* (essentially $L^\infty_t L^2_x$) and *semi-group estimates* in the spirit of [11]. This context allows the introduction of non-zero initial data, which are the setting in which LBM schemes are employed in practice. Since this is likely to rely on energy estimates for the underlying numerical scheme, we aim at leveraging the so-called "stability structure" [15] for LBM in order to obtain these estimates.

- Finally, we would like to adapt the work of [12] to show *convergence* of some simple LBM in presence of boundaries. This can possibly pass from their interpretation as multi-step algorithms and is now possible because these schemes are stable in presence of some natural kinetic boundary conditions.

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