Report

Title:	ESR - Executive Summary Report
Authors:	T. Van Hoof, B. Graille, Z. Alsalihi, L. Gouarin
Approver:	P. Schrooyen — Date : 2021/10/04
Ref:	LBMHYPE-ESR

Project identification

Cenaero references	
Project code :	2018070_LBMHYPE_ESA
Project short description :	LBM for hypersonic applications: Feasibility assessment study
Project manager :	T. Van Hoof
Client / Partner(s) references	
Purchase order / Grant agreement reference :	ESA_Contract_4000126149_18___NL_KML
Other reference :	
Contact person :	Richard Schwane, Maximilian Garre

Distribution list

ESA	Richard Schwane, Maximilian Garre
UPSud	Benjamin Graille, François Dubois, Filipa Caetano
CMAP	Loïc Gouarin, Marc Massot, Laurent Series
VKI	Zuheyr Alsalihi, Thierry Magin
Cenaero	Pierre Schrooyen, Ingrid Lepot

List of Revisions

Rev.	Status	Date	Author(s)	Purpose
00	DFT	2021/03/04	T. Van Hoof	Draft initialization
01	FIN	2021/10/04	T. Van Hoof	Version delivered to ESA

Contents

1 Project overview

The objective of the ESA TRP research project "LBMHYPE" is to evaluate the feasibility of Lattice Boltzmann Methods (LBM) for hypersonic space applications. LBM exhibits many interesting advantages for industrial applications (simple algorithm, ease to deal with complex geometries, high parallel computing efficiency, allows for multi-physics problems,...). However, the main limitation is the restriction to low velocity/weakly compressible flows which is incompatible with the hypersonic flow regime. The causes of the low compressibility limitation are still unclear, mainly because LBM is based on a bottom-up multiscale approach where the macroscopic quantities and their driving equations do not appear explicitly in the LBM scheme. In other words, the study of the relationships between the (microscopic) LBM scheme and the (macroscopic) flow behavior is not straightforward and requests the use of advanced mathematical and numerical tools. In this framework, the LBMHYPE initiative proposes to further analyze the capabilities and limitations of pure LBM schemes to simulate highly compressible flow behaviors.

Real highly compressible flows involve a lot of interacting physics (shock waves, rarefaction, thermal exchanges, reactive multi-species, etc). The simulation of such complex interacting phenomena is very challenging, even with the state of the art numerical methods. The objective of the LBMHYPE is to evaluate LBM step by step starting from simple test cases focusing on the main known limitation of LBM: the incompressible limit. To this aim, the analyses performed during the project focus exclusively on single specie, calorically perfect gas and inviscid compressible flows as modeled by the Euler equations. Furthermore, only 1D and 2D test cases with simple geometries and boundary conditions are used to focus on the study of the bulk LBM scheme behavior and to limit the computation costs of the simulations.

The LBMHYPE project has been divided into two phases. The first phase was devoted to the feasibility study itself: can we use LBM to simulate highly compressible flows? A literature review has been performed to identify promising LBM schemes able to simulate highly compressible flows (see TN1.1). In parallel, a set of 1D and 2D test cases of increasing complexity has been proposed to assess the LBM schemes step by step (see TN1.2). The proposed hyperbolic LBM schemes, based on an innovative vectorial scheme approach, where each conservation equation of the Euler system is solved by a different scheme, shows promising capabilities both in terms of accuracy and computational costs (see TN1.3). The main observed limitation is the occurrence of spurious oscillations in the vicinity of the flow discontinuities, as observed for most standard CFD methods (see TN1.3). The preliminary assessment also highlights the need of efficient numerical methods and tools to ease the study of LBM schemes limitations involving non-linear interactions between numerous parameters.

Based on the exciting conclusions of the first phase, the second phase of the project has focused on the development of the numerical methods and tools to ease the definition and analysis of compressible LBM schemes and simulations. A numerical platform with a user interface has been developed with the following targets:

- Didactic: LBM is conceptually different from conventional CFD method and newcomers need a numerical tool able to guide them through the theoretical and the practical aspects of the method.
- Research: the development and analysis of new LBM schemes is a challenging

task. Mathematical tools are needed to derive the macroscopic equations from the definition of the LBM scheme, and to ease the setup of large scale parameters sensitivity studies to further analyze the stability and accuracy of LBM simulations.

