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Department of Mechanics, Mathematics and Management
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Ph.D. Program
SSD: IIND-04/A–MANUFACTURING TECHNOLOGIES AND
SYSTEMS, MATH-05/A–NUMERICAL ANALYSIS
Final Dissertation

An Entropic Lattice Boltzmann Scheme for the Modeling of Wetting in Proton-Exchange Membrane Fuel Cells

by
Marco Desiderio Loffredo Senesi

Referees:

Prof. Dr. Ingenuin Gasser

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Prof. Giuseppe Casalino

Course n°38, 01/01/2023-31/12/2025



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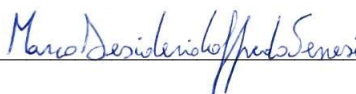
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- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
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- I have acknowledged all main sources of help.
- Where the thesis is based on work done by me jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

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The scientific work presented in this thesis benefited from discussions with professors and colleagues at Politecnico di Bari, Universität Hamburg, Università degli Studi di Padova, and Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg. In particular, I would like to thank Prof. Marco Torresi, Dr. Gianmarco Saponaro, Prof. Vito Di Noto, and Prof. Enrico Negro. I am truly grateful to my supervisors, Prof. Eng. Michele Dassisti and Prof. Alessandro Coclite, for their continuous encouragement and support. I express my appreciation to the members of the *Electrochemical Energy Storage and Conversion Laboratory* (Legnaro), Università degli Studi di Padova, with whom I spent a short but stimulating research stay in December 2023. I would also like to thank Prof. Dr. Ingenuin Gasser and his group at Universität Hamburg for the invaluable research experience I had at the Geomatikum during the winter 2024–2025.

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Sommario

La decarbonizzazione del settore dei trasporti richiede una rapida diffusione di sistemi di propulsione a basse emissioni di CO_2 e di inquinanti atmosferici. In affiancamento alle architetture puramente elettriche a batteria, le celle a combustibile a membrana a scambio protonico (PEMFC) rappresentano una soluzione promettente per l'integrazione nei veicoli elettrici. La loro adozione su larga scala rimane tuttavia limitata, principalmente, dai costi di sistema e dei materiali. In questa tesi, tali criticità vengono affrontate attraverso due strategie complementari: (i) la progettazione, fabbricazione e caratterizzazione sperimentale di un sistema PEMFC modulare per applicazioni *mobility* e (ii) lo sviluppo di un metodo numerico ad alta fedeltà, basato su metodi reticolari di Boltzmann, per il *modeling* e la simulazione di flussi multifase e fenomeni di bagnabilità, mirato a risolvere il trasporto d'acqua nei Gas Diffusion Layers (GDLs) delle PEMFC. Nell'ambito del progetto HYMOBITALY, è stato prodotto e testato uno stack modulare *twin* PEMFC da 2×16 celle, alimentato sia in aria/ H_2 che in O_2/H_2 , con un sistema simmetrico di distribuzione dei reagenti, raffreddamento a liquido distribuito e serpentine dimensionate per il trasporto dei reagenti. Il prototipo ha mostrato un funzionamento stabile nell'intervallo di densità di corrente considerato, con un'efficienza della configurazione *twin* prossima a quella dei singoli stack, validando così il concetto di modularità. Al contempo, le prove sperimentali hanno confermato che la gestione dell'acqua nel GDL costituisce un vincolo critico di progetto e di esercizio. Per studiare tale problematica sulla microscala, è stato sviluppato un metodo di reticolare di Boltzmann entropico tridimensionale con un operatore di collisione *cascaded*, accoppiato con un modello di tipo *pseudopotential* di Shan-Chen dotato di un'equazione di stato lineare a tratti, di una forza di interazione coesiva-adesiva unificata e di uno schema Coupled Boundary-Wettability per superfici curve non conformi al reticolo. Il metodo garantisce una segregazione di fase termodinamicamente consistente e un accurato controllo dell'angolo di contatto su un ampio intervallo di rapporti di densità e viscosità tra i fluidi, sopprimendo fortemente le correnti spurie, come verificato tramite benchmark su substrati piani e curvi. I risultati sperimentali e numerici congiunti forniscono un percorso coerente verso una progettazione predittiva dei componenti porosi delle PEMFC e di interi sistemi PEMFC modulari per la mobilità sostenibile.

Abstract

Decarbonizing the transport sector requires the deployment of propulsion systems with low emissions of both CO₂ and atmospheric pollutants. As a complement to established battery-electric architectures, Proton-Exchange Membrane Fuel Cells (PEMFCs) represent a promising technology for integration in electric powertrains. Their large-scale deployment, however, remains primarily constrained by system- and material-related costs. In this thesis, these challenges are addressed along two complementary directions: (i) the design, fabrication, and experimental characterization of a modular PEMFC power system for mobility applications, and (ii) the development of a high-fidelity lattice Boltzmann framework for modeling and simulation of multiphase flow and wetting, aimed at resolving water transport in PEMFC Gas Diffusion Layers (GDLs). Within the HYMOBITALY project, a twin 2×16-cell PEMFC stack with symmetric distribution of reactants, distributed liquid cooling, and tailored flow fields was built and tested under both air/H₂ and O₂/H₂ feeds. The prototype demonstrated stable operation over the investigated current-density range, with the efficiency of the twin configuration closely matching that of the single stacks, thereby validating the modular concept for scalable powertrains. However, the experiments confirmed that water management in the GDL is a critical design and operating constraint. To tackle this issue at the pore scale, a three-dimensional entropic cascaded lattice Boltzmann scheme, coupled with a Shan-Chen pseudopotential model, was developed, featuring a piecewise equation of state, a unified cohesive-adhesive interaction force, and a Coupled Boundary-Wettability scheme for off-grid curved surfaces. The method achieves thermodynamically consistent phase segregation and accurate contact-angle control over a wide range of density and viscosity ratios while strongly suppressing spurious currents, as verified through dedicated benchmark tests. The combined experimental and numerical results provide a consistent pathway toward a more accurate design of PEMFC porous components and modular fuel-cell power systems for sustainable mobility.

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Introduction

The concept of *sustainable mobility* is inherently broad, including the prioritization of efficient and affordable public transportation systems, the improvement of road-network design, and the operation of vehicles via renewable energy sources [1].

In 2025, the transport sector remains predominantly reliant on Internal Combustion Engine Vehicles (ICEVs) operating on fossil fuels. These systems offer clear end-user advantages, including practical fuel storage, high specific energy (e.g., 44 MJ/kg for gasoline), very short refueling times (<5 min), and conversion efficiencies that have substantially increased over more than a century of technological refinement [2]. Such benefits, however, come at a substantial cost: these technologies are responsible for one-third of CO₂ emissions from end-use sectors, with road transport accounting for ~ 73% of this share, as well as for the emission of pollutants such as particulate matter (PM) and carbon monoxide (CO) from incomplete combustion, along with nitrogen oxides (NO_x) and sulfur oxides (SO_x) [3]. Meeting the IEA *Net Zero Emissions by 2050 Scenario* requires a rapid shift toward low-carbon transport technologies, as the final energy consumption of the sector relies on oil products for more than 90%, which is only ~ 3% less than in the early 1970s, while current estimates suggest that proven reserves may be exhausted in roughly 50 years at today's consumption rates [4].

Electric vehicles (EVs) powered by renewable electricity might play a central role in this transition. Many governments in developed countries are actively promoting the adoption of EVs through policy instruments such as purchase incentives, reduced registration and circulation taxes, and other supportive measures aimed at accelerating market uptake [5]. EVs are typically classified according to the relative contribution of electric power to vehicle operation. This hierarchy spans from Hybrid EVs (ranging from mild to plug-in) and extended-range EVs, which still depend partly on internal combustion engines, to fully electric Battery-, Fuel Cell-, and Fuel Cell Hybrid EVs, namely BEVs, FCEVs, and FCHEVs [6]. Fully electric vehicles feature no tailpipe emissions, markedly reduce noise pollution, and exhibit high well-to-wheel efficiencies, reaching up to 70% when powered by renewable electricity, compared with 25–37% for diesel and 11–27% for gasoline vehicles. Currently, PHEVs and BEVs are dominant [7], with lithium-ion batteries being the primary storage technology due

to superior performances, including higher energy and power density, greater specific energy, minimal memory effect, and long cycle life [8].

Furthermore, The primary limitations of PHEVs and BEVs lie in the battery pack due to high upfront costs, long charging times (typically 4–8 h, reduced to ~ 30 min with fast charging), limited driving range, and substantial weight and volume. These constraints particularly affect taxi and car-sharing services and long-haul road transport [9]. The carbon footprint of manufacturing a battery pack is comparable to that generated by an entire conventional vehicle, which almost doubles for the full EV. Additionally, large-scale deployment of PHEVs and BEVs would require significant upgrades to the electrical distribution infrastructure, an investment that may be economically unattractive in rural or low-density regions. Safety risks also exist: mechanical, thermal, or electrical abuse can trigger parasitic exothermic reactions, and failures in the Battery Management System (BMS) may lead to hazardous overcharging or over-discharging. Battery swap stations (BSSs) could, in principle, mitigate long charging times; yet their practicality is constrained by the strong design heterogeneity among battery packs, which limits interoperability [8].

The limitations of a purely battery-based electrification of the transport sector open the road to a synergistic deployment of fuel cells [10]. These are electrochemical converters in which gas reactant streams are injected at the anode side (fuel) and at the cathode side (oxidant). Both electrodes are composed of porous materials that allow for the separation of reactants, ionic and electronic conduction, and catalytic activity, fostering the conversion of the chemical energy embedded in the fuel to electrical energy. A membrane separates the electrodes, preventing internal short circuits while enabling ionic conduction. The flow rate of the reactants is adjusted depending on the power required by the user. Heat is also produced from both reaction thermodynamics and irreversible transport phenomena. Fuel cells operating at low temperatures ($\sim 80^\circ\text{C}$), such as Proton-exchange Membrane Fuel Cells (PEMFCs) fed by a high-purity H_2 fuel stream, are particularly suitable for transport applications, integrating in a broader *hydrogen economy* which would also encompass stationary generation and green chemical industry [11]. PEMFC integration in FC(H)EVs promises (i) high efficiency, more than doubling traditional ICEs, and quick start-up times; (i) a longer driving range, achievable with properly distributed fuel tanks inside the car without compromising passenger habitability; (ii) the decoupling of energy storage and conversion, allowing flexible system design; (iii) short refueling time and (iv) lower station-level investment and milder impact on grid stability than the high-power fast-charging infrastructure required for BEVs [5, 12, 13].

At the end of 2024, 89 hydrogen fueling stations were present in the US, 74 of them in the state of California, while the number rises to 294 in the European Union, of which 113 in Germany, and to 748 in operation in Asia, 384 of them in China [14]. Fuel cell-based electrification efforts are of interest for a wide variety of vehicle classes, ranging from forklifts and passenger cars to light- and heavy-duty vehicles, as well as aircraft, trains, and ships. These exhibit substantial variability, both within and across types, in terms of daily traveling mileages, weight, volume, and power requirements. Addressing such a diversified demand would traditionally require the development of PEMFC stacks specifically tailored to each application, including the corresponding auxiliary components. This approach, though, significantly constrains the scalability of manufacturing processes and hinders straightforward maintenance of PEMFC electric powertrains. As a relevant challenge in stack manufacturing, the diversification in product requirements poses substantial economic risks to the eventual full automation of fabrication and assembly processes. On the other hand, manual and semi-automated procedures would stress operators due to product and process complexity [15]. Such challenges also extend to the frequent manual maintenance activities required on FCHEVs, as the U.S. Department of Energy (DOE) 2030 durability targets, ranging up to 25000 operational hours for heavy-duty vehicles with performance degradation below 10%, are currently far from being met [16].

In this context, the project *Hydrogen Mobility Made in Italy* (HYMOBITALY), a collaborative effort between the Polytechnic University of Bari and the University of Padova, aimed to demonstrate the potential for industrial scalability of PEMFC power systems intended for hydrogen-based mobility applications in terms of both their fabrication and maintenance. The project also targeted technologies for PEMFC disassembly and recycling, embedding circular-economy principles in sustainable mobility. Within HYMOBITALY, a modular PEMFC stack was designed, fabricated, and tested to promote the standardization of base units over a wide power range, supporting the implementation of modular production schemes and fostering specialized training programs for personnel involved in stack manufacturing and maintenance.

Peculiarities in the PEMFC stack response during the experimental campaign further confirmed a relevant issue widely reported in the literature: the control of liquid water within the cell, referred to as water management, acts as both a critical design and operating constraint [17]. The electrolyte membrane can indeed experience two detrimental limiting regimes: drying and flooding. Insufficient liquid water reduces proton conductivity, while its excess obstructs reactant transport pathways to the electrochemically active sites. Water management is strongly conditioned by the design

and properties of the gas diffusion layer (GDL), which forms the structural backbone of the electrodes [18]. The GDL must simultaneously facilitate reactant and product gas transport, regulate liquid-water removal and retention, provide heat removal, ensure mechanical integrity, protect the catalyst layer from corrosion, and maintain low-resistance electronic contact. In this framework, multiphase/multicomponent flow and the wettability of the fibrous structure play a central role in the design of the GDL. Starting from conventional carbon-fiber substrates [19], recent research has introduced novel materials and fabrication strategies, as electrospun PAN-based carbon nanofibers [20], carbon nanotube sheets [21], bio-based materials and composites [22], [23–25], and metal foams [26]. To support these developments, computational fluid dynamics (CFD) has become an increasingly important tool for performance prediction, particularly for analysing the effect of tailored pore morphologies and controlled deposition of hydrophobic agents [27]. Among CFD approaches, the lattice Boltzmann method (LBM) is a fully Eulerian, mesoscopic scheme that recovers the semi-incompressible Navier–Stokes equations through iterative collision and streaming of particle distribution functions on a lattice [28–31]. Pseudopotential extensions introduce effective interaction forces, allowing the LBM to model non-ideal fluids and thus simulate multiphase and multicomponent flows with interfacial tension and wetting effects [32–35]. Several studies have employed these models to investigate water transport and wetting in PEMFC GDLs [36–38]. However, many existing implementations rely on simplified collision operators and simplified prescriptions of wetting states, which may compromise physical consistency and induce spurious mass transfer at liquid–solid interfaces, thereby limiting their predictive capability.

Thesis Outline

This thesis is structured as follows:

- Chapter 1 describes the material selection, fabrication, and experimental characterization of the modular PEMFC stack prototype developed within the HY-MOBITALY project. The central role of water management in achieving high stack performance is highlighted, and the modeling strategy selected to address this issue is introduced.
- Chapter 2 presents the Lattice Boltzmann Method, introducing its mesoscopic foundations, deriving the governing equation, and defining the core algorithm. The analysis of the method, together with its recent advances and current limitations for the simulation of multiphase flows and wetting, is then discussed.

- Chapter 3 introduces the model developed for the accurate simulation of multiphase flows and wetting, starting from the initial–boundary value problem of interest, detailing the numerical method, and providing insights into the algorithmic structure and code implementation.
- Chapter 4 reports the validation tests performed on the proposed model and their outcomes, assessing its ability to reproduce both cohesive and adhesive phenomena.

Finally, the concluding chapter summarizes the main findings and outlines directions for future research.

CHAPTER 1

Construction and testing of a modular PEMFC stack

This chapter presents the design, construction, and experimental testing of a modular PEMFC stack developed within the framework of the *Hydrogen Mobility Made in Italy* (HYMOBITALY) project.

As a relevant issue hindering the performance of PEMFC stacks is the phenomenon of flooding, primarily occurring in the Gas Diffusion Layers (GDLs), this chapter also introduces a focus on this key component, stemming from the conference paper *A framework relating functions, properties and performances of GDLs for PEM Fuel Cells*, within the *Proceedings of the 10th International Conference on Materials Science and Smart Materials*.

Concluding this chapter, the role of multiphase-flow and wetting models in resolving transport phenomena within the GDL is critically assessed.

1. Fundamentals of PEMFCs

An increase in the market share of Fuel Cell Electric Vehicles (FCEVs) could mitigate the environmental impact of the transport sector, a major contributor to pollutant emissions [39, 40]. FCEVs are suitable for heavy-duty applications due to their short refueling time, long driving range, and optimal scalability in terms of size and power; however, they are expensive and require new fuel infrastructures [9]. Proton-exchange Membrane Fuel Cells (PEMFCs) fit perfectly into FCEVs powertrains due to their high efficiency, quick startup times, and good transient response; they are challenged, though by limited fuel flexibility, reduced durability, and high costs.

A PEMFC is fueled by a pure H_2 stream at the anode, where the Hydrogen Oxidation Reaction (HOR) takes place, and an air/ O_2 stream at the cathode, where the Oxygen Reduction Reaction (ORR) occurs, with water being the only reaction product. Electrical energy is produced, along with heat generated from both the thermodynamics of reactions and transport phenomena [12]. At a cell level, considering a symmetrical structure and spanning from its core component outwards, the unit includes the Proton-exchange Membrane (PEM), the Catalyst Layer (CL), the Gas Diffusion Layer (GDL), and the Bipolar Plate (BP). The PEM enables the conduction of protons (H^+) at an appropriate operating temperature ($\sim 80^\circ C$) and hydration level,

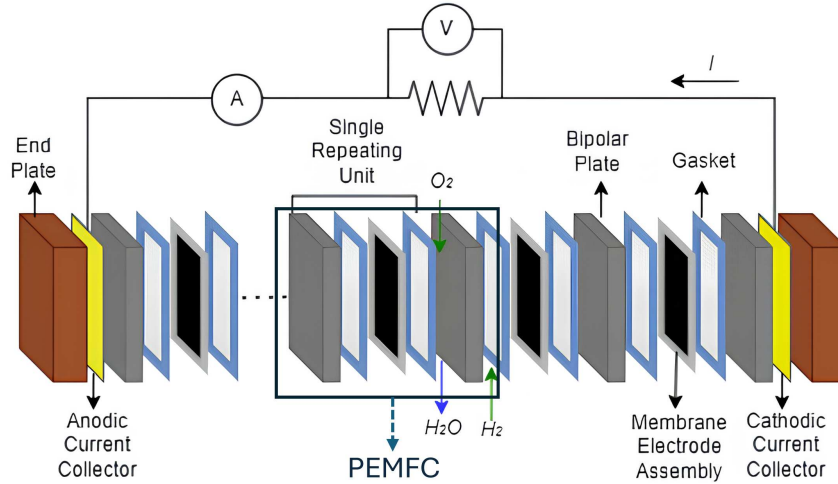


FIGURE 1. A PEMFC stack constituted of multiple Repeating Units and pairs of Current Collectors and End Plates, closing the system.

while simultaneously preventing electronic conduction and ensuring the separation of the reactant streams [41]. The CL is a porous, thin layer located on the GDL where the HOR and the ORR occur, respectively, at the anode and cathodic sides. Commercial electrocatalysts (ECs) consist of Pt on a carbon support in the form of nanocomposite Pt/C ECs. Both HOR and ORR are promoted by the Pt active sites; proton conduction is guaranteed by a dispersed ionomer, while electronic conduction is enabled by the carbonaceous support of the Pt/C EC [42]. The GDL is a porous structure that aids in gas distribution, water management, and mechanical support of the cell, while also ensuring electrical and thermal connection with the BP [43]. The Catalyst Layer (CL) and Gas Diffusion Layer (GDL) form the Gas Diffusion Electrode (GDEs), whereas interposing a Proton-exchange Membrane (PEM) between two GDEs yields a Membrane Electrode Assembly (MEA). Lastly, the bipolar plates (BP) enclose each cell, enabling the distribution of inlet and outlet reactant streams, providing electrical connections among multiple cells, and contributing to the overall thermal management of the stack [44, 45].

The power output of the system is increased by connecting multiple cells in series to form a PEMFC stack. Assembly methodology (e.g., screw or strap) and clamping pressure severely influence its performance [46].

A schematic depiction of a PEMFC stack is provided in Figure 1.

1.1. Polarization effects. The PEMFC polarization curve relates the cell voltage (V_c) to the produced current density (i), which is proportional to the mass flow rate of

reactants according to Faraday's law. As i increases, activation, ohmic, and concentration polarizations, each a monotonic function of i , progressively reduce V_c .

- Activation polarization (η_{act}) is related to the charge transfer mechanism at the CL, positively affected by high temperatures, appropriate catalyst selection and quantity, and electrode microstructure.
- Ohmic polarization (η_{ohm}) stems from the materials resistance to both electronic and ionic conduction, the latter being related to the PEM performance, peaking at $\sim 80^\circ\text{C}$ and a suitable level of humidification.
- Concentration polarization (η_{conc}) occurs due to the depletion of reactants at the CL active sites.

The impact of different polarization losses on V_c depends on i ; respectively, η_{act} , η_{ohm} , and η_{conc} most significantly affect the activation, ohmic, and mass transport regions of the polarization curve [47].

2. Construction of the modular PEMFC stack

The material selection for each component is first described, followed by the fabrication of a single cell, the assembly of a single stack, and finally, the assembly of the complete modular PEMFC stack.

