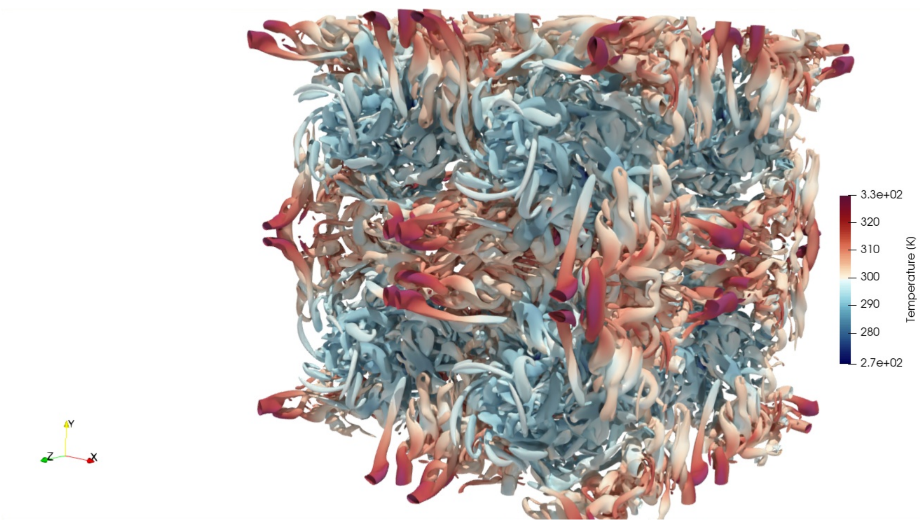
PhD Thesis Research Project Proposal

2024–2027

Exploring supercritical fluid thermodynamics through Lattice Boltzmann simulations for advanced energy-conversion turbomachinery

Ecole Centrale de Lyon / LMFA



Taylor-Green Vortex flow in a dense gas
Iso-surface of Q-criterion colored by temperature
Lattice-Boltzmann Method
Credit : Lucien Vienne

Context

Collecting energy from concentrated solar radiation, biomass combustion/gasification, geothermal reservoirs, and wasted heat sources plays a significant role in diversifying our energy sources. Cutting-edge technologies include Organic Rankine Cycle (ORC) and supercritical CO2 (scCO2) cycle power systems. Similar to the cycle found in steam power stations, ORC uses complex molecular fluids instead of water. The comprehension of these unconventional working fluids under thermodynamic conditions close to the critical point is a formidable physical and numerical challenge, in which high-fidelity simulations should provide insights into the fluid dynamics and enable engineers to improve efficiency.

Rooted in kinetic theory, the Lattice Boltzmann (LB) method has become a robust and versatile particle-based approach in the realm of computational fluid dynamics [Krüger, 2016]. The modularity and simplicity of LB algorithms facilitate their parallel implementation on modern computers incorporating accelerators such as GPUs. As a result, the LB method holds the promise to not only advance our exploration of non-ideal fluid behavior, but also to do so in a computationally very efficient manner, thereby mitigating the energy consumption associated with large-scale high-fidelity simulations [Giauque, 2023].

Today, the LB method makes it possible to safely simulate industrial configurations involving weakly compressible isothermal flows of ideal gas. Simulating non-ideal gas dynamics in the scope of our scientific program presents a challenge associated with two additional levels of complexity, namely

- Handling strong compressibility effects. In this case, an explicit resolution of internal energy dynamics becomes imperative. This entails an accurate consideration of kinetic and internal energy exchanges to suitably capture compressibility effects, guaranteeing the high fidelity of our simulations.
- Incorporating specific non-ideal thermal and calorific equations of state, i.e., $p(\rho, T)$ and $e(\rho, T)$, to account for the gas behavior under varying thermodynamic conditions. These equations play a pivotal role in reflecting the non-ideal nature of the gas dynamics.

Regarding strong compressibility effects, considerable progress has already been made by introducing more stable collision models or alternative off-lattice discretization strategy, correcting errors in Mach number and accounting explicitly for internal-energy dynamics by using either a second LB scheme or a finite-difference scheme [Farag, 2021][Wissocq, 2022]. However, despite the demonstrated effectiveness of these advancements, the application to complex geometries, such as flows in turbomachines, remains largely unexplored, as does the extension to non-ideal fluids, highlighting the need for more in-depth investigations [Hosseini, 2023].

Objectives and Methodology

Successive milestones define the time-line of the PhD candidate :

1. A comprehensive overview of the latest advances in the simulation of compressible non-ideal gas dynamics (without phase change) by the LB method. The PhD candidate will acquire in-depth knowledge of the LB method, physics related to compressible flows and non-ideal gases.
2. Cross-comparisons with simulations performed with the SU2 solver on academic test cases, focusing on the accuracy of the results and the computational cost. This detailed comparison will quantify the level of efficiency and accuracy of the LB approach compared to established solutions such as the SU2 solver.
3. Comparisons with experimental data. This phase represents an important step toward validating/anchoring numerical simulations in real-world. The PhD candidate will actively

engage with real experimental data, thereby obtaining valuable insights into the properties of real-world NICFD.

4. Simulation of a stator configuration representative of current or future turbomachines. This case is strategically chosen to emulate operational conditions and geometric complexity encountered in expected turbomachinery applications.

The PhD candidate will benefit from the expertise and support of Dr Lucien Vienne (LB method, coding), Dr Alexis Giauque (NICFD, turbomachines) and Dr Emmanuel Lévêque (LB method, turbulence). Simulations will use high-performance computing resources (including a GPU cluster) from the École Centrale de Lyon data center (PMSC2I).

References

T. Krüger et al. (2016) The Lattice Boltzmann Method : Principles and Practice, Springer Cham

G. Farag, et al. (2021), A unified hybrid lattice-Boltzmann method for compressible flows : Bridging between pressure-based and density-based methods, Physics of Fluids, 33 (8) : 086101.

G Wissocq, et al. (2022) Restoring the conservativity of characteristic-based segregated models : Application to the hybrid lattice Boltzmann method, Physics of Fluids 34 (4)

A. Giauque et al. (2023), High-fidelity numerical investigation of a real gas annular cascade with experimental validation, Physics of Fluids 35 (12)

S.A. Hosseini, I.V. Karlin (2023) Lattice Boltzmann for non-ideal fluids : Fundamentals and Practice, Physics reports vol. 1030, 1-137

Profile

This PhD thesis research project (starting date Oct 2024) will be carried out in the Fluid Mechanics and Acoustics Laboratory (LMFA) at Ecole Centrale de Lyon (ECL). Since it involves both physical modeling of turbulence and numerical developments in lattice boltzmann method, technical skills in fluid mechanics and applied mathematics are expected from the applicant. A marked taste for modeling and physical analysis in fluids will be an asset.

To apply send CV, Application letter and Transcripts to : alexis.giauque@ec-lyon.fr ; emmanuel.leveque@ec-lyon.fr ; lucien.vienne@ec-lyon.fr