A first prototype of the platform has been implemented to assess the proposed compressible LBM scheme and test the prospective methods developed during the project (mainly the tentative non-oscillating LBM scheme, the automatized parametric studies and the coupling with data analysis and optimization software 'Minamo'). In a second step, the prototype has been re-factorized into the more robust and user friendly interface called 'pylbm_ui' described in TN2.1 (code design), TN2.2 (code structure) and TN2.4 (code manual with tutorials). Eventually, the compressible LBM schemes implemented in the platform have been validated through comparisons with state of the art CFD methods (US3D) as presented in TN2.3. The validation highlights the promising capabilities of LBM for hypersonic applications in terms of ease of use, accuracy and computational performances.

2 State of the art

The references and related publications for lattice Boltzmann schemes that can be used for the highly compressible applications have been collected. For the reference collected, the level of physico-chemical fidelity has been reported. The investigation was not restricted to pure lattice Boltzmann schemes as very few showed good agreements with the applications: we also compared the results with those obtained with a more general class of finite volume schemes that involve somewhere a "Boltzmann ingredient." For each collected scheme that could simulate hypersonic fluid flows, the associated microscopic model (in particular the choice of the equilibrium) and the macroscopic equivalent equations have been described. That work has been summarized in a synthetic diagram allowing to compare the advantages and the drawbacks of the methods but also to anticipate on the possibility of coupling the ideas of each one in order to progress towards the targeted applications (see TN1.1 and the Final Report for further details). During the project, the 'pure' LBM schemes based on the vectorial approach have been favored for their expected flexibility, algorithmic simplicity and computational efficiency.

3 Vectorial LBM schemes for compressible flows

Several vectorial schemes can be proposed to simulate the 1D and 2D Euler equations that form a hyperbolic system. The following schemes have been developed during the project:

- The D_1Q_{222} vectorial scheme is the simplest 1D scheme able to model the 1D Euler equations. It involves three coupled D_1Q_2 schemes, one for each of the 1D Euler conservation equations. The velocity stencil contains only 2 velocities $(1, -1)$ and forms the smallest stencil in 1D leading to six populations (discrete particle distribution functions) and moments. The conserved moments are ρ (density), q (momentum), and E (energy). The scheme involves three relaxation rate parameters related to the diffusion of each conserved moment.
- The D_1Q_{333} vectorial scheme is build by coupling 3 D_1Q_3, one for each conservative equation. The velocity stencil involves 3 velocities $(0, 1, -1)$. The velocity 0 is added to the stencil of the D_1Q_{222} leading to nine populations and moments while the same conserved moments are considered ρ, q, and E. The scheme involves six relaxation

rate parameters to be adjusted to reach the desired flow properties (e.g. diffusion) and simulation stability. Two kinds of equilibrium functions have been proposed leading to two versions of the D_1Q_{333} vectorial scheme:

  - the $D_1Q_{333}-0$ aims at removing the non-linear terms according to the velocity in the second order equivalent equations.
  - the $D_1Q_{333}-1$ use equilibrium chosen to fit exactly the structure of the Navier-Stokes second-order operator.

- The $D_1Q_3L_2$ is a lattice Boltzmann scheme with three velocities and two levels of internal energy. The scheme is then defined by six populations and moments. It contains only three relaxation rates and another parameter related to internal energy splitting.

- The D_2Q_{4444} is the simplest 2D vectorial scheme able to simulate the 2D Euler equations. It involves four coupled D_2Q_4 schemes, one for each of the 2D Euler conservation equations. The velocity stencil contains only 4 velocities $((1,0),(0,1),(-1,0),(0,-1))$ and forms the smallest stencil in 2D. The conserved moments are ρ, q_x, q_y, and E. It involves sixteen populations and moments and nine relaxation rates.

These schemes have been implemented into the pylbm_ui platform (see Sec. 4) for further analysis. An extensive description of each scheme is provided in the user interface as shown in Figure 1. As highlighted in the Final Report, the proposed schemes are not exact and present numeric artifacts like diffusion or spurious oscillations in the vicinity of flow discontinuities. Guidelines and methods to control the diffusion and the spurious oscillations have been proposed in TN1.3 and the Final Reports.