2.1. Materials. The selected PEM is the GORE GFCG0316, characterized by a thickness of $8\mu\text{m}$ and consisting of perfluorosulfonic acid (PFSA) reinforced with porous polytetrafluoroethylene (PTFE), featuring high mechanical strength and durability [48]. A Pt/C EC is adopted, with a Pt loading set to 0.15 mg/cm^2 on the anode and 0.4 mg/cm^2 on the cathode, the latter being higher due to the slower electrochemical kinetics of the ORR in comparison with the HOR [43]. The SIGRACET 22BB from SGL carbon is selected as GDL, being a $215\mu\text{m}$ thick, non-woven carbon paper integrated with a Microporous Layer (MPL) and subjected to a hydrophobic treatment with PTFE. The selected component is inexpensive and recommended for automotive applications. Polyethylene naphthalate (PEN) is adopted in the sub-gasket frame due to its high thermal stability, good dielectric strength, and favorable mechanical properties [49]. The BPs consist of two half-plates made from a polymer-carbon composite, fabricated by molding a molten polymer (PVDF) binder mixed with carbon fillers, ensuring chemical stability while being lightweight and inexpensive [50]. The internal surface of the cathode half-plate incorporates parallel channels where distilled water circulates as a coolant, removing the heat absorbed at the BP-GDL interface (see Figure 2, left). Both half-plates on their electrode-facing sides feature multi-path serpentine flow-field channels for reactants (see Figure 2, right). This design enhances



FIGURE 2. Cathode coolant flow field (left), cathode and anode reactants flow fields (right).

under-rib convection, facilitating effective water removal and improving reactant transport to the catalyst layer (CL) [51]. The channels on the anodic side adopt a ‘V’ shape, whereas those on the cathodic side have a ‘U’ shape to accommodate higher flow rates. Closing the stack, the CCs are composed of silver-coated aluminum within a polyvinylidene fluoride (PVDF) frame, electrically connecting the stack to the load via dedicated terminals, while the two EPs are fabricated from anodized aluminum to withstand and evenly distribute the assembly clamping pressure [46].

2.2. Fabrication of a PEMFC. Multiple Catalyst Coated Membranes (CCMs) are fabricated initially. Each CCM is a multi-layered structure constituted of a PEM coated with a catalyst ink and is produced by the homonymous technique, which shows a higher quality of the final product compared to other methods such as the Catalyst Coated Substrate (CCS) [49]. The CCM requires a direct application of the catalyst ink on both sides of a PEM to obtain a slab, while other stack layers are assembled in subsequent steps. The adopted CCM is square-shaped, measuring 10 cm on each side, and is integrated into a PEN sub-gasket frame by the procedure detailed hereafter.

In the first step, the sub-gasket is prepared by cutting out a square opening slightly smaller than the MEA dimensions from a layered PEN structure. The CCM is then positioned within this opening and secured in place by an adhesive layer. Subsequently, the assembly is thermally bonded in an oven for a few minutes, activating the adhesive and ensuring a gas-tight seal along the CCM perimeter. Following the thermal bonding, the assembly is placed on a stencil with six predefined openings corresponding to the anode, cathode, and coolant circuit inlets and outlets, which are carved out by a press-cutting process that applies a force of 12 kN. The structure is then removed from the stencil, ready for the following steps (see Figure 3). The procedure is repeated for 32 cells to obtain the functional units needed to assemble the two PEMFC stacks within the modular system.



FIGURE 3. Structure constituted of CCM and sub-gasket after the cutting process. The apertures guarantees the stream of reactants and products within the PEMFC stack.

2.3. Assembly of a single PEMFC stack. The assembly procedure of a single stack starts by gluing an insulating sticker on the internal part of the anodic EP. The anodic CC, framed by a polyoxymethylene (POM) structure, is then positioned on top (see Figure 4-a). A cathodic monopolar half-plate is set, with its corresponding gasket, to ensure an adequate cooling on the anodic side (see Figure 4-b). Afterwards, the anodic half-plate and its gaskets are installed (see Figure 4-c). The layers being subsequently positioned comprise the anodic GDL, the CCM + sub-gasket assembly (see Figure 4-d) and the cathodic GDL (see Figure 4-e). A focus on the CCM sealing mechanism is provided in Figure 5. This sequence is repeated for each of the 16 cells included in each single PEMFC stack.

The cathodic CC is then laid, along with an additional POM frame and insulating sticker, concluding with the cathodic end plate (see Figure 4-f). The stack is secured by employing a screw-based clamping mechanism, as a simple and cost-effective technique. Stainless steel threaded bolts apply localized compressive force, optimized to ensure effective sealing without compromising the integrity of internal components [46]. This procedure results in a single 16-cell PEMFC stack.

2.4. Assembly of the modular PEMFC stack. The adoption of a modular PEMFC stack architecture would promote the development of standardized base units, enabling economies of scale in production and simplified, rapid maintenance via single-stack replacement in FCEVs, while also promoting regulated training for maintenance technicians. Recent literature suggests integrating small independent units, either solely

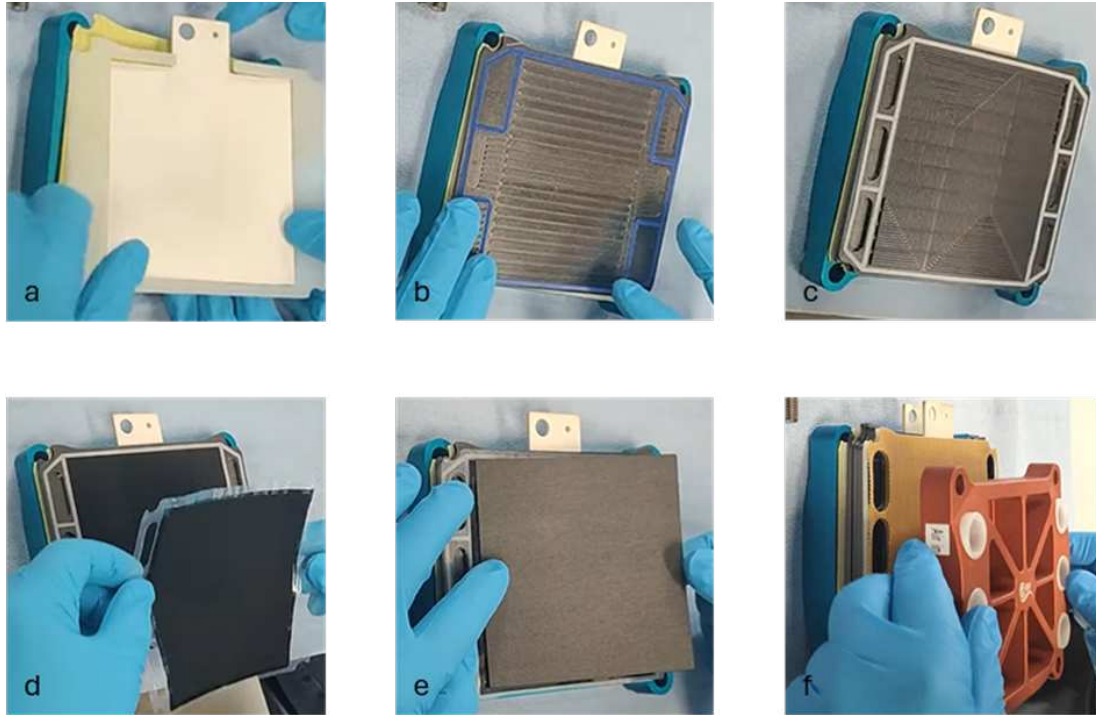


FIGURE 4. Assembly of a single PEMFC stack. Steps (a) - (b) are executed at the anodic side: positioning of the insulating sticker, current collector and cooling half-plate. Steps (c) - (e) are executed for the 16 cells. The procedure ends with the closure at the cathodic side (f), specularly to steps (a) - (b).

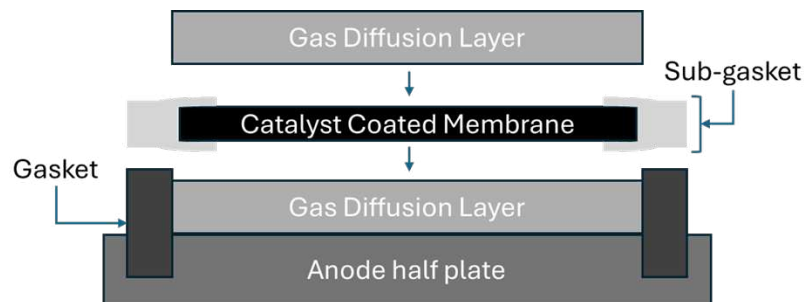


FIGURE 5. The sealing mechanism of the Catalyst Coated Membrane is constituted of embedded sub-gaskets and gaskets, preventing gas leak-ages.

electrically or also including fluid distribution and thermal subsystems, in PEMFC multi-stack system architectures. These latter branch in parallel or series fluidic configurations, with or without intermediate compression stages [52–54]

A modular PEMFC stack prototype is assembled in a 'twin' configuration, leveraging modularity also at the piping levels, exploiting composable manifolds, and guided by Internal Combustion Engine (ICE) research and development results, adopting common-rails for the H_2 , oxidant, and coolant stream circuits. Chrome plated brass piping and tee junctions of choice ensure good mechanical strength and corrosion resistance, complying with UNI EN 12165 CW617N and UNI EN 12164 CW614N. The symmetry of the piping system is essential to promote homogeneous performance among single stacks; thus, a regularly spaced layout is implemented. Additionally, the oxidant outlet piping would be inserted horizontally in each base unit to prevent gravity-driven water accumulation [55]. Each base unit is framed by a 5 mm thick composable POM structure, providing electrical and thermal insulation, as well as mechanical and chemical stability [56]. The favorable surface area-to-volume ratio enabled the placement of individual stacks with an interspacing of approximately 3 cm while expecting no detrimental impact on the thermal equilibrium of each unit.

3. Experimental testing of the prototype

To evaluate the effectiveness of the design, manufacturing, and assembly of both the single units and the LEGO-like twin-stack prototype (Figure 6), an experimental campaign is conducted, beginning with a preliminary break-in procedure followed by polarization testing.

A minimum stoichiometric current is set to 50 A to preserve the stack against fuel starvation, as this condition would induce anode catalyst degradation due to carbon corrosion. The selected values of anode and cathode inlet pressure, being respectively 100 and 80 kPa_g, would avoid unbearable stresses on the seals. The set coolant temperature, set to 65°C, is neither excessive, to avoid membrane drying, nor insufficient, thereby ensuring optimal PEM proton conductivity. Additionally, setting the anode and cathode (a/c) streams at +7°C with respect to the dew point temperature (DPT), here 70°C against 63°C, avoids water condensation [57]. The anode stream is free from contaminants of carbonaceous molecules, such as CO₂ or by-products of CH₄ steam reforming.

3.1. Break-in procedure. The break-in procedure is a crucial preliminary step, as it ensures optimal and stable stack performance. An activation protocol consists of applying a periodic current or voltage profile to the device (in galvanostatic or potentiostatic operation) until stable operating conditions are achieved. The progressive enhancement in performance is attributed to internal and interfacial phenomena within the PEM, the CL, and other stack components [58, 59]. Specifically, the PEM ionomer

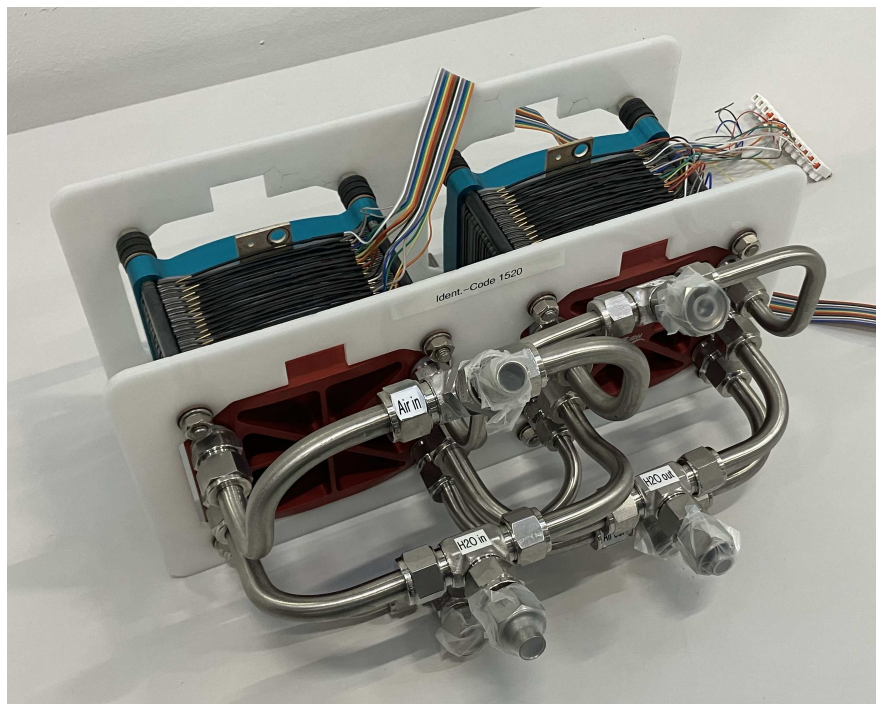


FIGURE 6. Modular twin-stack with symmetric piping system for the fuel, oxidant and coolant circuits.

is subject to hydration, internal structural modifications [60], surface skin rearrangement, and contaminants removal, all of which positively contribute to the PEM proton conductivity [61]. In the CL, the ionomer similarly experiences hydration, while the carbon support is partially oxidized [62]; contaminants are removed, and the size and distribution of Pt catalyst particles are altered, increasing the catalyst active surface area [63]. At the cell scale, the interface between the GDL and the BP undergoes morphological adjustments, reducing the area-specific resistance [64]. These activation processes collectively mitigate the negative impacts of manufacturing, transportation, and storage-induced imperfections.

An online galvanostatic break-in protocol is executed on the twin stack under air/H₂ feed by imposing a stepwise periodic current profile for approximately 7.5 hours. The load profile consists of alternating steps between low (30 A) and high (120 A) current set points, with short transients (100 s) in between. The switch criterion is based on the stability of the average cell voltage within ± 5 mV. To mitigate degradation driven by reactant starvation, stoichiometric ratios of 2.1 and 2.6 are set at the anode and cathode, respectively. Additionally, the coolant flow rate is fixed at 7 L/min to ensure effective thermal management [57]. The maximum, mean, and minimum cell voltages among the 32 units are displayed in Figure 7.

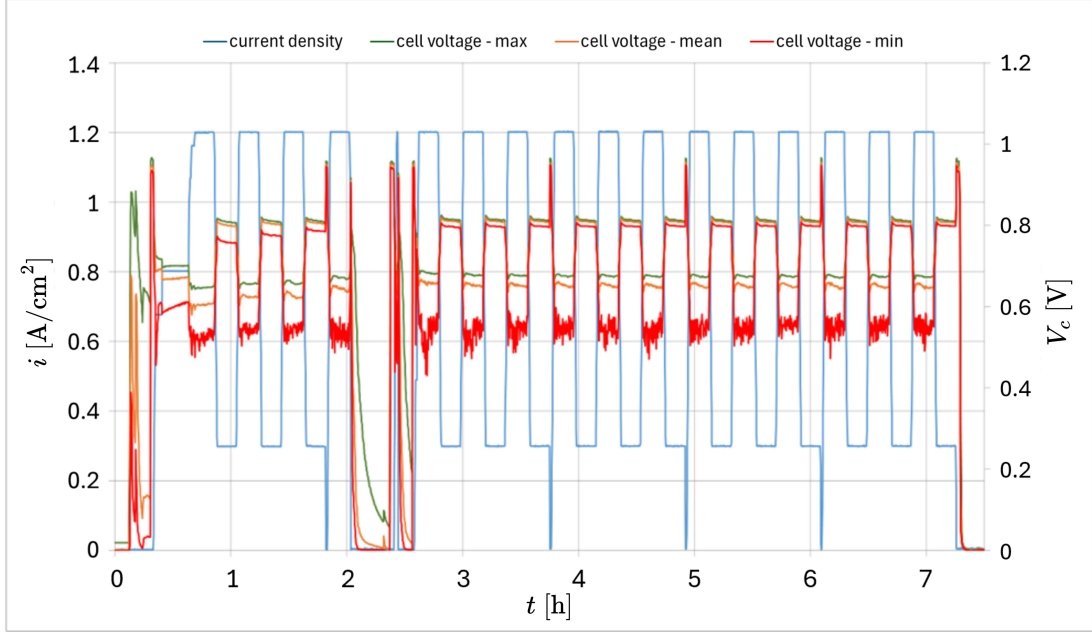


FIGURE 7. Results of the break-in procedure on the PEMFC twin stack. The current density, along with minimum, max and mean cell voltage are displayed.

Notably, during the break-in test, the time-averaged values at both low and high current half-periods increase significantly within the first three cycles. The test station was then temporarily shut down for approximately half an hour during the fourth load cycle due to technical reasons. Following the restart of the experiment, only a minor and transient improvement in high current performance is observed, diminishing gradually over the following cycle before stabilizing. Additionally, the maximum and mean cell voltage profiles show a higher consistency with the periodic load profile as the test progresses. At high current steps, a decrease in uniformity among the maximum, mean, and minimum cell voltages, as well as instability of the latter, is observed. These aspects are investigated in polarization testing.

3.2. Polarization testing. Polarization testing relates the measured device voltage to the generated current, enabling the computation of relevant performance metrics for PEMFC power systems [65]. This experimental procedure is conducted in galvanostatic operation through a stepwise adjustment of the stack current according to a predefined load profile to ensure reproducibility. The selected current set-points are: $I \in \{0, 10, 20, 40, 60, 80, 100, 120\}$ A.

Initially, the current is set to its peak target value; then, it is reduced stepwise (*descending phase*) to the stack open-circuit voltage (OCV) and then increased back

(*ascending phase*). This bidirectional current scan allows for the determination of the steady state behavior of the system while accounting for hysteresis effects induced by the varying stack conditioning at each load step [65]. The dwell time at each step is set to 5 minutes, except at OCV, in order to prevent excessive deterioration by the over-stoichiometric reactant flow rate. Stability during each step is ensured by a ± 5 mV criterion based on the mean cell voltage, guaranteeing reliable and consistent data acquisition [66]. Both stack and individual cell voltages are recorded; the latter are presented in their maximum, mean, and average at each step. In Table 1, specific settings of the test bench for polarization testing are displayed, including the stoichiometric ratio at the anode side (λ_a) and at the cathode side (λ_c), being the actual flow rate divided by the one required by the electrochemical reaction for the imposed load, along with the volume flow rate of coolant Q_c .

TABLE 1. Settings adopted for the polarization testing.

Case	Feed	# cells	λ_a [-]	λ_c [-]	Q_c [L/min]
single	air/H ₂	16	1.9	2.2	5
single	O ₂ /H ₂	16	1.9	2.2	5
twin	air/H ₂	32	2.0	2.5	8
twin	O ₂ /H ₂	32	1.9	2.2	9

The experimental results of the galvanostatic tests are shown in Figure 8 and Figure 9 for the single stack, respectively fed by air/H₂ and O₂/H₂ streams, and in Figure 10 and Figure 11 for the twin stack, tested under specular conditions of the reactants. In all the selected test cases, the cell voltage appears to be inversely proportional to the applied current; this occurs due to activation, ohmic, and diffusion polarization effects, with transport phenomena enhanced at high imposed loads [65].

At low generated current density, the cell voltage distribution within the stack appears uniform. However, at high load, especially in air-breathing configurations, the cell exhibiting the lowest voltage shows a significant loss in performance compared to both the maximum voltage cell and the calculated average one, alongside reduced operational stability. This behavior is attributed to increased water generation at higher power density, causing the accumulation of liquid water. The presence of excess water hinders reactant transport to active reaction sites, thus resulting in uneven voltage distribution within the stack [55].

The galvanostatic curves are not symmetric around the idle condition; instead, a clear effect of hysteresis manifests. Such behavior is attributed to a water-reservoir effect: the membrane is well hydrated in the initial stage of the descending phase due

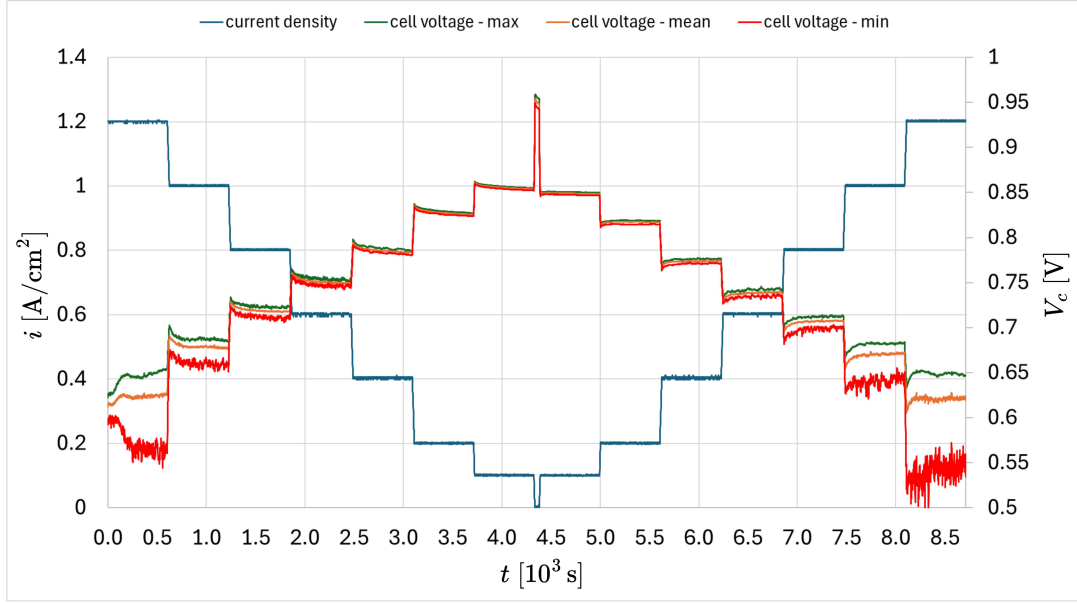


FIGURE 8. Galvanostatic polarization test: air/H₂ fed single unit.

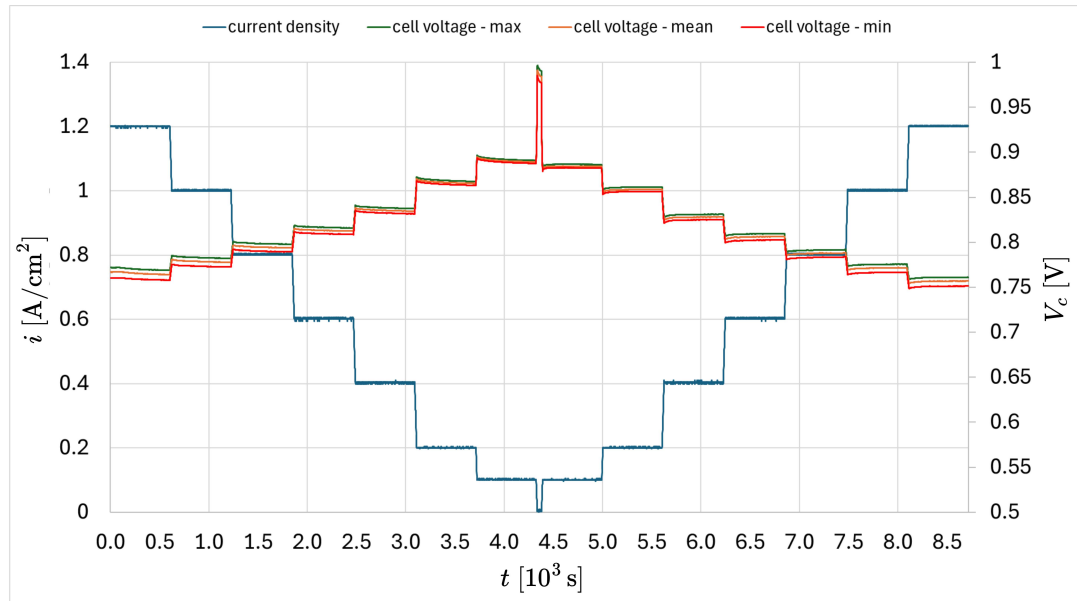
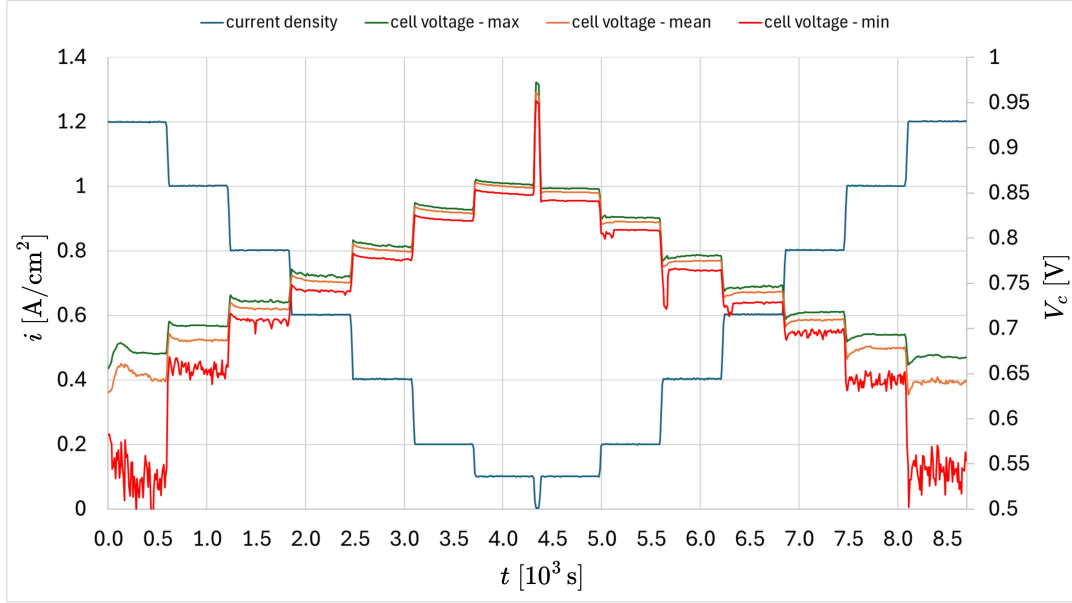
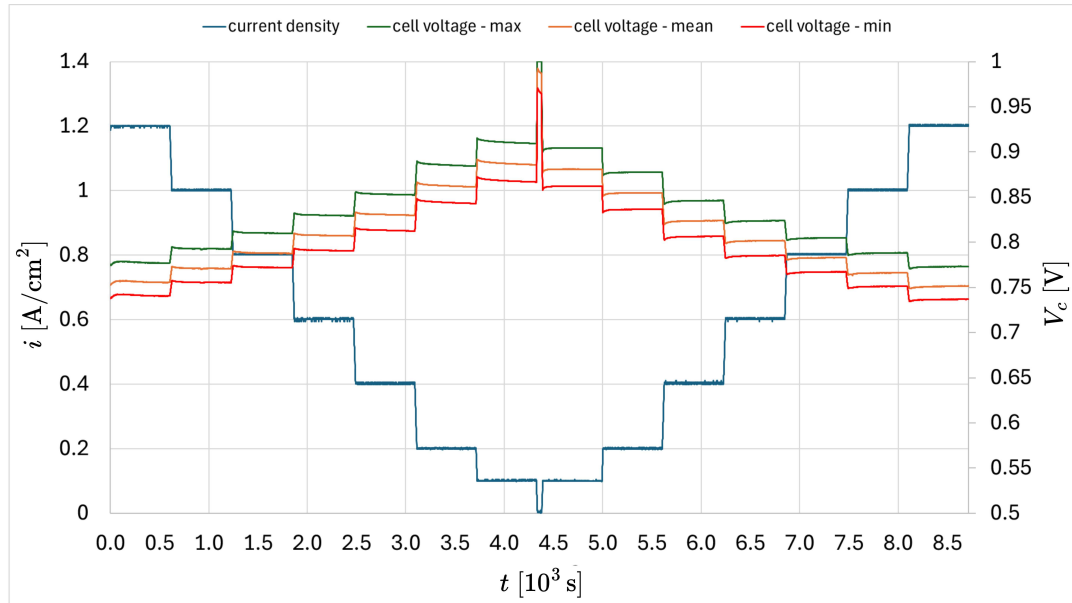


FIGURE 9. Galvanostatic polarization test: O₂/H₂ fed single unit.

to the high generated current density, enhancing the cell voltage in mid to low load conditions with respect to the corresponding values in the ascending phase. Considering the pairs of V_c after thermal equilibration, their proximity, especially the lack of crossing points, indicates, respectively, a sufficient test stabilization time and cell temperatures, and a satisfactory pre-humidification of reactant streams [67]. The polarization curve indicates the steady-state response of the system. It is computed as

FIGURE 10. Galvanostatic polarization test: air/H₂ fed twin stackFIGURE 11. Galvanostatic polarization test: O₂/H₂ fed twin stack

the arithmetic mean of the equilibrium values between the ascending and descending phases [66], and is presented here in Figure 12, normalized with respect to the chemical energy of the converted H₂, as the thermodynamic efficiency η . At peak current conditions, air-breathing cells operate within the mass-transport-limited region (*knee*) of their polarization curves, whereas cells fed on O₂/H₂ do not. The power curves relate the power density P_d , being the normalized electrical power per unit area, and

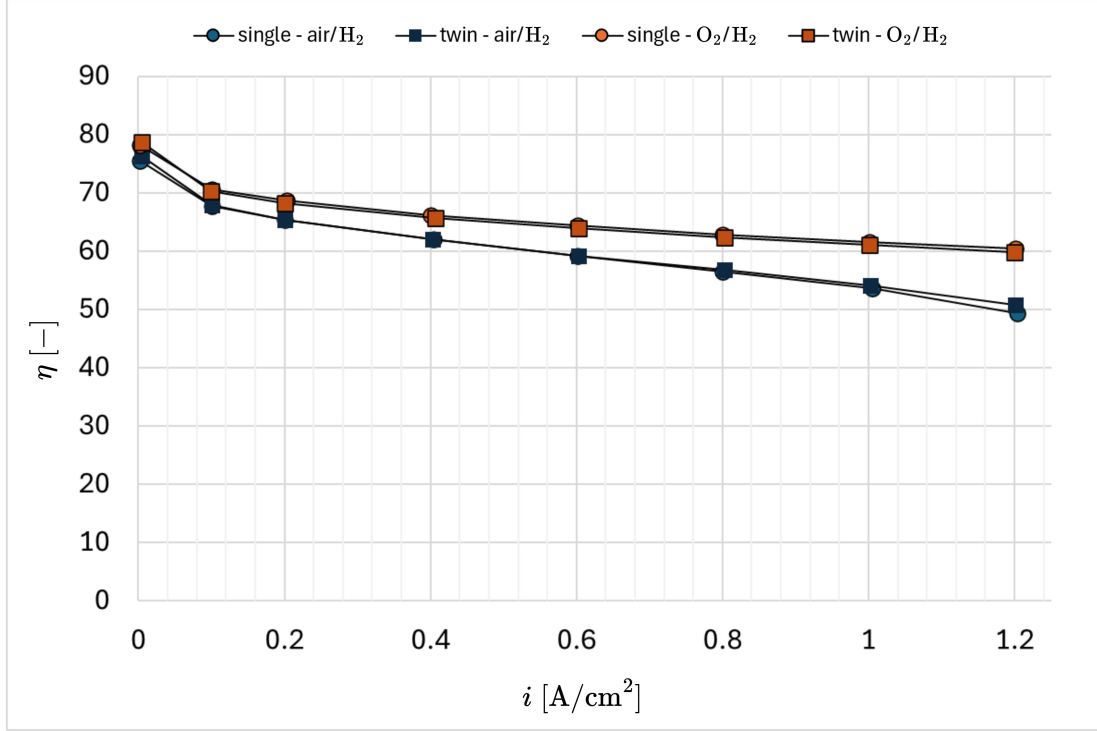


FIGURE 12. Efficiency at different imposed load for diverse experimental configurations. At fixed boundary conditions, η is linearly proportional to the corresponding polarization trends.

i. These are constructed with steady-state data and displayed in Figure 13, while the stack-level data, measured at maximum imposed load, are provided in Table 2, including the consumption of H₂ in terms of mass flow rate ($\dot{m}_{\text{H}_2}$).

TABLE 2. Stack-level polarization test results at maximum imposed load.

Case	Feed	Voltage [V]	Power [kW]	$\dot{m}_{\text{H}_2}$ [g/min]	η [-]
single	air/H ₂	9.914	1.187	1.194	49.43
single	O ₂ /H ₂	12.12	1.450	1.190	60.39
twin	air/H ₂	20.37	2.449	2.387	50.79
twin	O ₂ /H ₂	24.00	2.872	2.239	59.79

Both thermodynamic efficiency and power density curves demonstrate that feeding on pure O₂ leads to improved performance; this occurs due to a higher partial pressure of O₂ at the reaction sites, which increases the Nernst potential and the ORR activation overpotential while also reducing concentration losses.

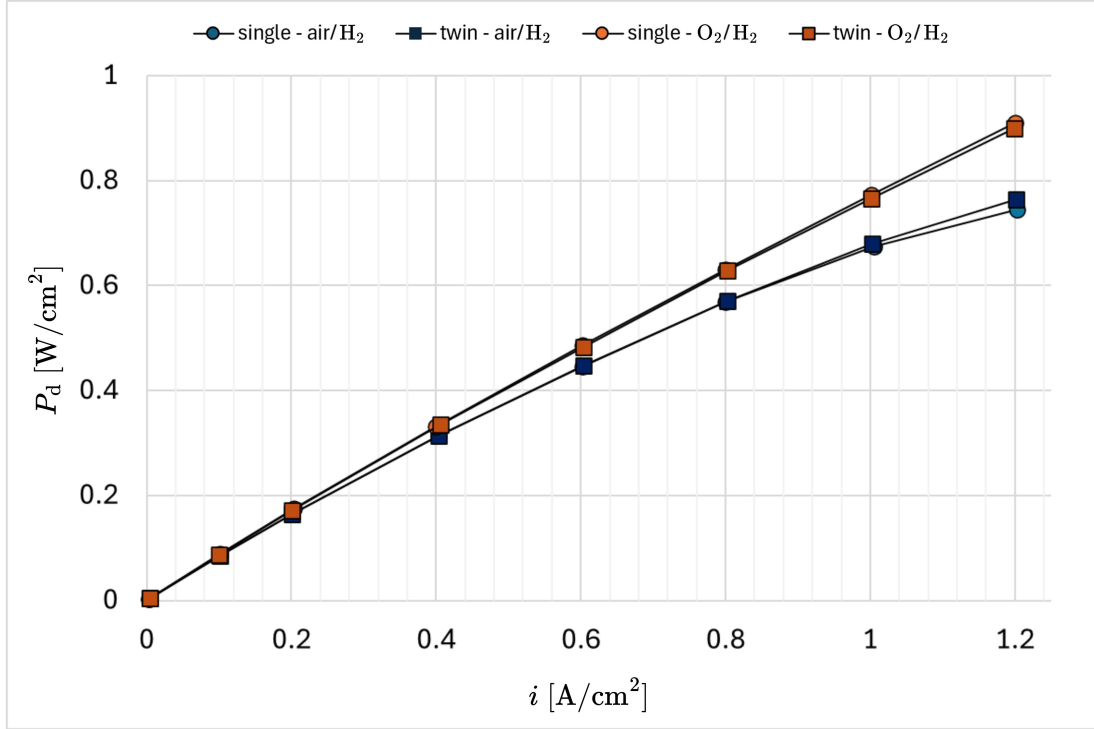


FIGURE 13. Power density curves evaluated for different experimental configurations.

More importantly for the present work, the curves for the single and twin stack configurations nearly overlap, indicating that an efficient coupling between the two single stacks was achieved.

4. PEMFC water management: bridging macroscale and microscale

Under air/H₂ feed, for a high imposed load, the stacks operate in the mass-transport-limited region of the polarization curve. In this regime, the minimum V_c within the stack deviates significantly from both the mean and maximum values, also showing unstable evolution over time. Such behavior could be attributed to the flooding phenomenon. The accumulation of liquid water hinders the transport of reactants towards the active sites of reaction and induces uneven voltage distribution among the cells. These phenomena are primarily governed by the morphology and material properties of the GDL; its design is thus crucial for water-management strategies [68].

4.1. A close look at the Gas Diffusion Layer. The GDL is a key performance-limiting component of a PEMFC, located between an internal and sensitive CL, which

hosts reaction sites, and an external and robust BP, which guides the streams of reactants and products. The positioning of the GDL defines its required functions: providing mechanical support and minimizing polarization effects due to transport phenomena. Several alternatives to traditional carbon paper-based materials for GDL are currently being investigated, including CNTs, bio-based materials, and metal foams. A GDL is typically composed of an external Macroporous Substrate (MPS) and an MPS. The most common base material for MPS is carbon paper (CP), ensuring a trade-off between durability, cost, and performance [19]. The MPL is characterized by a finer pore structure, ensuring a smooth transition towards the internal CL, thus minimizing electrical and thermal contact resistances, facilitating the CL deposition, and, in CP-GDL, protecting the CL by reducing catalyst dispersion and the chance of perforation by carbon fibers [69]. A relevant addition in the CP-GDL is the hydrophobic PTFE to aid in water management. Relevant industrial manufacturers include AvCarb Material Solutions, Toray Industries, and SGL carbon. Only the latter disclosed its fabrication process: polyacrylonitrile is subject to a sequence of heat treatments to break down organic compounds and produce carbon fibers, which are then chopped and subjected to wet laying. Carbon precursors are integrated through further heat treatments to obtain carbon paper, which being then subjected to a PTFE dip and, lastly, to MPL coating and sintering [19]. The main drawbacks of these CP-GDLs are their high costs [70], the adoption of fossil-fuel-derived carbon fiber precursors [22], and electrochemical degradation [71]. New kinds of GDLs are proposed in the literature, with alternative formulations of MPS, MPL, or both, claiming a more sustainable fabrication process or improved performance compared to traditional units. Among these are electrospun PAN-based carbon nanofibers [20], carbon nanotube sheets [21], bio-based materials and composites [22], [23–25], and metal foams [26].

A GDL is typically characterized by anisotropic material properties. These are labeled as *through-plane* and *in-plane*, respectively referring to those measured or computed across the component thickness or in a normal direction.

4.1.1. *Mechanical support.* GDL must both withstand high assembly loads and ensure long term durability during operation. High compressive, tensile, and shear limits, as well as bending stiffness, are required, the latter playing a significant role in the sub-freezing conditions expected in PEMFC transportation applications [72]. Thermal cycling could induce delamination of the MEA, resulting in a loss of performance due to a lack of contact between the constituent components. The mechanical support function is affected by bulk properties, thickness, and porosity; these are influenced by the PEMFC stack clamping pressure. an excessive load could induce significant elastic

or plastic deformation, resulting in possible fiber dislocation and loss of mechanical resistance, while reduced loads would lead to reactants and products leakages [73]. Durability is severely affected by electrochemical degradation effects, e.g., the catalytic (Pt) corrosion of carbon fibers at both low and high voltage, primarily occurring during startup, shutdown, and flooding [71]. Given that a strong backing layer would also protect the CL against degradation [74], the mechanical support function impacts all the polarization effects.

4.1.2. *Electrical connection.* A GDL must electrically connect the CL and the BP. The GDL internal resistance is affected by its thickness, bulk material properties, and the morphology of the structure. The effective electrical conductivity (σ_s^{eff}) corrects its bulk value (σ_s) by a function of ε only (Bruggeman model) or by more detailed relationships, e.g., including fiber properties for CP-GDL [75]. Among traditional GDL, the in-plane electrical conductivity is higher compared to its through-plane counterpart due to the anisotropic fiber alignment orientation. The first one shows almost no sensitivity to the applied pressure in the range of the clamping order of magnitude of the stack, while the second one, usually expressed as area resistance, shows much higher sensitivity. The content of PTFE is detrimental to the through-plane parameters, while it shows no impact on the in-plane values [76]. Interfacial resistance occurs due to a gradient in morphology and physico-chemical properties between the constituents, the role of the MPL is essential to ensure a smooth transition across the GDL/CL interface [76]. Interfacial resistance is reduced by increasing the assembly load, thus reducing porosity [77]. Experimental measurement of electrical resistances could be performed using the four-point probe method [76]. A proper electrical connection minimizes the series electrical resistance, reducing the ohmic polarization.

4.1.3. *Thermal dissipation.* Temperature build-up impacts the durability of materials and hinders proper H^+ conductivity of the membrane. Hotspots lead to dry areas, thus causing uneven reaction rates and stressing the components; proper thermal dissipation is thus required [75]. In a GDL, heat transfer by convective and radiative effects within the pores is negligible. The heat pipe effect affects water transport within the device and impacts hydrophilic structures more than hydrophobic ones. Conduction, however, is the main heat transfer mechanism, affected by both the effective thermal conductivity (k_{eff}) and the thermal contact resistances with CL and BP [78], where k_{eff} could be simply related to bulk material, properties of gas species, and liquid water (k_s , k_g , and k_l) and ε , or by more complex morphology-dependent formulations. Thermal resistances might be measured experimentally using a guarded heat flow meter. In CP-GDL, both in-plane and through-plane k_{eff} increase with decreasing porosity and

compression pressure; furthermore, the through-plane value might be enhanced by embedding carbon fibers in the through-plane direction [79]. Proper thermal management would profoundly aid PEM H^+ conductivity, affecting ohmic polarization.