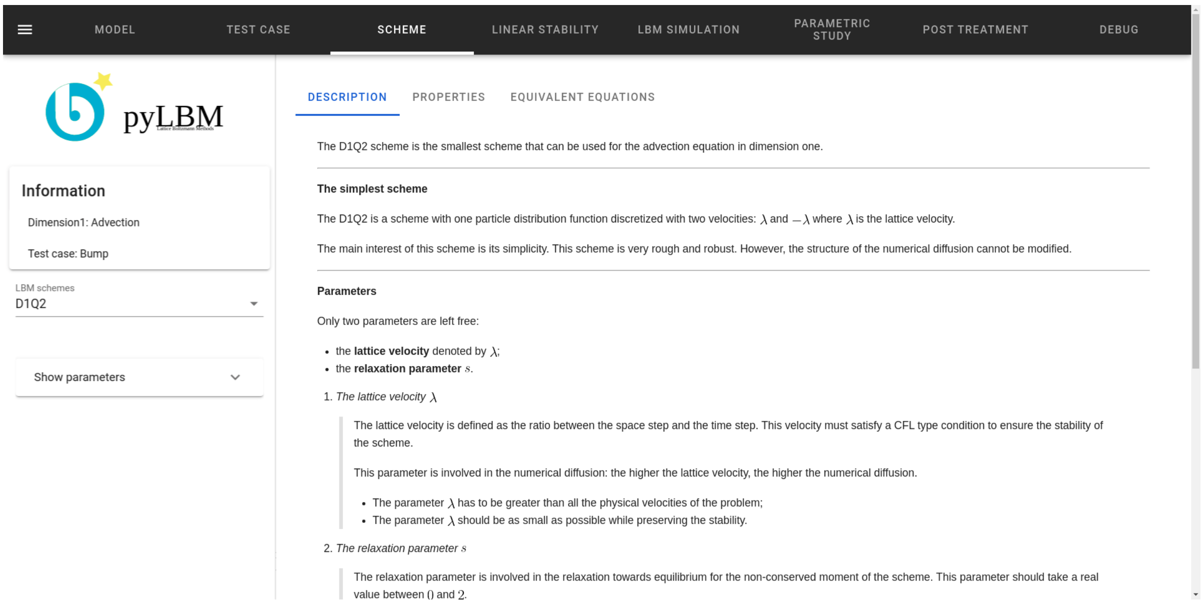

Figure 1: Snapshot of the SCHEME tab in the pylbm_ui platform.

4 Software infrastructure

During this project, a large number of lattice Boltzmann schemes have been studied to understand the difficulties related to hypersonic flows. We therefore needed a tool that would allow us to quickly describe the different schemes in a simple way with the possibility to make a fine analysis. We have therefore chosen to focus on the user experience rather than on the development of a large industrial code. The objectives of the infrastructure are the following:

- to have a clear vision of the project's test cases as well as the lattice Boltzmann schemes that can solve them
- to facilitate learning
- to better understand the LBM schemes and the influence of their parameters on the simulation
- to enrich the models
- to have a flexible UI to improve the user experience
- to be able to run test cases on supercomputers once the feasibility study is completed

In order to meet all these objectives, 4 tools have been developed and combined in a coherent platform:

- the **pylbm** software developed at the LMO and CMAP allowing to simulate physical problems using the lattice Boltzmann schemes in 1d, 2d and 3d. It allows to launch simulations on supercomputers and has a multi GPU implementation. It offers great flexibility in its use allowing to describe easily and quickly new lattice Boltzmann schemes and that is why we chose it. Morover, **pylbm** provides mathematical tools to derive the equivalent macroscopic equations and evaluate the linear stability of vectorial LBM schemes.
- a catalog software called **pylbm-catalog** allowing to describe test cases (see Sec. 5) and lattice Boltzmann schemes (see Sec. 3) and export them in JSON format. This software was developed within this project in order to list more easily the test cases and schemes studied, thus allowing ESA to have a clearer vision of the work done. It also offers other perspectives since it is possible to add other entries. It can therefore be useful to federate a community and have a common space where know-how and experience of users can be collected and documented.
- a user interface called **pylbm-ui** [1] has been developed during the project. **pylbm-ui** allows to query the catalog and to launch in real time a set of test cases, to change the parameters and to see their influence on the simulation, to offer analysis tools for the schemes, ...
- one of the analysis tools provided by **pylbm-ui** corresponds to the parameter sensitivity analysis method developed during the project (see Sec. 6). The output files containing the parametric study database are compatible with the **Minamo** software developed by CENAERO [2] which provides advanced data analysis tools.