4.1.4. *Gas distribution.* In a GDL, gases are transported by a combination of convection and diffusion through a porous matrix. Both mechanisms are enhanced by high porosity and limited thickness. From a macroscopic viewpoint, the bulk gas flow obeys Darcy-type behavior: the fluid velocity is controlled by the absolute permeability of the GDL and by the gas viscosity. Permeability is an intrinsic property of the medium and depends on porosity, tortuosity of the pore network, characteristic pore size, and, more generally, on the architecture of the carbon fibers, as described by Kozeny–Carman-type relations or fiber-based models such as those proposed by Tomadakis and Sotirchos [80, 81]. Porosity and pore-size distribution are typically characterized by standard porosimetry techniques [75]. Through-plane and in-plane permeabilities could be determined experimentally by imposing a known flow rate of a test gas (e.g., O_2 , N_2 , or air) across the GDL and measuring the resulting pressure drop [82], with permeability data usually reported in m^2 , Darcy, or Gurley units [19]. Diffusive transport superimposes on this convective flow and is driven by gradients in species concentration within the porous structure. The effective diffusion coefficient in the GDL is lower than in the bulk gas since transport takes place in a constricted and tortuous pore space. This reduction is captured by a so-called diffusibility factor, which accounts for porosity and the degree of water saturation [79]. As liquid water accumulates, it partially blocks pores and further decreases the effective diffusivity, thereby exacerbating mass-transfer limitations. Within the GDL, one usually distinguishes macropores (larger than about 7000 nm), mesopores (50–7000 nm), and micropores (smaller than 50 nm), the latter being especially abundant in the microporous layer. In these micropores, the mean free path of gas molecules becomes comparable to or larger than the pore diameter, and gas–wall collisions become dominant. Under such conditions, Knudsen diffusion contributes significantly to the overall transport mechanism [83]. Both convective permeability and effective diffusivity deteriorate under high clamping pressure, as compression reduces porosity and alters the pore network. Effective diffusion coefficients can be measured, for example, using Loschmidt-cell configurations [84].

4.2. The role of the Gas Diffusion Layer in water management. Water is generated as vapor at the cathode CL and can partially condense into liquid within the porous components. Both extremes of this process are detrimental: excessive drying

reduces proton conductivity in the membrane, whereas flooding obstructs gas pathways to the catalyst layer and can accelerate degradation, particularly under subzero conditions due to freeze–thaw damage [72]. Inside the cell, water is transported by diffusion driven by gradients in water activity, by electro-osmotic drag associated with proton motion through the membrane, and by bulk convection of liquid water and gas in the porous media. Across the GDL thickness, the convective motion of liquid water results from the balance between capillary forces and gas-pressure gradients. The liquid velocity increases with the absolute and relative permeability of the porous medium and decreases with the viscosity of water. The driving capillary pressure is determined by the air-water surface tension, the internal contact angle, and the microstructural features of the GDL, including porosity, permeability, and liquid saturation. These dependencies are often summarized through a Leverett-type function, which links capillary pressure to saturation and material properties [85–87]. The relative permeability to liquid water increases with porosity [88], while the internal contact angle, which effectively describes how water wets the internal pore surfaces, depends both on the intrinsic static contact angle and on the detailed morphology of the solid matrix. It can be inferred experimentally from breakthrough-pressure measurements, where the pressure required for water to percolate through the GDL is related to the curvature of the liquid-gas interface in the largest constrictions [89]. From a design standpoint, hydrophobic treatment with PTFE and the control of pore size distribution are fundamental for tailoring water management. High PTFE loading combined with larger pores facilitates drainage and promotes water discharge, which is advantageous at high relative humidity because it mitigates flooding. Conversely, lower PTFE content and smaller pores enhance water retention and help maintain membrane hydration at low relative humidity, but they can increase the risk of capillary blockage under wet conditions. Pore-graded structures are particularly attractive because they can simultaneously avoid severe flooding and drying over a broad range of humidity and load conditions [77, 86].

4.3. Modeling and simulation to address multiphase wetting. Recent computational studies have investigated the pore-scale modeling of liquid water permeation in GDL. Among these approaches, Niu et al. adopted a Volume-of-fluid (VOF) method to investigate realistic GDL microstructures, prescribing boundary conditions on the static contact angle to model hydrophobic treatments on carbon fibers at different PTFE loadings [27]. Numerous studies have been conducted adopting the Lattice Boltzmann Method (LBM) due to its advantages over macroscale-based CFD approaches, such as its intrinsic parallelism. In its basic formulation, LBM solves semi-incompressible,

single-phase Navier-Stokes equations through the mesoscopic dynamics of collision and streaming of discrete populations over a lattice, whereas Shan-Chen (SC) extensions introduce non-ideal forces to model multiphase and multicomponent flows with wetting. Notably, Wang et al. performed a multicomponent 2D study on a reconstructed microstructure of a GDL, investigating different PTFE distribution patterns to promote water management [36]. Guo et al. proposed an enriched multicomponent model including oxygen diffusion and electrochemical reactions, which is, however, limited by a unit density ratio between phases [37]. Zhou et al. proposed an alternative design of GDL to improve water management [38]. Despite these advances, existing LBM studies share several limitations, such as: (i) embedding collision operators with limited Galilean invariance, which being detrimental to physical consistency; (ii) modeling wetting through simplified forcing schemes that are known to generate spurious mass transfer at interfaces, spoiling the results of the simulations [90]. The modeling effort presented in the following chapters results in a multiphase SC-type framework capable of performing stable and consistent surface-resolved simulations of wetting flows, combining an advanced cascaded-entropic collision operator with a highly accurate and mass-conserving wetting formulation based on boundary-force interpolation. Such a framework is validated on canonical benchmark tests and is designed to be extended towards the modeling of realistic GDL microstructures to support PEMFC design and performance optimization.

CHAPTER 2

Fundamentals of multiphase Lattice Boltzmann Methods

In this chapter, the Lattice Boltzmann Method (LBM) is introduced, covering its principles, implementation, and extensions for modeling multiphase flows.

At first, essential topics of kinetic theory are presented, including the Boltzmann Equation and its compliance with macroscopic conservation laws. Its discretization in velocity space, followed by discretization in physical space and time, is discussed. The core streaming-collision algorithm is outlined, alongside boundary treatments of interest. Furthermore, fundamental topics on multiphase flows are introduced, such as the constraints on non-ideal equations of state, stress discontinuity at the separation interface, and adhesion to solid surfaces. Finally, the pseudopotential model, being the extension of choice for modeling multiphase flows with LBM, is introduced by outlining its basic formulation, weaknesses, and recent developments in the literature, along with persistent gaps.

1. The essence of kinetic theory

The description of fluid systems admits different approaches, spanning a hierarchy of space and time scales; the appropriate level of focus is dictated by the phenomena of interest. In length, one may target the particle (atom/molecule) diameter l_p , the mean free path l_{mfp} , a hydrodynamic gradient scale l and/or the size of a typical engineering device, as a turbine, l_s ; one usually has $l_p \ll l_{\text{mfp}} \ll l \leq l_s$. In time, the level of focus might span between the interparticle collision duration t_p , the mean flight time between collisions t_{mfp} or hydrodynamic time-scales as diffusive t_d or convective t_{cv} ones; typically, $t_p \ll t_{\text{mfp}} \ll t_d \approx t_{\text{cv}}$. The proposed scale ordering, though, is not always compliant with the physics of the problem.

In studies concerning the *microscale*, the individual motion of a limited number of particles is tracked, while for *macroscale* systems, one must resort to a description based on macroscopic observables, such as mass and momentum density.

Defining the Knudsen number as $\text{Kn} = l_{\text{mfp}}/l$, the macroscopic/continuum approach is valid only for $\text{Kn} \ll 1$.

As $\text{Kn} \gtrsim 1$, one must resort to the kinetic theory description, which lies in the *mesoscale*, depicting how the distribution of particles in a fluid system evolves around

the mean collision time t_{mfp} . The state of the system is described by the probability density distribution $f = f(\mathbf{x}, \xi, t) : \mathcal{D} \times \mathbb{R}^3 \times \mathbb{R}_+ \rightarrow \mathbb{R}_+$, being the probability density of finding a particle in $\mathbf{x} \in \mathcal{D}$ with a particle-velocity ξ at time $t \geq 0$. The statistical moments of f with respect to the particle-velocity space yield macroscopic quantities of interest, such as mass density and momentum density, respectively:

$$(1) \quad \rho(\mathbf{x}, t) = \int f(\mathbf{x}, \xi, t) d^3 \xi,$$

$$(2) \quad \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) = \int \xi f(\mathbf{x}, \xi, t) d^3 \xi.$$

with $\mathbf{u}$ being the macroscopic velocity.

Considering an elastic collision between hard spheres, as a dilute monatomic gas, the equilibrium state f^{eq} is described by the Maxwell-Boltzmann distribution:

$$(3) \quad f^{\text{eq}}(\mathbf{x}, |\mathbf{v}|, t) = \rho \left(\frac{1}{2\pi RT} \right)^{3/2} \exp \left[-\frac{|\mathbf{v}|^2}{2RT} \right],$$

where R is the universal gas constant and $\mathbf{v} = \xi - \mathbf{u}$ is the relative velocity. Such a distribution is constructed to preserve mass, momentum, and energy.

The Boltzmann Equation describes the evolution of f in space and time, and reads:

$$(4) \quad \frac{\partial f}{\partial t} + \xi \cdot \nabla_{\mathbf{x}} f + \frac{\mathbf{F}}{\rho} \cdot \nabla_{\xi} f = \Omega, \quad \text{with } \mathbf{x} \in \mathcal{D}, t \geq 0.$$

The system non-equilibrium behavior is influenced by both the collision operator Ω and a total external body force $\mathbf{F}$ [91].

The Chapman-Enskog expansion of the Boltzmann Equation recovers the Navier-Stokes-Fourier equations (NSFE) to a first order approximation in the Knudsen number $f \approx f^{\text{eq}} + \text{Kn} f^{(1)}$, as in the continuum limit ($\text{Kn} \ll 1$) higher order terms are negligible.

Transport coefficients are determined via molecular cross sections and are embedded in the Boltzmann collision operator, which reads:

$$(5) \quad \begin{aligned} \Omega(f, f) = & \underbrace{\int_{\mathbb{R}^3} \int_{S^2} B(|\mathbf{g}|, \cos \theta) f(\xi^*, t) f(\tilde{\xi}^*, t) d\omega d\tilde{\xi}}_{\Omega^+(f, f) \text{ (gain)}} \\ & - \underbrace{\int_{\mathbb{R}^3} \int_{S^2} B(|\mathbf{g}|, \cos \theta) f(\xi, t) f(\tilde{\xi}, t) d\omega d\tilde{\xi}}_{\Omega^-(f, f) \text{ (loss)}}, \end{aligned}$$

with (*) and (˜) identifying post-collision values and dummy particle/neighbor values. B is the collision kernel, as a function of the relative speed $\mathbf{g} = \xi - \tilde{\xi}$ and the differential cross section $\cos \theta = \hat{\mathbf{g}} \cdot \boldsymbol{\omega}$, with $\boldsymbol{\omega} \in S^2$ representing the scattering direction and S^2 the unit sphere in $\mathbb{R}^3$.

Given the complexity of the Boltzmann operator, one might model the collision process through a local and simplified counterpart, the Bhatnagar-Gross-Krook (BGK) operator, from the seminal work by Bhatnagar et al. [92], expressed as:

$$(6) \quad \Omega(f) = -\frac{1}{\tau}(f - f^{\text{eq}}),$$

prescribing a single-time relaxation of both hydrodynamic and non-hydrodynamic modes toward a local equilibrium state.

The BGK formulation yields the correct NSFE structure in terms of conservation laws and constitutive closure for a generic Newtonian fluid, with dynamic viscosity $\mu = \rho c_s^2 \tau$, fixed thermal conductivity, and Prandtl number $\text{Pr} = 1$.

Microscopic features might be fully expressed in terms of equations of state or transport coefficients.

This concept is of paramount importance for establishing the suitability of mesoscopic-level inspired schemes in describing multiphase fluid physics at the macroscale.

2. The Lattice Boltzmann Equation

The Boltzmann Equation, even in the BGK formulation, is more complex to treat analytically than the Navier-Stokes Equations (NSE), since f is defined in a seven-dimensional space. By contrast, discrete numerical schemes based on mesoscopic physics could be more straightforward and convenient to implement than traditional fluid solvers.

2.1. Discretization in the velocity space. The discretization procedure starts in the velocity space and, from a hydrodynamic perspective, entails no loss of macroscopic information.

It is indeed sufficient to enforce conservation laws as low-order moment constraints on the discrete f , as finer mesoscopic details are irrelevant at the macroscale.

The continuum equilibrium distribution f^{eq} is expanded in Hermite polynomials, and velocity integrals are computed by the Gauss-Hermite quadrature rule. The dependence on the continuous-valued $\xi \in \mathbb{R}^3$ discretized by introducing a finite quadrature set of nodes and weights $\{\mathbf{e}_i, w_i\}$. Such a set, denoted as DdQq [93], is defined by q discrete velocity directions and their associated isotropic weights. Here, each $\mathbf{e}_i \in \{-1, 0, 1\}^d$ is a d -dimensional discrete particle velocity, with $i \in \{0, 1, \dots, q-1\}$ labeling the q directions, while $w_i \in \mathbb{R}^+$ is the corresponding isotropy weight.

In the following, a compact Dirac notation is adopted to represent local lattice quantities in velocity space. Any set of q directional components $\{a_i(\mathbf{x}, t)\}_{i=0}^{q-1}$ is collected into the q -dimensional column vector $|a(\mathbf{x}, t)\rangle := (a_0(\mathbf{x}, t), \dots, a_{q-1}(\mathbf{x}, t))^T \in$

$\mathbb{R}^q$. The corresponding bra $\langle a|$ denotes transposition, while the bracket $\langle X|Y\rangle$ denotes a inner product in $\mathbb{R}^q$ that is defined subsequently.

The Hermite series expansion for the equilibrium distribution is truncated at second order, which is sufficient to recover the hydrodynamic laws. Within the isothermal assumption, each value $f_i^{\text{eq}} : \mathcal{D}_f \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$, $i \in \{0, q-1\}$, is expressed as:

$$(7) \quad f_i^{\text{eq}} = w_i \rho \left(1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right)$$

constituting $|f_i^{\text{eq}}(\mathbf{x}, t)\rangle = (f_0^{\text{eq}}(\mathbf{x}, t), \dots, f_i^{\text{eq}}(\mathbf{x}, t), \dots, f_{q-1}^{\text{eq}}(\mathbf{x}, t))^\top$, the discrete equilibrium set. The term c_s identifies the lattice speed of sound.

The weights are computed so that moments up to the required order are integrated exactly; equivalently, one might impose tensor constraints requiring rotational isotropy. For the isothermal NSE, non-negative weights and isotropy up to the fourth order are required; thus:

$$(8) \quad \begin{aligned} \sum_{i=0}^{q-1} w_i &= 1, \quad \sum_{i=0}^{q-1} w_i e_{i\alpha} = 0, \quad \sum_{i=0}^{q-1} w_i e_{i\alpha} e_{i\beta} = c_s^2 \delta_{\alpha\beta}, \\ \sum_{i=0}^{q-1} w_i e_{i\alpha} e_{i\beta} e_{i\gamma} &= 0, \quad \sum_{i=0}^{q-1} w_i e_{i\alpha} e_{i\beta} e_{i\gamma} e_{i\delta} = c_s^4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}), \end{aligned}$$

with $(\alpha, \beta, \gamma, \delta \in \{1, \dots, d\})$.

By analogy with its equilibrium counterpart, the distribution function f is discretized into a finite set of *populations* $f_i : \mathcal{D}_f \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$, $i \in \{0, q-1\}$, resulting in $|f_i(\mathbf{x}, t)\rangle = (f_0(\mathbf{x}, t), \dots, f_i(\mathbf{x}, t), \dots, f_{q-1}(\mathbf{x}, t))^\top$.

The raw moments of $|f_i\rangle$ of order $n = n_x + n_y + n_z$ are defined as

$$(9) \quad k_{n_x n_y n_z} = \langle f_i | e_{ix}^{n_x} e_{iy}^{n_y} e_{iz}^{n_z} \rangle = \sum_{i=0}^{18} f_i e_{ix}^{n_x} e_{iy}^{n_y} e_{iz}^{n_z},$$

and allow for the construction of macroscopic properties of interest.

The discrete-velocity force $|R_i(\mathbf{x}, t)\rangle = (R_0(\mathbf{x}, t), \dots, R_i(\mathbf{x}, t), \dots, R_{q-1}(\mathbf{x}, t))^\top$ with $R_i : \mathcal{D}_f \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$, $i \in \{0, q-1\}$, is approximated, in the scheme proposed by He et al. [94], by considering small deviations of the continuous f from its equilibrium state

$$(10) \quad |R_i\rangle = \mathbf{F} \cdot \nabla_\xi f \approx \mathbf{F} \cdot \nabla_\xi f^{\text{eq}} = -\frac{f_i^{\text{eq}}}{\rho} \frac{(\mathbf{e}_i - \mathbf{u})}{c_s^2} \cdot \mathbf{F}.$$

2.2. Discretization in the physical space and time. Unlike conventional CFD methods, the classical LBM requires spatial discretization via a uniform and structured grid. Moreover, each population f_i displaces with a velocity $\mathbf{e}_i$ towards its neighboring

site, landing exactly there after a single time step Δt . This not only imposes a constant spacing Δx , with diagonal neighbors distant $\sqrt{2}\Delta x$ and $\sqrt{3}\Delta x$, but also enforces a constraint on the discrete velocities, such that $e_{i\alpha} = n\Delta x/\Delta t$.

The discrete-velocity Boltzmann equation reads:

$$(11) \quad \frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla_{\mathbf{x}} f_i = \Omega_i(f) + R_i, \quad \text{for } i = 0, \dots, q-1, \quad \text{with } \mathbf{x} \in \mathcal{D}, t \geq 0,$$

Integrating Eq. (11) over a time step:

$$(12) \quad \int_t^{t+\Delta t} \frac{df_i}{d\zeta} d\zeta = \int_t^{t+\Delta t} (\Omega_i + R_i) d\zeta \quad \text{for } i = 0, \dots, q-1.$$

The advection step is exact according to the method of characteristics. Applying a second-order time discretization to the LHS yields the Lattice Boltzmann Equation:

$$(13) \quad |f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t)\rangle - |f_i(\mathbf{x}, t)\rangle = \Delta t |\Omega_i(\mathbf{x}, t)\rangle + \left(1 - \frac{\Delta t}{2\tau}\right) |R_i(\mathbf{x}, t)\rangle,$$

with $\mathbf{x} \in \mathcal{D}_f, t \geq 0$, being $\mathcal{D}_f = \mathcal{D} \cap \mathbb{N}^3$ the lattice.

Complying with Eq. (13), one can easily compute:

$$(14) \quad \rho = k_{000}, \quad \rho \mathbf{u} = (k_{100}, k_{010}, k_{001}) + \frac{\mathbf{F} \Delta t}{2}.$$

Within a Single Relaxation Time (SRT) approach, the BGK collision operator for the LBE reads [28]:

$$(15) \quad |\Omega_i\rangle = -\frac{1}{\tau}(|f_i\rangle - |f_i^{\text{eq}}\rangle).$$

A Chapman-Enskog analysis then yields the kinematic viscosity

$$(16) \quad \nu = c_s^2 \left(\tau - \frac{\Delta t}{2} \right).$$

To ensure physical consistency, one imposes $\nu > 0$, which implies $\tau/\Delta t \in (1/2, \infty)$. Differently from its continuous counterpart, $|f_i\rangle$ could be subject to *under-relaxation*, if $\tau/\Delta t > 1$, *full-relaxation*, if $\tau/\Delta t = 1$, or *over-relaxation*, if $\tau/\Delta t \in (1/2, 1)$.

2.3. Nondimensionalization and discrete velocity sets. In LBM, physical variables are often expressed in lattice units (l.u.). These are obtained through a nondimensionalization procedure. Conversion factors C_α (typically for length, time, and density) map experimental units to lattice units in accordance with the Buckingham - π theorem [95].

Given the constraints on velocity, space, and time discretization, as well as the nondimensionalization argument, adopting $\Delta x = 1$ l.u. and $\Delta t = 1$ l.u. (as customary in LBM) implies $|e_{i\alpha}| \in \{0, 1\}$ for the standard 3D lattices. The discrete velocities connect nearest-neighbor nodes and are therefore also referred to as *lattice links*. In

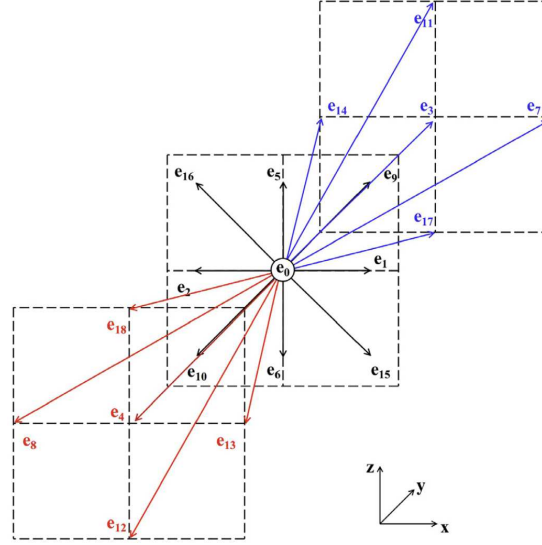


FIGURE 14. The D3Q19 velocity set. From [96].

this work, the D3Q19 set is adopted (see Figure 14) as a compromise between accuracy and computational burden cost [93].

Each e_i is represented as a row vector of the matrix:

$$(17) \quad e = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & -1 & 1 & -1 & 1 \end{bmatrix}^T,$$

with e_i components in the α_{th} direction being collected in column vectors $|e_{i\alpha}\rangle \in \{-1, 0, 1\}^q$. Lattice weights $w_0 = 1/3, w_{1-6} = 1/18$ and $w_{7-18} = 1/36$ approximate the continuous isotropic behavior. In D3Q19, the speed of sound is $c_s = \Delta x / (\sqrt{3}\Delta t)$.

3. The core algorithm of LBM

The Lattice Boltzmann Method is a mesoscopic Navier-Stokes solver based on the collision and streaming of distribution functions (*populations*) on a lattice. Macroscopic fields, such as mass density, velocity, and components of the pressure tensor, are computed as statistical moments of the population set.

The streaming phase is linear, favoring the parallelization of computational codes, while the collision process is non-linear but local [28].

A basic implementation of the Lattice Boltzmann Method features a minimal structure consisting of several steps, which are briefly discussed here [31].

3.1. Initialization. While proper initial conditions are required for time-dependent problems, the initialization procedure is essential, even for steady-state problems.

Populations are initialized by adopting a scheme that is consistent with the applied force field, leading to [97]:

$$(18) \quad |f_i\rangle(\mathbf{x}, t = 0) = |f_i^{eq}\rangle(\rho_0(\mathbf{x}), \bar{\mathbf{u}}_0(\mathbf{x})), \quad \text{with} \quad \bar{\mathbf{u}}_0 = \mathbf{u}_0 - \frac{\mathbf{F}\Delta t}{2\rho_0}$$

where $\rho_0, \mathbf{u}_0$ are, respectively, the imposed initial mass density and macroscopic velocity fields.

3.2. Main loop. A set of operations must be executed up to a prescribed final time. If the problem is expected to reach a steady state, one should impose a convergence criterion, e.g., the drop of the L^2 -norm of an error function below a specified tolerance.

3.2.1. *Update of macroscopic moments.* Relevant macroscopic fields are computed as moments of the populations set. Mass and momentum density, from Eq. (14), are required for the subsequent steps of the algorithm. Additional quantities of interest might be retrieved, such as the fluid pressure and stress components. Selected fields are then written to disk for diagnostics and post-processing.

3.2.2. *Computation of the equilibrium state.* The equilibrium distribution function is computed at every lattice node by the updated mass density and macroscopic velocity. This step might be resource-intensive; however, some advanced LBM formulations substantially reduce its cost [98].

3.2.3. *Collision step.* The LBE in Eq. (13) is conveniently decomposed in two distinct parts: *collision* and *streaming*. The collision step is local and nonlinear; populations are updated by the collision operator and an external forcing term, as follows:

$$(19) \quad |f_i^*(\mathbf{x}, t)\rangle = |f_i(\mathbf{x}, t)\rangle + \Delta t |\Omega_i(\mathbf{x}, t)\rangle + \left(1 - \frac{\Delta t}{2\tau}\right) |R_i(\mathbf{x}, t)\rangle,$$

where $|f_i^*(\mathbf{x}, t)\rangle$ is the post-collision population set.

3.2.4. *Streaming step.* The set $|f_i^*(\mathbf{x}, t)\rangle$ must be shifted towards the target neighboring lattice site, avoiding memory-overwriting, as:

$$(20) \quad |f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t)\rangle = |f_i^*(\mathbf{x}, t)\rangle$$

The streaming operator is linear. This peculiarity is particularly favorable for domain decomposition and efficient parallel implementations. Note that the *rest population* f_0 , associated with $\mathbf{e}_0 = (0, 0, 0)^\top$, does not, in practice, stream (Figure 15).

3.2.5. *Application of Boundary Conditions.* Given the update equations for the populations, boundary conditions (BCs) determine the evolution of the system within a well-posed problem. Among these, two categories are relevant to this work: periodic and wall BCs.

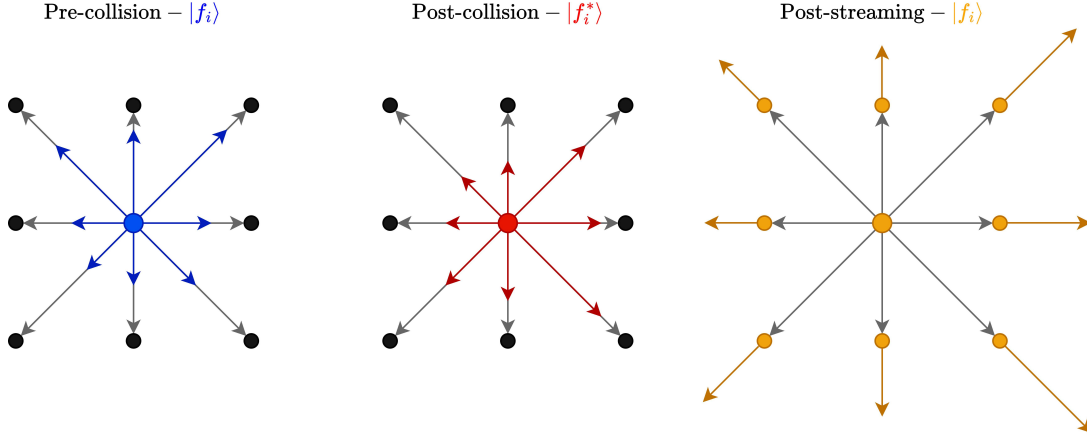


FIGURE 15. At each lattice node, the discrete populations f_i are first relaxed by the collision operator and then streamed along lattice links to neighboring sites; the rest population f_0 updates without propagating.

Periodic BCs exploit flow symmetries to model a representative unit cell of a spatially repeating configuration. On a domain $\mathcal{D}_f = \{0, \dots, N_x - 1\} \times \{0, \dots, N_y - 1\} \times \{0, \dots, N_z - 1\}$, with triply-periodic BCs, topologically a 3-torus, one imposes [99]:

$$(21) \quad f_i^*(\mathbf{x}, t) = f_i^*(\mathbf{x} + \mathbf{L}, t),$$

where $\mathbf{L}$ describes the direction of periodicity and the length of the pattern. This condition can also be imposed on macroscopic fields, even to reconstruct their derivatives, if required. By construction, periodic BCs conserve total mass and momentum.

Wall BCs are required to preserve the impermeability of the solid surface and the no-slip condition. The *halfway bounce-back* is a commonly adopted one, being both local and mass-conserving. The missing populations required to complete the streaming step at the boundary nodes are reconstructed by reflecting outgoing populations in the opposite direction, enforcing both impermeability and a null slip velocity [100].

For a static wall:

$$(22) \quad f_{\bar{i}}(x_f, t + \Delta t) = f_i^*(x_f, t),$$

where $\bar{i}$ denotes the direction opposite to i .

An advanced curved-geometry and force-consistent wall scheme is presented in the next chapter.

4. Stability and accuracy in BGK-LBM

4.1. Stability. Instability in LBM occurs when the errors of populations and macroscopic variables grow exponentially, leading to overflow and underflow errors in simulations. A standard route to assess stability is the linear von Neumann analysis [101]; although it does not quantify nonlinear destabilization mechanisms, it is an essential tool for evaluating the accuracy and robustness of a numerical scheme.

In traditional NSE solvers based on the direct NSE discretization, a Courant number $C = |\mathbf{u}| \Delta x / \Delta t$ exceeding unity is a sufficient condition for instability, as the information on fluid advection cannot be propagated quickly enough.

The analysis of LBM presents additional complexity, as it involves q equations and a relaxation time τ . Relevant necessary constraints are imposed by physics, as $\tau / \Delta t \in (1/2, \infty)$, to avoid negative viscosity, and non-negative equilibrium populations. These latter contribute to determine stability charts, mapping the maximum obtainable velocity modulus $|\mathbf{u}|_{\max} \Delta x / \Delta t$ over $\tau / \Delta t$.

Analytical results obtained with the implementation of the BGK operator are presented for the bulk LBE. A conservative stability condition, obtained numerically, results in $|\mathbf{u}|_{\max} \rightarrow 0$ as $\tau \rightarrow 1/2$ [102].

As a guideline to simulate a single-phase flow with an imposed Re , one might set τ in full-relaxation mode and control/monitor the reference velocity magnitude such that $|\mathbf{u}| \leq c_s$. If the latter condition is not satisfied, one should reduce τ while adjusting $|\mathbf{u}|$, complying with stability charts [31].

The required Re might not be achievable due to the BGK-LBE strict stability limits; in this case, one must resort to advanced collision operators, which are discussed afterward.

4.2. Accuracy. In an approximation scheme, a truncation error ε_{tr} is introduced when an infinite representation, such as a series or a differential operator, is approximated by a finite number of terms. A discretization is consistent if the truncation errors vanish as the time and space discretization steps tend to zero; thus, such errors can be represented as $\varepsilon_{tr,t} = \mathcal{O}(\Delta t^{p_t})$ and $\varepsilon_{tr,x} = \mathcal{O}(\Delta x^{p_x})$ with rates of decay p_t and p_x .

The discretization error ε_d results from the approximation of continuous PDEs by a system of algebraic equations. For linear problems, ε_d can be directly related to $\varepsilon_{tr,t}$ and $\varepsilon_{tr,x}$ while for nonlinear ones, the relationship is non-trivial. If the scheme is stable, the order of accuracy can be approximated by the order of convergence to the analytical or a high fidelity numerical solution.

For the LBE, additional complexity arises as ε_d depends not only on space and time discretization but also on one or more relaxation parameters. This latter is a relevant drawback of the BGK-LBE, as τ affects both the fluid viscosity and ε_d .

The LBE can be reformulated in terms of finite difference stencils [103, 104]. As a relevant result, one finds that the truncation contributions in space and time also depend on polynomials of τ , as $\mathcal{O}(\Delta t^2, \text{pol}_t[\tau])$ and $\mathcal{O}(\Delta x^2, \text{pol}_x[\tau])$.

Holding the relaxation time fixed while refining Δx and Δt , the LBM approximates the NSE with second-order accuracy in space and time, provided that modeling errors remain negligible. Standard velocity sets would indeed introduce a cubic-velocity error term $\mathcal{O}(|\mathbf{u}|^3)$ that both affects the viscous stress tensor and violates Galilean invariance. Additionally, compressibility effects contribute to an error scaling with $\mathcal{O}(\text{Ma}^2)$ [105]. If these errors are not suppressed by operating in the low-Mach and low velocity-regime, LBM temporal accuracy degrades to first order.

5. Introducing advanced collision operators

A collision operator relaxes the populations towards a local equilibrium state. This latter is determined by the macroscopic quantities of local mass density and velocity.

Recently, Coreixas et al. investigated the discrete-velocity, force-free Boltzmann Equation and proved that, without accounting for the physical-space and time discretization, the collision model does not impact the asymptotic behavior of LBM, which is solely affected by the selection of a proper equilibrium state and velocity set. Differently, numerical properties such as stability, accuracy, and computational cost could be significantly improved by a proper selection of the collision operator [106].

The Single-Relaxation-Time (SRT) framework, embedding the BGK approximation, yields a compact operator that guaranties high computational efficiency by relaxing the system on a unique characteristic time scale. Importantly, this method achieves this enhancement while rigorously maintaining essential physical properties, such as mass and momentum conservation. While straightforward to implement and featuring the lowest computational cost, this scheme suffers from instability at high Reynolds numbers and reduced accuracy at low Reynolds numbers [30].

5.1. The Multiple-Relaxation-Time Scheme. The Multiple-Relaxation-Time (MRT) scheme broadens the stable viscosity range by re-routing the collision process to increase its parametric degrees of freedom [107]. Populations are mapped into the raw moments space, relaxed, and then anti-transformed to obtain their post-collision values. Relaxation parameters acting on non-hydrodynamic moments are free to tune,

allowing one to extend the stability and accuracy of the scheme [107, 108]. These advantages come at a substantial cost, as two dense matrix-vector operations per node, significantly increasing the computational burden, even with an efficient implementation. Tuning the full set of relaxation rates in an MRT collision operator typically requires extensive, case-specific parameter studies. In practice, many of these degrees of freedom can increase implementation complexity and computational overhead while slightly improving accuracy or stability.

5.2. The Two-Relaxation-Time Scheme. The Two-Relaxation-Time (TRT) scheme provides a compromise between SRT and MRT by introducing only two relaxation rates. The distribution functions are decomposed into symmetric (even) and anti-symmetric (odd) components and are relaxed independently. This separation is sufficient to decouple the control of viscosity from numerical artifacts associated with odd modes, improving stability and boundary-performance tuning while avoiding the high-dimensional parameter space of MRT. With a careful implementation, TRT requires only a small overhead relative to SRT, as the even/odd decomposition and recombination is partly compensated by the halved number of collision operations, while being less expensive than MRT [109].

5.3. The Cascaded Lattice Boltzmann Method. Further developments led to the cascaded Lattice Boltzmann Method (CLBM), based on the collision of central moments. These are computed in a reference frame co-moving with the macroscopic fluid velocity. This requires mapping the populations to raw moments and subsequently shifting these to the central moments space, where the collision occur. Post-collision populations are reconstructed by inverse transformations. This approach enhances Galilean invariance and mitigates moment crosstalk, being the spurious coupling between the relaxation of low- and high-order moments that can otherwise introduce grid-dependent artifacts, especially on coarse lattices [110–114].

Although CLBM appears much more computationally demanding than SRT, its overhead can be negligible in optimized implementations. For instance, Gruszczyński et al. compared SRT, MRT, and CLBM within a multiphase framework and reported that MRT was about 14% slower than SRT, whereas CLBM was only about 2% slower [98]. They attributed this to the fact that, while central-moment handling adds operations, the CLBM formulation can simplify the evaluation of equilibria and forcing terms relative to a MRT approach. It must be considered, though, that exact overheads remain implementation- and hardware-dependent.

TABLE 3. Comparison of common LBM collision operators.

Operator	Advantages	Limitations
SRT	The simplest and cheapest scheme; directly based on the BGK approximation of the Boltzmann Equation.	Unstable at low viscosity; inaccurate at high viscosity; no control of non-hydrodynamic modes.
MRT	Improved stability and/or accuracy via independent relaxation of raw moments; broader stable viscosity range; control on non-hydrodynamic modes.	High per-node cost due to moment transforms; case-dependent parameters tuning; increased implementation complexity.
TRT	Near-SRT costs; two rates provide additional control; improved stability without the full MRT parameter space.	Less flexible than MRT; benefits depend on boundary treatment and flow regime.
CLBM	Improved Galilean invariance; reduced moment crosstalk and grid artifacts; very efficient within an optimized implementation.	Complex formulation and implementation.
(Entropic–)	Physics-based stabilization by enforcing a discrete-entropy constraint.	Increased complexity and computational overhead.

Efforts to increase the stability and accuracy of lattice Boltzmann schemes extend beyond the definition of the collision operator.

According to the Boltzmann H -theorem, a nearly-ideal gas should evolve in time following the minimization path of a convex entropy functional. However, the standard lattice Boltzmann formulation does not inherently satisfy a discrete version of this theorem [115]; thus, a class of models, usually referred to as *entropic* lattice Boltzmann methods, has been developed.

In entropic schemes, the relaxation process is constrained to minimize a discrete entropy functional in the post-collision state, resulting in increased stability, achieved by improving the method’s physical consistency. Entropic schemes have been developed within the multiple relaxation time schemes and cascaded lattice Boltzmann frameworks [116–119]. The entropic-cascaded collision operator would support stable and accurate simulations [114].

A concise summary of the advantages and disadvantages of the aforementioned collision operators is provided in Table 3.

6. Modeling multiphase flows and wetting with LBM

Several numerical approaches have been developed to model multiphase and multicomponent flows and related wetting phenomena.

Among the most prominent ones are those established on the direct NSE discretization and others based on the Lattice Boltzmann Methods.

Within the first category, volume-of-fluid methods are inherently mass-conserving and well-suited for large-scale multiphase simulations, but they can suffer from smeared interfaces and difficulties in precise contact-angle implementation [120]. Level-set techniques offer smooth interface delineation and accurate curvature computation; however, they require re-initialization for mass loss control [121]. Phase-field models, based on diffuse-interface formulations, naturally incorporate surface tension and wettability effects, but at the cost of solving additional differential equations and potential artificial interfacial thickening [122].

LBM offers a mesoscopic alternative to traditional NSE solvers that excels in its intrinsic parallelism. The proper LBM multiphase modeling is an active field of research, with common approaches including the color gradient [123], the free-energy [124], the interface tracking [94], and the pseudopotential method.

Among these, the latter, proposed by Shan and Chen (S-C), aligns naturally with the LBM mesoscopic perspective and, even in its basic implementation, is simple and efficient, allowing for straightforward handling of complex geometries and easy incorporation of wetting physics through localized solid-fluid interaction rules [125, 126].

Before assessing the strengths and limitations of such a model, essential concepts in multiphase flows and wetting are introduced.

6.1. Fundamentals of multiphase flows and wetting. Multiphase and multicomponent flows comprise two or more different fluids that differ by their physical properties, such as mass density and viscosity.

For single-component multiphase flows, the liquid and vapor phases of the same substance coexist and can interconvert from one to another, as a system comprising liquid water and water vapor. The distinction between the two phases is given by the order parameter, which could conveniently be the fluid mass density, with a minimum in the vapor phase, ρ_v , and a maximum in the liquid phase, ρ_l .

In nature, such parameters change abruptly across a separation interface, which can be approximated as a discontinuity in the mass density and pressure fields.

6.1.1. Equations of state for multiphase systems. In a single-component multiphase system, the equation of state (EOS) relate the bulk pressure and mass density (or

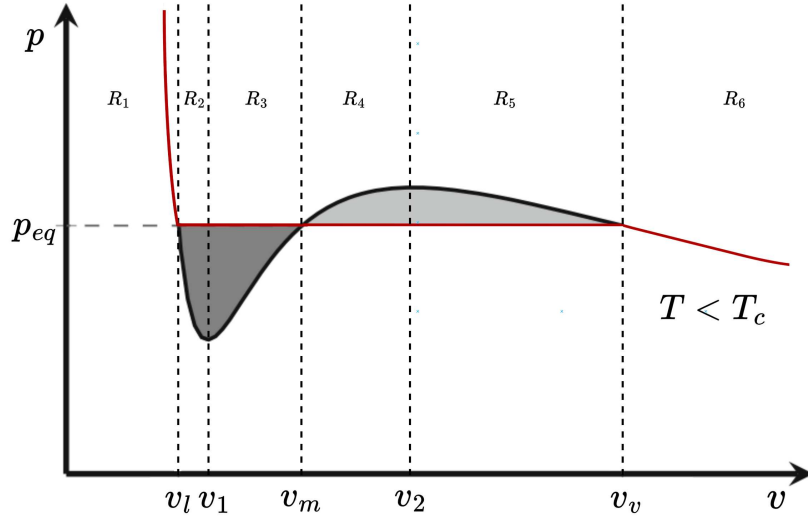


FIGURE 16. An equation of state for a real fluid below the critical temperature. The shaded areas must be equal, as prescribed by the Maxwell construction rule, leading to the red curve. In red, the equivalent experimental curve, with constant pressure p_{eq} within phase transition.

molar volume v) for a given temperature T , as $p = p(\rho, p, T)$. A pioneering equation of state (EOS) for real fluids is the one formulated by van der Waals [127]:

$$(23) \quad p = \frac{RT}{v-b} - \frac{a}{v^2},$$

with a and b substance-dependent parameters that, respectively, quantify molecular attraction and repulsion beyond the ideal-gas elastic collision dynamics.

Consider a generic non-ideal EOS in its $p-v$ plane representation. Above the critical temperature T_c , the fluid behaves similarly to an ideal gas. At T_c , a horizontal inflection point emerges at the critical molar volume and pressure (v_c, p_c) . Below T_c (see Figure. 16), three distinct values of v appear within a wide pressure range. The latter is of interest for modeling liquid-vapor coexistence.

In regions R1 and R2, the fluid is, respectively, in the liquid and vapor phases, being $v < v_l$ and $v > v_v$. The fluid features single-phase physics, characterized by

$$(24) \quad \left(\frac{\partial p}{\partial v}\right)_T < 0 \leftrightarrow K_T = -v \left(\frac{\partial p}{\partial v}\right)_T > 0$$

where K_T is the (positive) bulk modulus.

In contrast, regions R2 to R5 exhibit distinct multiphase traits, showing a minimum and maximum at *spinodal* points, where, respectively, $v = v_1$ and $v = v_2$.

In regions R3 and R4, one spots a mechanically unstable branch, where $K_T < 0$. As a pure substance in a multiphase system manifests a constant pressure in regions R2

to R5, the analytical EOS would be replaced by the horizontal equilibrium isotherm $p = p_{eq}$, where phase mass/volume fractions vary according to the lever rule. Such a physical feature is accounted for by the Maxwell equal area rule, which imposes:

$$(25) \quad \int_{v_l}^{v_v} (p_{eq} - p(v', T)) dv' = 0$$

with $p_{eq} = p(v_v, T) = p(v_l, T)$.

This rule requires that both the liquid and vapor phases are in chemical equilibrium, determined by equal chemical potential, and in mechanical equilibrium, set by equal pressure; therefore, the shaded areas in Figure. 16 must be equal.

For a given T and EOS, if the coexistence triplet (p_{eq}, v_l, v_v) satisfies the Maxwell rule, then it is *thermodynamically consistent*.

From a practical viewpoint, to represent multiphase fluid behavior at $T < T_c$, one considers an analytical, non-ideal EOS, imposes T and substance-dependent parameters, and then computes p_{eq} , v_v , and v_l using the Maxwell rule.

6.1.2. *The separation interface and surface tension.* The equal-pressure argument is valid exclusively in the bulk of the two phases, where a fluid particle experiences isotropic non-ideal interactions.