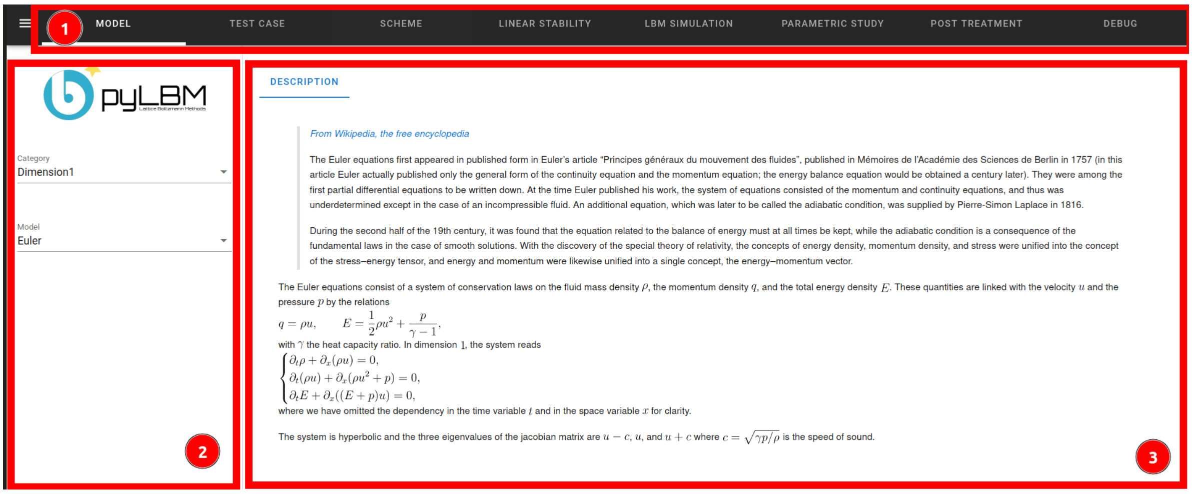

Figure 2: Snapshot of the pylbm_ui user interface with three different areas.

The tools are written in Python, widely used in the scientific community. The user interface relies on the Jupyter project which offers many tools for scientific computing, and ipyvuetify which allows to use a set of widgets (slider, text area, ...) for the interaction with the user. Figure 2 illustrates **pylbm-ui** which consists of 3 areas:

- Zone 1 corresponds to the tabs available in the application and allows to navigate in the different features of the application.
- Zone 2 is a menu dedicated to each tab. This one can be hidden, which is useful when the screen size is small.
- And finally the zone 3 is the main window of the functionality of the chosen tab.

The codes are open source in order to offer our expertise of lattice Boltzmann methods to the largest number of people and to encourage the emergence of new collaborations, the improvement of these tools and the construction of a community around them. The code source is freely available from the github project page [1].

5 Test cases and validation

The strategy that was followed in the project was to propose different test cases of increasing complexity to evaluate and test the capabilities and limitations of different LBM schemes for hypersonic flows. The cases were devoted to the investigation of the LBM methods for the Euler equations, the compressible inviscid flows since the compressibility is the major limitation of the method for hypersonic flow applications. The working gas in all the test cases was selected to be calorically perfect air. All the test cases are documented, input and comparison data were established.

In 1D, the classical Sod Shock Tube problem, which has an analytical solution, is the best first step to begin. Modified Toro problems, which are more extreme Riemann problems, are designed to test the robustness of the numerical schemes. The Shu-Osher problem, a shock wave entering into an oscillating density field, is another problem with an exact solution. This unsteady problem is an ideal test for the LB solvers which are inherently transient.