At the separation interface, a stress jump is present, represented by the Laplace pressure Δp , which is governed by the surface tension σ . This latter is defined as the energy per unit area required to form the interface.

Given $\mathbf{P}$ as the symmetric pressure tensor, and $\mathbf{n}$ the unit normal to a given planar interface, $\mathbf{P} = \mathbf{P}(s)$ where s is the coordinate along $\mathbf{n}$ crossing the interface. The normal and tangential stresses are defined, respectively, as $p_n(s) = \langle \mathbf{n} | \mathbf{P}(s) | \mathbf{n} \rangle$ and $p_t(s) = [\text{tr}(\mathbf{P}(s)) - p_n(s)]/2$. The surface tension reads:

$$(26) \quad \sigma = \int_{-\infty}^{+\infty} [p_n(s) - p_t(s)] ds,$$

Imposing static equilibrium ($\nabla \cdot \mathbf{P} = 0$), for a weakly curved interface, one finds the Young-Laplace law [128, 129]:

$$(27) \quad \Delta p = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

with R_1, R_2 the principal radii of curvature.

The separation interface acts like a membrane, exhibiting complex viscoelastic behavior, even if the fluid, in both the liquid and vapor bulk phase regions, obeys Newtonian rheology [130].

The interface area is minimized at equilibrium; if not constrained, this yields $R_1 = R_2$, resulting in spherical droplets or bubbles.

6.1.3. *Wetting.* In nature and in most engineering applications, the liquid and vapor fluid phases interact with a solid material, showing different affinities.

At thermodynamic equilibrium, a droplet located on top of a solid surface forms a *contact angle* θ , determined by the balance between fluid-fluid cohesion and solid-fluid adhesion effects. The condition of mechanical stability at the contact line, where the liquid, vapor and solid phases interact, is given by Young's equation:

$$(28) \quad \cos \theta = \frac{\gamma_{sv} - \gamma_{sl}}{\sigma}$$

where γ_{sv} and γ_{sl} respectively denote the solid-vapor and solid-liquid surface tension. If $\theta < 90^\circ$, the surface is *lyophilic*, $\theta = 90^\circ$ implies a condition of *neutral wetting*, while if $\theta > 90^\circ$ the surface is *lyophobic*.

6.2. The pseudopotential model. In their seminal works [32,33], Shan and Chen proposed a *bottom-up* mesoscopic model for multiphase flow in which a mean-field attractive interparticle force is introduced via an *effective mass* (or *pseudopotential*).

Above a lattice-dependent threshold of an *interaction strength* $\mathcal{G}$, two phases with distinct mass density values could coexist in the system and would distribute depending on the set initial conditions. The separation interface and surface tension manifest spontaneously, without requiring any auxiliary interface-tracking equations. The mesoscopic nature of the pseudopotential model, with self-emerging properties, is fully consistent with the rationale behind the single-phase LBM.

Assuming periodic boundaries (thus no fluid-solid coupling) on the fluid domain $\mathcal{D}_f$, adopting the single-speed ($|e_i| = 1$) D2Q6 lattice and assuming $\Delta t = 1$ l.u., the original force is formulated as:

$$(29) \quad \mathbf{F}(\mathbf{x}, t) = -\mathcal{G} \psi(\mathbf{x}, t) \sum_{i=1}^{q-1} \psi(\mathbf{x} + \mathbf{e}_i, t) \mathbf{e}_i, \quad \text{with } \mathbf{x} \in \mathcal{D}_f$$

Due to the hexagonal symmetry of D2Q6, all nearest neighbors contribute equally to the total non-ideal interaction at a lattice site. On multiple-speed lattices (e.g., D3Q19), directional weights w_i are typically embedded.

In their original formulation, Shan and Chen demonstrated that their interaction force would induce the following equation of state [32]:

$$(30) \quad p = c_s^2 \rho + \frac{1}{2} \mathcal{G} c_s^2 \psi^2,$$

comprising an ideal-gas term and an effective potential tail. Liquid-vapor separation requires a mechanically unstable branch; this condition is only achievable when (i) $\mathcal{G}$ is sufficiently negative, (ii) $\psi = \psi(\rho)$, and (iii) ψ is monotonically increasing yet bounded, thus saturating towards an asymptotic value.

In their seminal paper, Shan and Chen proposed:

$$(31) \quad \psi(\rho) = \rho_0[1 - \exp(-\rho/\rho_0)]$$

with $\psi \rightarrow \rho$ as $\rho \rightarrow 0$, also $\psi \rightarrow \rho_0$ as $\rho \rightarrow +\infty$, with ρ_0 being the saturation value. Adopting such a formulation for ψ , the critical point is computed at $(\mathcal{G}_c, \rho_{0,c}) = (-4, \rho_0 \ln(2))$. Phase separation requires $\mathcal{G} < \mathcal{G}_c$; thus, the interaction strength acts as a temperature-like parameter.

Considering the physics of the separation interface, assuming a planar surface located at $x = 0$, Eq. (26) yields:

$$(32) \quad \sigma = -\frac{c_s^4 \mathcal{G}}{2} \int_{-\infty}^{+\infty} \left(\frac{d\psi}{dx} \right)^2 dx.$$

Aside from fluid-fluid interactions, fluid-solid interactions can be easily modeled by introducing halfway bounce-back boundary conditions and a simple force acting on boundary nodes, formulated by Sukop and Thorne [29] as:

$$(33) \quad \mathbf{F}_{adh}(\mathbf{x}, t) = -\mathcal{G}_{adh} \psi(\mathbf{x}, t) \sum_{i=0}^{q-1} w_i \mathbf{e}_i.$$

The term $\mathcal{G}_{adh}$ corresponds to the adhesive interaction strength; wetting states of interest are achieved by its trial-and-error tuning.

The algorithmic implementation of the pseudopotential force is originally proposed via the sole modification of the equilibrium velocity, as:

$$(34) \quad \mathbf{u}^{eq} = \frac{1}{\rho} \left(\sum_{i=1}^{q-1} f_i \mathbf{e}_i + \tau \mathbf{F} \right).$$

6.2.1. Main weaknesses. While commendable, the basic model proposed by Shan and Chen suffers from several drawbacks, namely thermodynamic inconsistency, the development of spurious currents, and the inability to strictly reproduce the behavior of a given real fluid [131].

6.2.1.1. Thermodynamic inconsistency. The chemical equilibrium for the pseudopotential EOS imposes [34]:

$$(35) \quad \int_{\rho_v}^{\rho_l} \left(p_{eq} - c_s^2 \rho - \frac{1}{2} \mathcal{G} c_s^2 \psi^2 \right) \frac{1}{\rho^2} d\rho = 0,$$

where p_{eq} is the coexistence pressure.

While the mechanical equilibrium reads:

$$(36) \quad \int_{\rho_v}^{\rho_l} \left(p_{eq} - c_s^2 \rho - \frac{1}{2} \mathcal{G} c_s^2 \psi^2 \right) \frac{\psi'}{\psi} d\rho = 0,$$

with $\psi' = d\psi/d\rho$.

The Maxwell construction rule requires both Eq.s (35)-(36) to be simultaneously satisfied for any arbitrary pair of coexistence densities, imposing the following constraint on ψ :

$$(37) \quad \frac{\psi'}{\psi} = \frac{1}{\rho^2} \quad \rightarrow \quad \psi(\rho) \propto \exp\left(-\frac{1}{\rho}\right).$$

This choice, however, is proven to amplify discretization artifacts, leading to instabilities [131]; thus Eq. (31), is widely adopted and preferred over Eq. (37) despite its lack of thermodynamic consistency.

6.2.1.2. *Spurious currents.* Spurious currents are small amplitude, parasitic velocity components that manifest mainly in the proximity of the diffuse liquid-vapor interface. These spoil complex flow simulations and can be easily detected and quantified only in controlled static benchmark tests. Spurious currents represent a discretization artifact induced by the imperfect isotropy of the interaction force. These significantly intensify at lower T (equivalently, higher $|\mathcal{G}|$) as the density ratio between phases $DR = \rho_l/\rho_v$ increases, along with the interparticle force magnitude and Laplace pressure. These also intensify as the relaxation time is reduced ($\tau \rightarrow 0.5$). When the peak speed exceeds the lattice speed of sound, numerical instability develops [132–134]

6.2.1.3. *Unrealistic fluid behavior and properties coupling.* In the original S-C scheme, Eq.s (30)-(31) allow for the correct reproduction of a key element of a non-monotonic EOS, which being the mechanically unstable branch; this peculiarity is shared with commonly adopted EOS such as van der Waals, Redlich-Kwong, and Peng-Robinson. A central limitation, though, is that the S-C EOS does not represent any real-world fluid behavior. Furthermore, the surface tension is uniquely set by the interaction strength, which induces a property-coupling constraint: σ and DR are not independent model parameters [133]. This is particularly detrimental for studies in surface engineering, where independent control of surface properties and coexistence properties is required, e.g. when introducing surfactants in the system. In addition, the S-C algorithmic implementation of the discrete force (see Eq. (34)) introduces further coupling, as tuning τ would affect the density ratio and surface tension, altering the equilibrium thermodynamics in an unphysical manner [135].

6.2.2. *Literature advances and gaps.* Within the cohesive force model, the aforementioned issues of thermodynamic inconsistency, limited achievable density ratios, flow spoiling due to intense spurious currents, and the lack of representativeness of real-fluid behavior are extensively addressed in the literature.

Yuan and Schaefer proposed constructing the pseudopotential from a selected EOS in order to impose a real-fluid behavior to the system. Concretely, they isolate ψ from

Eq. (30) and enforce the target pressure $p(\rho, T, a_1, \dots, a_n)$, where the coefficients a_i (and their number n) are determined by the structure of the specific EOS [136]. In the Yuan-Schaefer formulation, the interaction force results effectively insensitive to the interaction strength $\mathcal{G}$, as the equilibrium properties are instead completely dictated by the temperature and parameters of the real-fluid EOS.

Shan inquired about the isotropy properties of the interaction force, identifying the source of spurious currents in the high-order anisotropic truncation errors induced by the finite-support force stencil [132].

These findings were subsequently corroborated and deepened by Sbragaglia et al., who also investigated strategies for properties-decoupling [133]. These topics were also deepened by Kupershtokh et al., along with the enhancement of the model thermodynamic consistency by introducing a composite force expression [135].

In the pioneering work by Wang et al. [137], stability and accuracy of multiphase simulations were improved by the implementation of an entropic-stabilized CLBM framework embedding a consistent forcing scheme [138].

Despite recent advances, scholars have abandoned the idea of implementing high-order isotropic forcing to push the maximum achievable density and viscosity ratios. Specifically, the literature lacks an investigation on how an extended force-stencil support would affect the numerical performance of the pseudopotential method within modern central-moment Lattice Boltzmann schemes with entropic stabilization.

Adhesive forces require careful consideration on their own: over the last two decades, the pioneering wetting model by Sukop and Thorne (Eq.(33)) [29] has been revised and extended to improve its flexibility for diverse wetting conditions and its accuracy .

Benzi et al. proposed a formulation which mildly mimics the structure of the cohesive force, defining a virtual wall density that could be tuned to match the target surface wettability [139].

To inhibit the formation of a nonphysical mass transfer layer and spurious currents, Li et al. proposed the computation of the virtual density from a corrected weighted average on neighboring fluid nodes [140].

More recently, Peng et al. introduced a virtual effective-mass approach and suggested an analytical correlation for contact angles valid on flat walls [90].

Although the approaches by Li and Peng reduce discretizations and modeling artifacts, the disjointed integration of cohesive and adhesive forces is believed to limit stability at high density ratios. Furthermore, despite the extensive investigations on adhesion models in the literature, most applications investigating complex geometries

rely on the simplest boundary discretization approach, adopting a *staircase boundary approximation* supported by the halfway bounce-back (HBB).

The staircase-HBB approach yields a grid-aligned series of orthogonal steps, which may lead to modeling errors. To deal with this issue, a plethora of boundary conditions has been developed to account for complex geometries, mostly designed for the single-phase LBM; among these: Ghost Methods [141, 142], Immersed Boundary Methods [143–146], and Interpolated Bounce Back (IBB) [147].

Notably, the latter operates independently from the collision process, but it does not hold a mass-preserving property. Specifically, Yu et al. [148] demonstrated that the mass leakage induced by the interpolated bounce back within the Shan-Chen model is unacceptably high, and shape deformation is induced in liquid droplets wetting curved surfaces. This analysis was corroborated and extended by Xu et al. [149]. The main drivers of mass leakage are identified as the local boundary orientation and curvature, the tangential momentum density, and the presence of an inhomogeneous force field. The normal gradients of mass density, momentum, and momentum flux also influence the average mass leakage.

In this context, Yu et al developed a scheme for compensating for this mass leakage on curved boundaries using extrapolation methods. While commendable, their approach imposes a single relaxation time collision step at the boundary. Furthermore, their work is focused on a low density ratio ($\mathcal{O}(1)$) in a 2D domain.

Building on the state of the art in cohesive and adhesive force modeling, an original Lattice Boltzmann Method was designed to address the aforementioned gaps in the literature. The formulation and implementation are detailed in the following chapter.

CHAPTER 3

A model for the accurate simulation of wetting

The aim of the proposed model is to compensate for the gaps in the literature highlighted in the previous chapter by formulating a Lattice Boltzmann Method that embeds:

- a central-moments-based collision operator enhanced by an entropic stabilization approach;
- a unified formulation of the pseudopotential force that allows for extending treatments adopted to refine the cohesive interaction to the adhesive interaction;
- an improved mass refill strategy for the interpolated bounce-back scheme, addressing its native mass-leakage by exploiting local interaction force data, here termed Unidirectional Coupled Boundary Wettability (U-CBW) scheme;
- a refined U-CBW approach able to impose wall-location-sensitive wettability conditions within a compact force stencil, here termed Bidirectional Coupled Boundary Wettability (B-CBW) scheme.

The target initial-boundary value problem is first presented, and the model structure is detailed; then the method is completely characterized; additionally, the proof of the H -theorem for the discrete problem at hand is provided. Testing strategies and the results of an extensive experimental campaign are presented in the following chapter.

1. The initial-boundary value problem

Consider a *multiphase* fluid domain $\mathcal{D} \subset \mathbb{R}^3$ with boundary $\partial\mathcal{D} \subset \mathbb{R}^3$, where the liquid and vapor phases of a substance of interest coexist.

Within the monolithic mixture assumption, the state of the system is characterized by two unique fields varying in space and time, the mass density $\rho : \mathcal{D} \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$ and velocity $\mathbf{u} : \mathcal{D} \times \mathbb{R}^+ \rightarrow \mathbb{R}^3$.

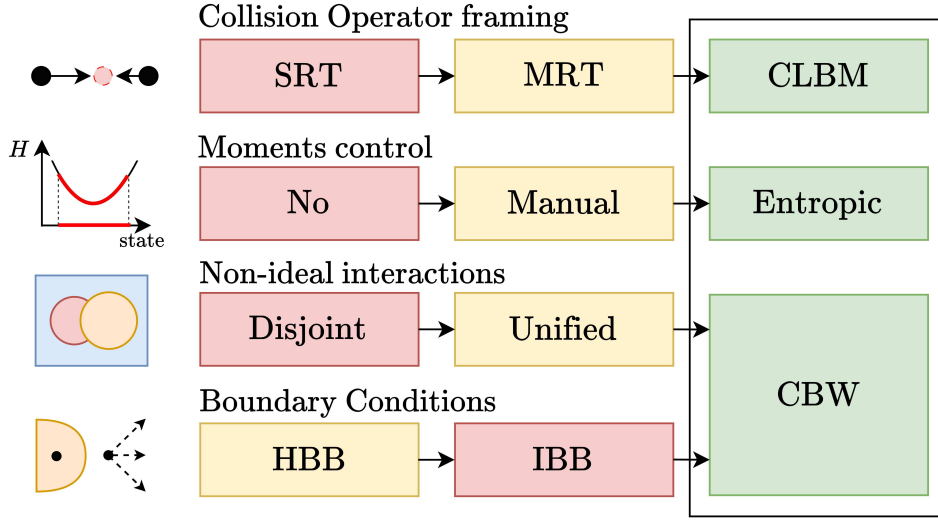


FIGURE 17. Main features of the proposed model: a cascaded collision operator (CLBM) controls the relaxation of high-order moments with entropic stabilization, furthermore a unified non-ideal interaction force and a mass-deficient IBB are embedded within the Coupled Boundary-Wettability (CBW) scheme.

The initial-boundary value problem of interest reads:

$$(38) \quad \begin{cases} \partial_t \rho(\mathbf{x}, t) + \nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) = 0, & \mathbf{x} \in \mathcal{D}, t > 0 \\ \partial_t (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) + \nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \otimes \mathbf{u}(\mathbf{x}, t)) = \\ \quad = \nabla \cdot \mathbf{P}(\mathbf{x}, t) + \nabla \cdot \boldsymbol{\sigma}'(\mathbf{x}, t) + \mathbf{F}_{ext}(\mathbf{x}, t), & \mathbf{x} \in \mathcal{D}, t > 0 \\ \rho(\mathbf{x}, t) = \rho_b(\mathbf{x}, t), & \mathbf{x} \in \partial \mathcal{D}, t > 0, \\ \mathbf{u}(\mathbf{x}, t) = \mathbf{u}_b(\mathbf{x}, t), & \mathbf{x} \in \partial \mathcal{D}, t > 0 \\ \rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}), & \mathbf{x} \in \mathcal{D} \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), & \mathbf{x} \in \mathcal{D} \end{cases}$$

where $\rho_b : \partial \mathcal{D} \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$, $\mathbf{u}_b : \partial \mathcal{D} \times \mathbb{R}^+ \rightarrow \mathbb{R}^3$ and $\rho_0 : \mathcal{D} \rightarrow \mathbb{R}^+$, $\mathbf{u}_0 : \mathcal{D} \rightarrow \mathbb{R}^3$ are some given functions defining boundary and initial conditions; and $\mathbf{F}_{ext} : \mathcal{D} \times \mathbb{R}^+ \rightarrow \mathbb{R}^3$ is the total external force density.

The fluid rheology is Newtonian; thus, the viscous stress tensor reads:

$$(39) \quad \boldsymbol{\sigma}'(\mathbf{x}, t) = \rho(\mathbf{x}, t) \nu (\nabla \mathbf{u}(\mathbf{x}, t) + (\nabla \mathbf{u}(\mathbf{x}, t))^{\top}) + \rho(\mathbf{x}, t) \left(\zeta - \frac{2}{3} \nu \right) (\nabla \cdot \mathbf{u}(\mathbf{x}, t)) \mathbf{I},$$

where ν and ζ are the kinematic shear and bulk viscosities.

The pressure tensor $\mathbf{P}$ is implicitly defined by the local momentum transfer rate, embedding the contribution of the isothermal fluid pressure, namely $\rho(\mathbf{x}, t) c_s^2$ (where

c_s is the speed of sound), and the contribution of the mutual interaction between phases in a total interaction force $\mathbf{F}_u : \mathcal{D} \times \mathbb{R}^+ \rightarrow \mathbb{R}^3$:

$$(40) \quad \nabla \cdot \mathbf{P}(\mathbf{x}, t) = -\nabla(\rho(\mathbf{x}, t)c_s^2) + \mathbf{F}_u(\mathbf{x}, t).$$

$\mathbf{F}_u$ is modeled as the superposition of pairwise forces governed by the *effective mass*, an auxiliary density-dependent field ψ that drives phase separation and the interfacial dynamics. Its functional form critically influences properties such as surface tension and phase equilibria. Due to this, for any couple of points $\mathbf{x}, \tilde{\mathbf{x}} \in \mathcal{D}$ the pairwise force results proportional to the product $\psi(\mathbf{x})\psi(\tilde{\mathbf{x}})$. Such interactions are, indeed, additive and decay with the distance between two selected points in $\mathcal{D}$. Profiting from the superposition principle, the total interaction force is thus defined as:

$$(41) \quad \mathbf{F}_u(\mathbf{x}, t) = \int_{\mathcal{R}_\delta(\mathbf{x})} G(\|\mathbf{x} - \tilde{\mathbf{x}}\|) \psi(\mathbf{x}, t) \psi(\tilde{\mathbf{x}}, t) (\mathbf{x} - \tilde{\mathbf{x}}) d\tilde{\mathbf{x}}.$$

The kernel $G : [0, \delta) \rightarrow \mathbb{R}$ ($\delta \in \mathbb{R}^+$) is a compactly supported function which depends uniquely on the Euclidean distance between the target and the dummy sites; the interaction force is isotropic.

Such a force integral is computed over an open ball of radius δ : $\mathcal{R}_\delta(\mathbf{x}) = \{\tilde{\mathbf{x}} \in \mathbb{R}^3 : \|\mathbf{x} - \tilde{\mathbf{x}}\| < \delta\}$ (see Figure 18). The effective mass is defined on the extended domain $\mathcal{D}_e = \mathcal{D} \cup \bigcup_{\mathbf{x} \in \mathcal{D}} \mathcal{R}_\delta(\mathbf{x})$ as $\psi : \mathcal{D}_e \times \mathbb{R}^+ \rightarrow \mathbb{R}$. As such, the function ψ extends beyond the boundary of the domain $\mathcal{D}$, as reported in Figure.18. Exploiting the isotropy requirement on $\mathbf{F}_u$, its definition is conveniently written by employing a change of variables $\mathbf{x} \rightarrow \mathbf{r} = \mathbf{x} - \tilde{\mathbf{x}}$, with $\mathbf{r} = (r_1, r_2, r_3)$ and $r = \|\mathbf{r}\|_2$:

$$(42) \quad \mathbf{F}_u(\mathbf{x}, t) = \psi(\mathbf{x}, t) \int_{r < \delta} G(r) \psi(\mathbf{x} - \mathbf{r}, t) \mathbf{r} d\mathbf{r}.$$

Approximating $\mathbf{F}_u$ at the third order by involving the multivariate Taylor expansion of ψ in $\mathbf{r}$, the 0-th order and second-order terms vanish by parity, while the first-order and third order terms benefit from the integral kernel isotropy:

$$(43) \quad \begin{aligned} \mathbf{F}_u(\mathbf{x}, t) \approx & \underbrace{\psi^2(\mathbf{x}, t) \int_{r < \delta} G(r) \mathbf{r} d\mathbf{r}}_{=0} - \underbrace{\psi(\mathbf{x}, t) \nabla \psi(\mathbf{x}, t) \int_{r < \delta} G(r) (\mathbf{r} \otimes \mathbf{r}) d\mathbf{r}}_{\kappa \mathbf{I}} \\ & + \underbrace{\frac{\psi(\mathbf{x}, t)}{2} \nabla \nabla \psi(\mathbf{x}, t) \int_{r < \delta} G(r) (\mathbf{r} \otimes \mathbf{r} \otimes \mathbf{r}) d\mathbf{r}}_{=0} \\ & - \underbrace{\frac{\psi(\mathbf{x}, t)}{6} \nabla \nabla \nabla \psi(\mathbf{x}, t) : \int_{r < \delta} G(r) (\mathbf{r} \otimes \mathbf{r} \otimes \mathbf{r} \otimes \mathbf{r}) d\mathbf{r}}_{\mu (\delta_{ij} \delta_{k\ell} + \delta_{ik} \delta_{j\ell} + \delta_{i\ell} \delta_{jk})} \\ & = -\kappa \psi(\mathbf{x}, t) \nabla \psi(\mathbf{x}, t) - \frac{\mu}{2} \psi(\mathbf{x}, t) \nabla (\nabla^2 \psi(\mathbf{x}, t)), \end{aligned}$$

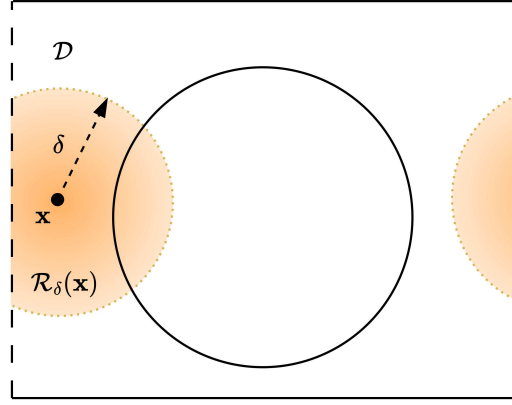


FIGURE 18. Depiction of the domain $\mathcal{D} \cup \mathcal{R}_\delta(\mathbf{x})$. The ball $\mathcal{R}_\delta(\mathbf{x})$ here interacts with periodic (---) and solid boundaries (—).

$$\text{being } \kappa = \frac{1}{3} \int_{r < \delta} G(r) r^2 dr, \quad \mu = \frac{1}{15} \int_{r < \delta} G(r) r^4 dr.$$

Substituting Eq. (43) into Eq. (40), the constraint on the pressure tensor reads:

$$(44) \quad \nabla \cdot \mathbf{P}(\mathbf{x}, t) = -\nabla(\rho(\mathbf{x}, t) c_s^2) - \kappa \psi(\mathbf{x}, t) \nabla \psi(\mathbf{x}, t) - \frac{\mu}{2} \psi(\mathbf{x}, t) \nabla(\nabla^2 \psi(\mathbf{x}, t)).$$

A symmetric tensor whose divergence satisfies Eq. (44) is:

$$(45) \quad \mathbf{P}(\mathbf{x}, t) = \left[-\rho(\mathbf{x}, t) c_s^2 - \frac{\kappa}{2} \psi^2(\mathbf{x}, t) + \frac{\mu}{4} |\nabla \psi(\mathbf{x}, t)|^2 \right] \mathbf{I} - \frac{\mu}{2} \psi(\mathbf{x}, t) \nabla \nabla \psi(\mathbf{x}, t),$$

and holds an equivalent representation, redistributing isotropic parts, of the form:

$$(46) \quad \mathbf{P}(\mathbf{x}, t) = \left[\rho(\mathbf{x}, t) c_s^2 - \frac{\kappa}{2} \psi(\mathbf{x}, t)^2 - \frac{\mu}{2} \psi(\mathbf{x}, t) \nabla^2 \psi(\mathbf{x}, t) + \frac{\mu}{4} |\nabla \psi(\mathbf{x}, t)|^2 \right] \mathbf{I} + \frac{\mu}{2} \nabla \psi(\mathbf{x}, t) \otimes \nabla \psi(\mathbf{x}, t).$$

Considering the bulk of each phase, where $\nabla \psi = 0$, or a first-order approximation of Eq. (43), the pressure tensor $\mathbf{P}$ reduces to a scalar field, the hydrodynamic pressure:

$$(47) \quad \mathbf{P}(\mathbf{x}, t) \approx \left[\rho(\mathbf{x}, t) c_s^2 + \frac{\kappa}{2} \psi^2(\mathbf{x}, t) \right] \mathbf{I} = p(\mathbf{x}, t) \mathbf{I}.$$

One can impose p to be ruled by a piecewise linear equation of state [150]:

$$(48) \quad p(\mathbf{x}, t) = \begin{cases} \rho(\mathbf{x}, t) \theta_v, & \text{if } \rho(\mathbf{x}, t) \leq \rho_1 \\ \rho_1 \theta_v + (\rho(\mathbf{x}, t) - \rho_1) \theta_m, & \text{if } \rho_1 < \rho(\mathbf{x}, t) \leq \rho_2 \\ \rho_1 \theta_v + (\rho_2 - \rho_1) \theta_m + (\rho(\mathbf{x}, t) - \rho_2) \theta_l, & \text{if } \rho(\mathbf{x}, t) > \rho_2 \end{cases}.$$

The parameters θ_v , θ_m , and θ_l represent the slopes of the equation of state in the vapor phase, the mechanically unstable region, and the liquid phase, respectively (see Figure 19). θ_l has the most significant influence on thermodynamic consistency, while θ_m primarily controls the surface tension [35].

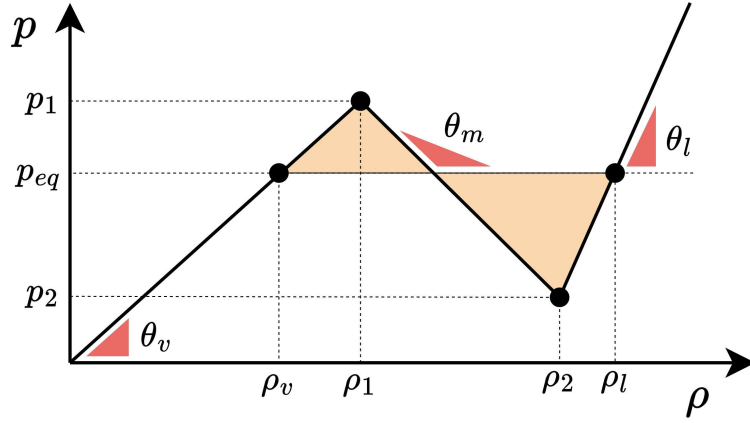


FIGURE 19. Plot of the piecewise linear equation of state in the p - v . Shaded regions are obtained through the Maxwell construction rule.

The two *spinodal* points ρ_1 and ρ_2 in Eq. (48) are obtained for two fixed values of vapor (ρ_v) and liquid (ρ_l) phase densities by adopting the mechanical and chemical equilibrium constraints:

$$(49) \quad \int_{\rho_v}^{\rho_l} dp = (\rho_1 - \rho_v)\theta_v + (\rho_2 - \rho_1)\theta_m + (\rho_l - \rho_2)\theta_l = 0,$$

$$(50) \quad \int_{\rho_v}^{\rho_l} \frac{1}{\rho} dp = \log\left(\frac{\rho_1}{\rho_v}\right)\theta_v + \log\left(\frac{\rho_2}{\rho_1}\right)\theta_m + \log\left(\frac{\rho_l}{\rho_2}\right)\theta_l = 0.$$

The local effective mass is thus computed by recasting the definition of the hydrodynamic pressure p in Eq. (47) as [136]:

$$(51) \quad \psi(\mathbf{x}, t) = \sqrt{\frac{2[p(\mathbf{x}, t) - \rho(\mathbf{x}, t)c_s^2]}{\kappa}}, \quad \mathbf{x} \in \mathcal{D}.$$

The elastic potential tail in Eq. (47) is forced to comply with the non-monotonic behavior in Eq. (48) by Eq. (51), being consistent with non-ideal fluid thermodynamics dictated by the equation of state. This condition is sufficient to support a stable (non-dissolving) interface between fluid phases in $\mathcal{D}$ separating regions of bulk densities ρ_v and ρ_l , given $\rho_v < \rho_l$.

For $\mathbf{x} \in \mathcal{D}_e \setminus \mathcal{D}$, the effective mass is reconstructed by an averaging procedure restricted to the fluid domain sites:

$$(52) \quad \psi(\mathbf{x}, t) = \phi \cdot \frac{\int_{\mathcal{R}_\delta(\mathbf{x}) \cap \mathcal{D}} G(\|\mathbf{x} - \tilde{\mathbf{x}}\|) \psi(\tilde{\mathbf{x}}, t) d\tilde{\mathbf{x}}}{\int_{\mathcal{R}_\delta(\mathbf{x}) \cap \mathcal{D}} G(\|\mathbf{x} - \tilde{\mathbf{x}}\|) d\tilde{\mathbf{x}}}, \quad \mathbf{x} \in \mathcal{D}_e \setminus \mathcal{D}.$$

where $\phi \in \mathbb{R}^+$ controls the balance between adhesive and cohesive forces.

2. The numerical method

2.1. The cascaded collision operator. The flow Reynolds number, $Re = UL/\nu$, impacts both the stability and the accuracy of LBM simulations, where U and L are, respectively, the characteristic velocity and length of the problem.

The implementation of the SRT model leads to inaccurate results at low Re and instability developing at high Re [30]. Moments based collision methods, as the Multiple Relaxation Time (MRT) scheme, are thus adopted to address these criticalities [107].

Within the MRT scheme, populations are transformed into raw moments of order n , collisions occur via a relaxation matrix, then $f_i^*, i \in \{0, \dots, q-1\}$ are recovered by an antitransformation and, lastly, streamed towards nearby lattice nodes. Relaxation parameters related to non-hydrodynamic (*ghost*) moments are tuned to maximize stability or accuracy [108].

The MRT scheme still exhibits unstable behavior at higher Re due to both insufficient Galilean invariance and interactions between high- and low order moments relaxation [110, 151].

The first issue stems from the fixed reference frame imposed by the raw moments collision process, which destabilizes and introduces negative hyper-viscosity effects $\propto Ma^2$. Meanwhile, the second issue, referred to as moments (*crosstalk*), induces artifacts that lead to instability on coarse grids.

These problems are addressed by the Cascaded Lattice Boltzmann Method (CLBM), where relaxation occurs in the central moment space. Thus, the coordinate systems move jointly with $\mathbf{u}(\mathbf{x}, t)$, leading to a stabilizing and positive hyper-viscosity effect $\propto Ma^4$ [151].

The crosstalk is addressed by computing central moments: $\tilde{k}_{n_x n_y n_z} : \mathbb{R}_+ \times \mathbb{R}^3 \rightarrow \mathbb{R}$

$$(53) \quad \tilde{k}_{n_x n_y n_z} = \langle f_i | (e_{ix} - u_x)^{n_x} (e_{iy} - u_y)^{n_y} (e_{iz} - u_z)^{n_z} \rangle = \sum_{i=0}^{18} f_i \left[\prod_{\alpha \in \{x,y,z\}} (e_{i\alpha} - u_\alpha)^{n_\alpha} \right],$$

from raw moments of lower order by the binomial expansion:

$$(54) \quad \prod_{\alpha \in \{x,y,z\}} [(e_{i\alpha} - u_\alpha)^{n_\alpha}] = \prod_{\alpha \in \{x,y,z\}} \left[\sum_{k=0}^{n_\alpha} \binom{n_\alpha}{k} e_{i\alpha}^k (-u_\alpha)^{n_\alpha-k} \right],$$

resulting in a one-way coupling.

The relaxation procedure is thus controlled in an ascending order (*cascaded*) [111].

The CLBM collision process is expressed as:

$$(55) \quad |f_i^*\rangle = \Delta t \mathbf{M}^{-1} \mathbf{N}^{-1} [(\mathbf{I} - \mathbf{S}) \mathbf{N} \mathbf{M} |f_i\rangle + \mathbf{S} \mathbf{N} \mathbf{M} |f_i^{eq}\rangle + (\mathbf{I} - \mathbf{S}/2) \mathbf{N} \mathbf{M} |R_i\rangle].$$

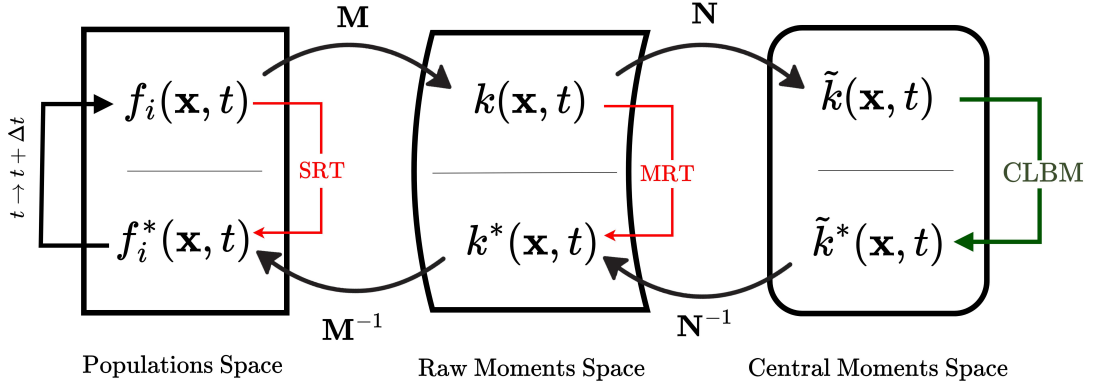


FIGURE 20. In the cascaded framework, populations are mapped first in the raw moments space, then in the central moments space, where they update and then are anti-transformed back, ready for the streaming step.

Collisional elements are transformed into raw moments by $\mathbf{M} \in \mathbb{Z}^{q \times q}$, shifted to central moments by $\mathbf{N} \in \mathbb{R}^{q \times q}$, relaxed by $\mathbf{S} \in \mathbb{R}^{q \times q}$, and lastly, anti-transformed by $(\mathbf{M}^{-1}\mathbf{N}^{-1})$ (see Figure 20).

Both the shift matrix $\mathbf{N}$ and its inverse $\mathbf{N}^{-1}$ are lower triangular, differing only by opposite signs in the odd order velocity terms.

The raw and central moments sets of $|f_i\rangle$, respectively $|K_i\rangle$ and $|\tilde{K}_i\rangle$, are defined as:

$$(56) \quad |\tilde{K}_i\rangle = \mathbf{N}|K_i\rangle = \mathbf{N}\mathbf{M}|f_i\rangle,$$

adopting an analogous notation for other collisional elements, Eq. (55) is expressed as:

$$(57) \quad |f_i^*\rangle = \Delta t \mathbf{M}^{-1} \mathbf{N}^{-1} [(\mathbf{I} - \mathbf{S})|\tilde{K}_i\rangle + \mathbf{S}|\tilde{K}_i^{eq}\rangle + (\mathbf{I} - \mathbf{S}/2)|\tilde{K}_i^R\rangle].$$

The construction of both $\mathbf{M}$ and $\mathbf{N}$ is sensitive to the choice of moments to be relaxed, the selected raw and central moment sets are [114]:

$$(58) \quad |K_i\rangle = \mathbf{M}f_i = \left(k_{000}, k_{100}, k_{010}, k_{001}, k_{110}, k_{101}, k_{011}, k_{\sigma,T}, k_{\sigma,xy}, k_{\sigma,xz}, k_{120}, k_{102}, k_{201}, k_{012}, k_{021}, k_{220}, k_{202}, k_{022} \right)^\top,$$

$$(59) \quad |\tilde{K}_i\rangle = \mathbf{N}|K_i\rangle = \left(\tilde{k}_{000}, \tilde{k}_{100}, \tilde{k}_{010}, \tilde{k}_{001}, \tilde{k}_{110}, \tilde{k}_{101}, \tilde{k}_{011}, \tilde{k}_{\sigma,T}, \tilde{k}_{\sigma,xy}, \tilde{k}_{\sigma,xz}, \tilde{k}_{120}, \tilde{k}_{102}, \tilde{k}_{201}, \tilde{k}_{012}, \tilde{k}_{021}, \tilde{k}_{220}, \tilde{k}_{202}, \tilde{k}_{022} \right)^\top,$$

with:

$$(60) \quad k_{\sigma,T} = k_{200} + k_{020} + k_{002}, \quad k_{\sigma,xy} = k_{200} - k_{020}, \quad k_{\sigma,xz} = k_{200} - k_{002}.$$

These moments reflect macroscopic quantities of interest: aside from the mass and momentum density, one notices that k_{200} , k_{020} , and k_{002} are normal stresses; thus, $k_{\sigma,T}$ constitutes the trace of the pressure tensor, while $k_{\sigma,xy}$ and $k_{\sigma,xz}$ represent the normal stress differences [113].

The transformation matrix $\mathbf{M}$ is defined row by row as:

$$\begin{aligned}
 (61) \quad & M_{0,:} = \mathbf{1}_{1 \times 18}, \quad M_{1,:} = |e_{ix}\rangle^\top, \quad M_{2,:} = |e_{iy}\rangle^\top, \quad M_{3,:} = |e_{iz}\rangle^\top, \\
 & M_{4,:} = (|e_{ix}\rangle \circ |e_{iy}\rangle)^\top, \quad M_{5,:} = (|e_{ix}\rangle \circ |e_{iz}\rangle)^\top, \quad M_{6,:} = (|e_{iy}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{7,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle + |e_{iy}\rangle \circ |e_{iy}\rangle + |e_{iz}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{8,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle - |e_{iy}\rangle \circ |e_{iy}\rangle)^\top, \quad M_{9,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle - |e_{iz}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{10,:} = (|e_{ix}\rangle \circ |e_{iy}\rangle \circ |e_{iy}\rangle)^\top, \quad M_{11,:} = (|e_{ix}\rangle \circ |e_{iz}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{12,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle \circ |e_{iy}\rangle)^\top, \quad M_{13,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{14,:} = (|e_{iy}\rangle \circ |e_{iz}\rangle \circ |e_{iz}\rangle)^\top, \quad M_{15,:} = (|e_{iy}\rangle \circ |e_{iy}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{16,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle \circ |e_{iy}\rangle \circ |e_{iy}\rangle)^\top, \quad M_{17,:} = (|e_{ix}\rangle \circ |e_{ix}\rangle \circ |e_{iz}\rangle \circ |e_{iz}\rangle)^\top, \\
 & M_{18,:} = (|e_{iy}\rangle \circ |e_{iy}\rangle \circ |e_{iz}\rangle \circ |e_{iz}\rangle)^\top.
 \end{aligned}$$

where $\mathbf{1}_{1 \times 18}$ is a unitary row vector and $(\circ)$ denotes the element-wise Hadamard product.

The shift matrix $\mathbf{N}$ incorporates the binomial expansion coefficients from Eq. (54). Explicit expressions for $\mathbf{M}$ and $\mathbf{N}$ are provided in Appendix A.

The central moment transformation of both $|f_i^{\text{eq}}\rangle$ and $|R_i\rangle$ is approached differently.

Consider the Gaussian character of the continuous Maxwell-Boltzmann distribution f^{MB} , as $|f_i^{\text{eq}}\rangle$ is constructed to preserve the conservation of hydrodynamic moments, one computes these in the continuum space [111], resulting in:

$$(62) \quad |\tilde{K}_i^{\text{eq}}\rangle = (\rho, 0, 0, 0, 0, 0, 0, 3\rho c_s^2, 0, 0, 0, 0, 0, 0, \rho c_s^4, \rho c_s^4, \rho c_s^4)^\top.$$

In the scheme proposed by He et al. [94], the forcing term is approximated by considering small deviations of the continuous function f from its equilibrium state:

$$(63) \quad R = \mathbf{F} \cdot \nabla_\xi f \approx \mathbf{F} \cdot \nabla_\xi f^{MB} = -\mathbf{F} \cdot \frac{(\xi - \mathbf{u})}{c_s^2} f^{MB},$$

thus, in an analogous procedure, one finds [138]:

$$(64) \quad |\tilde{K}_i^R\rangle = (0, F_x, F_y, F_z, 0, 0, 0, 0, 0, 0, F_x c_s^2, F_x c_s^2, F_y c_s^2, F_z c_s^2, F_y c_s^2, F_z c_s^2, 0, 0, 0)^\top.$$

2.2. The entropic relaxation process.

2.2.1. *The H-theorem in the continuum.* In classical kinetic theory, the H -theorem asserts that a convex functional H , the Boltzmann entropy, tends to decrease over time as a system evolves through particle collisions, in a mesoscopic formulation of the second law of thermodynamics.