The D_1Q_{333} and D_1Q_{222} LBM schemes have been successfully applied to all the selected

1D test cases (see TN1.3 and TN2.3 for more details). The numerical study shows that for the same spatial resolution, D_1Q_{333} has higher accuracy than D_1Q_{222}. On the other hand, the CFL stability criteria are lower leading to an increase in the number of iterations to complete the simulation. The accuracy of LBM seems similar to most of the standard methods presented in [3]. It could be further increased through specific adaptations to locally smooth the spurious oscillations to obtain a non-oscillating LBM scheme, as initaly proposed by Canana [3], and later adapted to the LBM framework using out-of equilibrium moments leading to improved performances and robustness, as described in the Final Report and Sec. 6.

A set of 2D test cases has been proposed to evaluate both the accuracy and the computational costs of LBM in more complex configurations. The assessment methodology relies on the comparison of LBM with the state of the art CFD code 'US3D,' developed by Graham V. Candler of University of Minnessota, for similar space and time resolutions. The D_2Q_{4444} scheme has been evaluated using three test cases (see TN2.3 and Final Report for more details):

- The supersonic wedge case is the deflection of an inviscid flow over a wedge. In the limit of small diffusion, LBM is able to reproduce the shock angle as a function of the wedge angle and the flow velocity. However, the lack of slip boundary condition for a wall not aligned with the computational grid (the lattice) induces wrong flow patterns in the vicinity of the wall. This highlights the need of realistic boundary conditions adapted to each LBM scheme.
- The implosion problem involves complex interactions between moving shocks and contact discontinuities. LBM is able to preserve the flow symmetry over long period which is not necessary the case for most standard methods as explained in [4]. The overall flow pattern is reproduced even for large diffusion, while smaller patterns appears for vanishing diffusion.
- The forward facing step test case is a seminal case where a Mach 3 flow hits a step creating a complex evolving shock pattern. Unlike the supersonic wedge case, slip boundary conditions have been easily imposed because the walls are aligned with the grid. Here again, LBM converges towards the reference solution for vanishing diffusion while reasonable overall flow pattern are observed even for non zero diffusion. Furthermore, LBM provides better results than US3D in the corner region as shown in Figure 3.

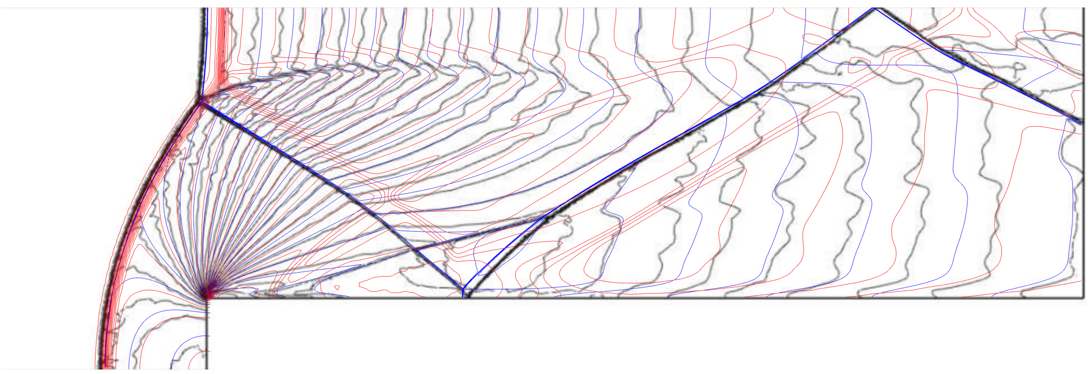

Figure 3: Density isolines of the US3D Euler solution in red, 4801 x 801 LBM in blue, and the scanned reference solution, black.

The assessment highlights the high computational efficiency of LBM. For all tested cases, LBM CPU times are several orders of magnitudes smaller than US3D. Moreover, the setup of LBM simulations is also significantly shorter and easier, mainly due to the absence of preliminary meshing procedure. The cases computed with LBM clearly demonstrate that the method is competitive with one of the best hypersonic codes in the world, with absolute superiority in terms of CPU and possibly programming and mesh generation. We have seen the limitations with the diffusion of the scheme, but this can be overcome using local grid refinement or using non-oscillatory scheme. The main shortcomings were the definition the boundary conditions on the sloped or curved surfaces. The striking accuracy and the success of the method for the forward facing step clearly shows the potential and necessity to further exploit the method in very complicated flows.

6 Toward efficient LBM analysis tools

During the first phase of the project, an empirical analysis showed interesting behaviors of the hyperbolic LBM schemes applied to highly compressible inviscid (Euler) test cases. The main observations are summarized as follows (see TN1.3 for more details):

- Stability:
  - Is mainly driven by the well known "Courant–Friedrichs–Lewy" criteria (CFL) which, for LBM, corresponds to a minimum value for the scheme velocity $\lambda = \Delta x/\Delta t$.
  - Unstable LBM simulation can also be observed for relaxation rate (s) close to the maximal theoretical value of 2.
- Accuracy:
  - The LBM solution converges toward reference Euler solution for vanishing values of the diffusion coefficient $Diff = \sigma\lambda\Delta x = 1/(0.5 + s)\lambda\Delta x$. The expression of the diffusivity further highlights one of the common difficulty of LBM: the flow behavior is a function of three parameters: the time step (Δx), the scheme velocity λ (ultimately related to the time step since $\Delta t = \Delta x/\lambda$) and the relaxation rate S.
  - As the overall accuracy increases in the whole domain for vanishing $Diff$ values, spurious oscillations emerge in the vicinity of flow discontinuities. The empirical analysis indicates that the onset of the spurious oscillation is related to the criteria $Diff/\Delta x = \sigma\lambda < U_{disc}/2$, where U_{disc} is the velocity of the fastest discontinuity in the system (shock, contact or rarefaction front/tail).
  - Further decrease of $Diff$ leads to an increase of the spurious oscillations amplitude and, eventually, to unstable LBM simulation.

The empirical analysis highlights the need of an analysis method able to fill the gap between the mathematical analysis of the LBM scheme (e.g. linear stability and equivalent PDE derivation) and the real capabilities of LBM to simulate test cases involving complex combinations of physical states and boundary conditions. In practice, the empirical analysis was an embryonic parametric study involving a large number of LBM simulations with varying scheme and discretization parameters. However, the definition, execution and analysis of such a large set of LBM simulations is time consuming and the repetitive tasks involved makes it prone to human errors. As a consequence, during the second phase of the project, a significant effort has been devoted to the improvement of the analysis method.

The development of the systematic LBM analysis method takes advantage of the pre-existing expertise and tools of Cenaero in the field of data analysis and optimization. A first demonstrator has been developed using the coupling capabilities of the Minamo data analysis software from Cenaero [2] to interact with pylbm in order to automatize the setup and analysis of large scale parameter sensitivity and optimization studies. The demonstrator allows to assess the method and the results further confirm the tendencies observed during the first phase of the project regarding the LBM behavior.

However, the complexity of the chain quickly appears as strong limitations since a high level of expertise was requested to define and run a parametric study which makes it impracticable for non experts. To tackle that issue, a prototype of platform with a user interface has been developed as a first step toward a coherent and user friendly software solution to study LBM. The prototype is fully integrated with the catalog of LBM schemes and test cases developed during the project and allows to easily define and run a parametric study with few 'clicks' while strongly reducing the risks of errors through an automatic adaptation of the available parameters and responses to the selected catalog elements. The prototype provides a standalone tool for parameter sensitivity studies thanks to the implementation of basic sampling and parallel coordinate plot features. Meanwhile, advanced users can unleash the full potential of the developed systematic LBM analysis method thanks to the Minamo coupling giving access to a large catalog of cutting edge data analysis tools including surrogate model assisted optimization. pylbm_ui re-factorizes the main features of the parametric study for a better integration with the underlying pylbm library and an improved overall user experience as shown in Figure 4 and described in Sec. 4.

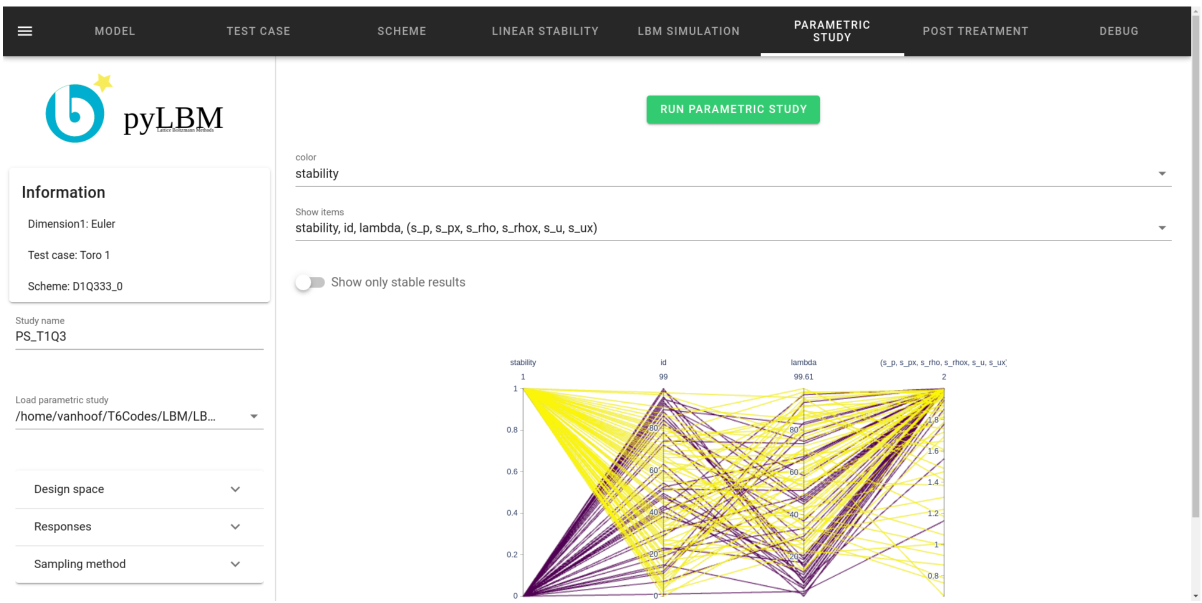

Figure 4: Snapshot of the PARAMETRIC STUDY tool in the *pylbm_ui* platform.

Meanwhile, some efforts have been devoted to the development of non-oscillating LBM schemes to tackle the standard CFD issue related to the spurious oscillations. During the first phase of the project, M. Canana initiated the adaptation of the well knows artificial viscosity method to LBM [3]. The resulting non-oscillating scheme is based on standard pressure discontinuity detector and the local adaptation of the diffusion thanks to modification of the relaxation rate in each LBM cell. The approach provides very promising results but do not take full advantage of the LBM framework. During second phase, the standard discontinuity detector has been replaced by a detector based on the out-of-equilibrium moments available in LBM. The resulting non-oscillatory scheme appears to be numerically efficient (even if the current implementation can certainly be improved), flexible (various moments and moments combination can be defined to tailor the detector), and easy to use (generic parameters values appears to give good results in most test cases in 1D and 2D). Further details about the non-oscillating scheme are provided in the Final Report.

7 Conclusions

The LBMHYPE project aims to study the feasibility of LBM for hypersonic applications. Given the complexity of both the targeted physics and numerical method, the LBMHYPE consortium has proposed to focus on the main known limitation of LBM with respect to hypersonic applications: the simulation of (highly) compressible flows. LBM appears as an efficient method for the simulation of highly compressible flows but the development of new schemes is difficult since the targeted macroscopic equations do not appear explicitly in LBM and the relationships between the scheme parameters on the resulting flow behavior are not straightforward. To tackle these issues, several tools have been proposed and unified into a coherent and user-friendly platform called **pylbm-ui** [1]. The platform provides a user interface with an intuitive workflow to guide new users in their first steps with LBM with a lot of theoretical and practical informations to ease the definition, run and post-treatment of LBM simulations. Experienced users can benefit from the advanced LBM scheme analysis features proposed during the project (derivation of equivalent PDE, linear stability analysis, parameter sensitivity studies and coupling with Minamo) to ease the development and study of new schemes.

References

[1] "Pylbm_ui - platform for LBM simulation and analysis." https://github.com/pylbm/pylbm_ui.

[2] "Minamo - advanced data analysis and optimization software by cenaero." https://www.cenaero.be/.

[3] M. Canana, "Development of Non-Oscillatory Lattice Boltzmann Method for Flows with Shock waves," in *ESA FAR Conference*, 2019.

[4] R. Liska and B. Wendroff, "Comparison of Several Difference Schemes for the Euler Equations in 1D and 2D," in *Hyperbolic Problems: Theory, Numerics, Applications*, 2003, pp. 831–840.