To evaluate whether an entropic-stabilized numerical scheme is suited to solve the problem at hand, namely a Boltzmann Equation embedding a body force with null velocity-divergence and also periodic and reflecting boundary conditions, its compliance with the H -theorem is investigated.

The system of equations (38), (39), (41), (48), (50), (51), (52) could be derived by applying the Chapman-Enskog analysis to the forced Boltzmann Equation in Eq.(4).

The H -functional is defined as,

$$(65) \quad H(\mathbf{x}, t) = \int_{\mathcal{V}} f \ln(f) d\xi.$$

By differentiating H with respect to time, applying the Leibniz and chain rules, and subsequently substituting Eq. (4), the contributions stemming from the streaming, forcing, and collision phases become evident:

$$(66) \quad \begin{aligned} \frac{\partial H}{\partial t} &= \int_{\mathcal{V}} (1 + \ln(f)) \frac{\partial f}{\partial t} d\xi = \\ &= \int_{\mathcal{V}} (1 + \ln(f)) \left(\underbrace{(-\xi \cdot \nabla_{\mathbf{x}} f)}_{\text{streaming}} + \underbrace{\left(-\frac{\mathbf{F}}{\rho} \cdot \nabla_{\xi} f \right)}_{\text{forcing}} + \underbrace{\Omega(f)}_{\text{collision}} \right) d\xi. \end{aligned}$$

By observing that,

$$(67) \quad \nabla_{\mathbf{x}} (f \ln(f)) = \nabla_{\mathbf{x}} f + \ln(f) \nabla_{\mathbf{x}} f = (1 + \ln(f)) \nabla_{\mathbf{x}} f,$$

$$(68) \quad \nabla_{\mathbf{x}} \cdot \xi = 0,$$

and using the Leibniz rule, the streaming term reads,

$$(69) \quad \begin{aligned} I_{str} &= - \int_{\mathcal{V}} (1 + \ln(f)) (\xi \cdot \nabla_{\mathbf{x}} f) d\xi = - \int_{\mathcal{V}} \xi \cdot \nabla_{\mathbf{x}} (f \ln(f)) d\xi \\ &= - \int_{\mathcal{V}} \nabla_{\mathbf{x}} \cdot (\xi f \ln(f)) d\xi = - \nabla_{\mathbf{x}} \cdot \int_{\mathcal{V}} \xi f \ln(f) d\xi = - \nabla_{\mathbf{x}} \cdot \mathbf{J}_H, \end{aligned}$$

where $\mathbf{J}_H$ is the H -flux density.

Consider now the forcing contribution, by applying the chain rule as in Eq. (67) and factoring the body force in the velocity-divergence form, it holds:

$$(70) \quad \begin{aligned} I_{for} &= - \int_{\mathcal{V}} (1 + \ln(f)) \left(\frac{\mathbf{F}}{\rho} \cdot \nabla_{\xi} f \right) d\xi = - \int_{\mathcal{V}} \frac{\mathbf{F}}{\rho} \cdot \nabla_{\xi} (f \ln(f)) d\xi \\ &= - \int_{\mathcal{V}} \nabla_{\xi} \cdot \left(f \ln(f) \frac{\mathbf{F}}{\rho} \right) d\xi + \int_{\mathcal{V}} f \ln(f) \nabla_{\xi} \cdot \left(\frac{\mathbf{F}}{\rho} \right) d\xi = I_{F1} + I_{F2}. \end{aligned}$$

Due to the divergence theorem, the independence of $\mathbf{F}$ from ξ , and the decay to zero of the integrand as $\|\xi\| \rightarrow \infty$ [152, 153], I_{F1} and I_{F2} read:

$$(71) \quad I_{F1} = - \int_{\mathcal{V}} \nabla_{\xi} \cdot \left(f \ln(f) \frac{\mathbf{F}}{\rho} \right) d\xi = - \int_{|\xi| \rightarrow \infty} \left(f \ln(f) \frac{\mathbf{F}}{\rho} \right) \cdot d\mathbf{S}_{\mathcal{V}} = 0,$$

$$(72) \quad I_{F2} = \int_{\mathcal{V}} f \ln(f) \nabla_{\xi} \cdot \left(\frac{\mathbf{F}}{\rho} \right) d\xi = 0,$$

where $d\mathbf{S}_{\mathcal{V}}$ is the $\mathcal{V}$ oriented boundary element.

Lastly, embedding the mass conservation constraint in I_{coll} leads to a strictly non-positive contribution for the Boltzmann collision operator [91],

$$(73) \quad I_{coll} = \int_{\mathcal{V}} (1 + \ln(f)) \Omega(f) d\xi = \int_{\mathcal{V}} \ln(f) \Omega(f) d\xi = \sigma_H(\mathbf{x}, t) \leq 0.$$

Given the computations above, Eq. (66) results in:

$$(74) \quad \frac{\partial H}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{J}_H = \sigma_H \leq 0,$$

being the local H -balance for a distribution function evolving in time according to Eq. (4).

By integrating Eq. (74) and applying the divergence theorem, it results that,

$$(75) \quad \int_{\mathcal{D}} \left(\frac{\partial H}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{J}_H \right) d\mathbf{x} = \frac{d\mathcal{H}}{dt} + \int_{\partial \mathcal{D}} \mathbf{J}_H \cdot d\mathbf{S}_{\mathcal{D}} = \int_{\mathcal{D}} \sigma_H d\mathbf{x},$$

where $\mathcal{H}$ is the total entropy of the system and $d\mathbf{S}_{\mathcal{D}}$ is the $\mathcal{D}$ oriented boundary element.

Let the boundary region be the union of two disjoint parts $\partial \mathcal{D} = \partial \mathcal{D}_p \cup \partial \mathcal{D}_r$, where periodic and Dirichlet boundary conditions are applied, respectively.

Opposite periodic faces come in pairs of points $\mathbf{x}^+ \in \partial \mathcal{D}_p^+$ and $\mathbf{x}^- \in \partial \mathcal{D}_p^-$; periodicity implies $f(\mathbf{x}^+, \xi, t) = f(\mathbf{x}^-, \xi, t)$, thus $\mathbf{J}_H(\mathbf{x}^+, t) = \mathbf{J}_H(\mathbf{x}^-, t)$ and $d\mathbf{S}_{\mathcal{D}}(\mathbf{x}^+) = -d\mathbf{S}_{\mathcal{D}}(\mathbf{x}^-)$, hence the fluxes cancel pair-wise:

$$(76) \quad \int_{\partial \mathcal{D}_p} \mathbf{J}_H \cdot d\mathbf{S}_{\mathcal{D}} = \int_{\partial \mathcal{D}_p^+} \mathbf{J}_H \cdot d\mathbf{S}_{\mathcal{D}} + \int_{\partial \mathcal{D}_p^-} \mathbf{J}_H \cdot d\mathbf{S}_{\mathcal{D}} = 0.$$

At the Dirichlet boundary, $f(\mathbf{x}, \xi_{\tau}, \xi_n, t) = f(\mathbf{x}, \xi_{\tau}, -\xi_n, t)$, being ξ_{τ} and ξ_n the tangential and normal components of ξ with respect to $d\mathbf{S}_{\mathcal{D}}$, respectively.

The integrand is odd on $\partial \mathcal{D}_r$ [154], resulting in:

$$(77) \quad \int_{\partial \mathcal{D}_r} \mathbf{J}_H \cdot d\mathbf{S}_{\mathcal{D}} = 0.$$

Given Eq.s (76)–(77), Eq. (75) reads

$$(78) \quad \frac{d\mathcal{H}}{dt} = \int_{\mathcal{D}} \sigma_H d\mathbf{x} \leq 0.$$

Thus, the system of interest complies with the Boltzmann H -theorem.

2.2.2. *The H-theorem in LBM.* The existence of a perfect entropy functional in LBM (H_d) allows the implementation of a discrete H -theorem to enhance the physical consistency and stability of the method [116].

In a time-discrete framework, the continuous decrease in H is approximated by minimizing the post-collisional entropy at each time step. An early approach achieves this by constructing consistent equilibrium populations, complying with mass and momentum conservation and the recovery of the momentum flux density tensor, and imposing an entropy balance condition between the pre-collisional state and an entropic mirror state [117].

As a more recent approach, within the over-relaxation regime [$\tau/\Delta t \in (1/2, 1)$], the KBC model combines the unsupervised update of low-order moments with a controlled relaxation of high-order moments dictated by an adaptive stabilizer. This latter is a function of local macroscopic fields computed by imposing entropy minimization, resulting in a dynamic and local constraint on the relaxation process. The implementation of the KBC model is proven to yield positive results, enhancing the stability of 2D [118] and 3D lattices [155], even within a CLBM framework [137].

The discrete entropy functional $H_d \in \mathbb{R}_+^q \rightarrow \mathbb{R}_+$ is [156]

$$(79) \quad H_d = \sum_{i=0}^{q-1} f_i \ln(f_i/w_i),$$

being minimized in the post-collisional state

$$(80) \quad |f_i^*\rangle = (1 - \delta)|f_i\rangle + \delta|f_i^m\rangle \quad \text{with} \quad \delta = \frac{1}{2} \frac{\Delta t}{\tau} \in \left(\frac{1}{2}, 1\right),$$

where $|f_i^m\rangle$ identifies a mirror state [118, 155]. The entropic stabilizer is now constructed.

The central moments set (Eq. 59) is sectioned into a kinematic, shear, and high order part [155]

$$(81) \quad |\tilde{K}_i\rangle = |\tilde{K}_i^K\rangle + |\tilde{K}_i^h\rangle + |\tilde{K}_i^s\rangle$$

where

$$(82) \quad |\tilde{K}_i^K\rangle = (\tilde{k}_{000}, \dots, \tilde{k}_{001}, 0, \dots, 0)^\top,$$

$$(83) \quad |\tilde{K}_i^s\rangle = (0, \dots, 0, \tilde{k}_{110}, \tilde{k}_{101}, \tilde{k}_{011}, 0, \tilde{k}_{\sigma,xy}, \tilde{k}_{\sigma,xz}, 0, \dots, 0)^\top,$$

$$(84) \quad |\tilde{K}_i^h\rangle = |\tilde{K}_i\rangle - (|\tilde{K}_i^K\rangle + |\tilde{K}_i^s\rangle).$$

The discrete distribution function $|f_i\rangle$ is thus constructed as

$$(85) \quad |f_i\rangle = |\kappa_i\rangle + |s_i\rangle + |h_i\rangle,$$

$$(86) \quad |\kappa_i\rangle = \mathbf{M}^{-1} \mathbf{N}^{-1} |\tilde{K}_i^k\rangle$$

$$(88) \quad |h_i\rangle = \mathbf{M}^{-1} \mathbf{N}^{-1} |\tilde{K}_i^h\rangle$$

[illegible]

The Chapman-Enskog analysis allows to recover the NSE as expressed in Eq. 38, with a kinematic viscosity complying with Eq. 16 and a bulk viscosity [155]:

$$(97) \quad \zeta = c_s^2 \left(\frac{\tau}{\gamma^*} - \frac{\Delta t}{2} \right)$$

Notice that, being ω_v prescribed by the physics of the problem and $\gamma^* = \gamma^*(\mathbf{x}, t)$ computed, one has no degree of freedom to manually act on the relaxation process.

2.3. The unified interaction force.

2.3.1. *The cohesive interaction.* Hereafter, if not otherwise specified, $\mathbf{x} \in \mathcal{D}_f$, also $\Delta x = 1$ and $\Delta t = 1$.

In their seminal works [32, 33], Shan and Chen proposed a microscopic model of two-phase systems by introducing the pairwise interaction force in Eq. (29).

As points $\mathbf{x} \in \mathcal{D}_s$ are not involved in the computation of the cohesive interaction, here denoted as $\mathbf{F}_{ch}$, a switch function is defined $s_f : \mathcal{D}_+ \rightarrow \{0, 1\}$ to check whether the neighbor node is fluid:

$$(98) \quad s_f(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \in \mathcal{D}_f \\ 0, & \text{if } \mathbf{x} \in \mathcal{D}_s \end{cases}.$$

Considering also the extension of the S-C model to non-hexagonal lattices, Eq. (29) become:

$$(99) \quad \mathbf{F}_{ch}(\mathbf{x}, t) = -\mathcal{G}_{ch} \psi(\mathbf{x}, t) \sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) w_i \psi(\mathbf{x} + \mathbf{e}_i, t) \mathbf{e}_i,$$

with a support extending to a lattice link distance. Such a force discretizes Eq. (43) within the cohesive (*ch*) interaction as $\delta \rightarrow 0$. where $\mathcal{G}_{ch} \in \mathbb{R}$ is the cohesive interaction strength, with $\mathbf{F}_{ch} : \mathcal{D}_f \times \mathbb{R}^+ \rightarrow \mathbb{R}^3$ and $\psi : \mathcal{D}_+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$ defined on $\mathcal{D}_+$.

$\mathcal{D}_+ = \mathcal{D}_f \cup \mathcal{D}_s$ is an extended discrete domain with $\mathcal{D}_s \cap \mathcal{D}_f = \emptyset$, being $\mathcal{D}_s$ the set of solid nodes spanned by the sum in Eq. 99.

The expression in Eq. (99) considers a sum of individual neighbor contributions acting on the joining line between two fluid points. A spontaneous phase separation is induced within a diffuse interface below critical conditions. The effective mass ψ is computed on fluid nodes through Eq. (51).

Recently, Luo et al. proposed an additional forcing term, tuned by $\lambda \in \mathbb{R}$, to control the surface tension with minimal impact on equilibrium properties [114]:

$$(100) \quad \begin{aligned} \mathbf{F}_{ch}^{(l)}(\mathbf{x}) = & -\frac{\lambda}{3} \mathcal{G} \psi(\mathbf{x}) \sum_l^L \omega(|\mathbf{e}_l|^2) \psi(\mathbf{x} + \mathbf{e}_l) \mathbf{e}_l + \frac{\lambda}{6} \mathcal{G} \sum_l^L \omega(|\mathbf{e}_l|^2) \psi^2(\mathbf{x} + \mathbf{e}_l) \mathbf{e}_l + \\ & -\frac{\lambda}{6} \mathcal{G} \left\{ 2 \sum_l^L \omega(|\mathbf{e}_l|^2) [\psi(\mathbf{x} + \mathbf{e}_l) - \psi(\mathbf{x})] \right\} \sum_l^L \omega(|\mathbf{e}_l|^2) \psi(\mathbf{x} + \mathbf{e}_l) \mathbf{e}_l, \end{aligned}$$

where the term within $\{\}$ is the finite difference approximation of $\nabla^2 \psi$.

2.3.2. *The adhesive interaction.* Within the model proposed by Shan and Chen, Sukop and Thorne prescribed a simple formulation [29] for such adhesive interactions, as expressed in Eq 33.

By introducing $s_s : \mathcal{D}_+ \rightarrow \{0, 1\}$ to check whether the target node is solid:

$$(101) \quad s_s(\mathbf{x}) = 1 - s_f(\mathbf{x}),$$

the adhesive force is recast as:

$$(102) \quad \mathbf{F}_{adh}(\mathbf{x}, t) = -\mathcal{G}_{adh} \psi(\mathbf{x}, t) \sum_{i=0}^{q-1} s_s(\mathbf{x} + \mathbf{e}_i) w_i \mathbf{e}_i.$$

Unlike the Sukop and Thorne expression, the popular model by Benzi et al. [139] mildly resembles the structure of the cohesive interaction force, through:

$$(103) \quad \mathbf{F}_{adh}(\mathbf{x}, t) = -\mathcal{G}_{adh} \psi(\mathbf{x}, t) \sum_{i=0}^{q-1} s_s(\mathbf{x} + \mathbf{e}_i) w_i \psi(\rho_w) \mathbf{e}_i,$$

where $\mathcal{G}_{adh} = \mathcal{G}_{ch}$. The virtual wall density is set as a parameter in the range of gas and liquid coexistence values $\rho_w \in [\rho_v, \rho_l]$ such that, if $\rho_w = \rho_v$, then $\theta \approx 180^\circ$; if $\rho_w = \rho_l$, then $\theta \approx 0^\circ$. As in Eq. (102), the wetting state would be set as constant over $\partial \mathcal{D}_s$.

Li et al. [140] proposed a local definition of the wall density as:

$$(104) \quad \rho_w(\mathbf{x}, t) = \begin{cases} \phi \rho_{\text{avg}}(\mathbf{x}, t), & \phi > 1 \quad \text{for} \quad \theta < 90^\circ \\ \rho_{\text{avg}}(\mathbf{x}, t) - \Delta \rho, & \Delta \rho > 0 \quad \text{for} \quad \theta > 90^\circ \end{cases}, \text{ with } \mathbf{x} \in \mathcal{D}_s,$$

where a limiter is set on ρ_w , such that if $\rho_w < \rho_v$, then $\rho_w \leftarrow \rho_v$, and if $\rho_w > \rho_l$, then $\rho_w \leftarrow \rho_l$; ρ_{avg} is the local weighted average of the surrounding fluid neighbors and corresponds to:

$$(105) \quad \rho_{\text{avg}}(\mathbf{x}) = \frac{\sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) w_i \rho(\mathbf{x} + \mathbf{e}_i)}{\sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) w_i}, \text{ with } \mathbf{x} \in \mathcal{D}_s.$$

This method can both eliminate the non-physical mass-transfer layer near the solid boundary and reduce spurious currents [140].

Peng et al. [90] extended the model by Li et al. with the aim of making it easily adaptable for partially miscible multicomponent flows. They adopted the direct computation of a virtual wall pseudopotential as $\psi(\mathbf{x}, t) = \phi \psi_{\text{avg}}(\mathbf{x}, t)$ with:

$$(106) \quad \psi_{\text{avg}}(\mathbf{x}, t) = \frac{\sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) w_i \psi(\mathbf{x} + \mathbf{e}_i, t)}{\sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) w_i}, \text{ with } \mathbf{x} \in \mathcal{D}_s.$$

Under certain simplifying assumptions, the prescribed ϕ and the consequent θ may be analytically correlated.

2.3.3. *The unified interaction.* A unified interaction force is proposed as:

$$(107) \quad \mathbf{F}_u(\mathbf{x}, t) = \mathbf{F}_{ch}(\mathbf{x}, t) + \mathbf{F}_{adh}(\mathbf{x}, t).$$

Eq. (107), combined with Eqs (99), (98) and (101), results in:

$$(108) \quad \mathbf{F}_u(\mathbf{x}, t) = -\mathcal{G} \psi(\mathbf{x}, t) \sum_{i=0}^{q-1} w_i \psi(\mathbf{x} + \mathbf{e}_i, t) \mathbf{e}_i,$$

Notably, there is no distinction between a fluid or solid neighbor within this force expression; these are simply considered *interacting material nodes*. Wettability conditions are exclusively applied to ψ and comply with the Peng approach [90].

Eq. (108) is reformulated for a generic L -element stencil:

$$(109) \quad \mathbf{F}_u(\mathbf{x}, t) = -g c_s^2 \psi(\mathbf{x}, t) \sum_{l=0}^{L-1} \omega(\|\mathbf{e}_l\|^2) \psi(\mathbf{x} + \mathbf{e}_l, t) \mathbf{e}_l,$$

in which each site $l \in \{0, 1, \dots, L-1\}$ is related to a distance vector $\mathbf{e}_l$ and an interaction weight $\omega(\|\mathbf{e}_l\|)$ [133]. The weights set is uniquely determined by L .

Consider a Taylor expansion around the l -th neighbor of $\mathbf{x}$:

$$(110) \quad \psi(\mathbf{x} + \mathbf{e}_l, t) = \sum_{n=0}^{\infty} \frac{1}{n!} \nabla^{(n)} \psi(\mathbf{x}, t) : \mathbf{e}_l^{\otimes n}.$$

Each scalar term is computed by a tensor contraction, with $\nabla^{(n)}$ and $\otimes n$ representing the n -times applications of the gradient and the outer product, respectively.

Due to Eq. (110), Eq. (109) could be expressed as,

$$(111) \quad \mathbf{F}_u(\mathbf{x}, t) = -\mathcal{G} \psi(\mathbf{x}) \sum_{n=0}^{\infty} \frac{1}{n!} \nabla^{(n)} \psi(\mathbf{x}, t) : \mathbf{E}^{(n+1)},$$

with:

$$(112) \quad \mathbf{E}^{(n)} = \sum_{l=0}^{L-1} \omega(\|\mathbf{e}_l\|^2) \mathbf{e}_l^{\otimes n}.$$

The force $\mathbf{F}_u$ recovers the continuum isotropic behavior, i.e. it remains parallel to $\nabla \psi$, only if the tensors $\mathbf{E}^{(n)}$ satisfy the corresponding isotropy conditions at all relevant

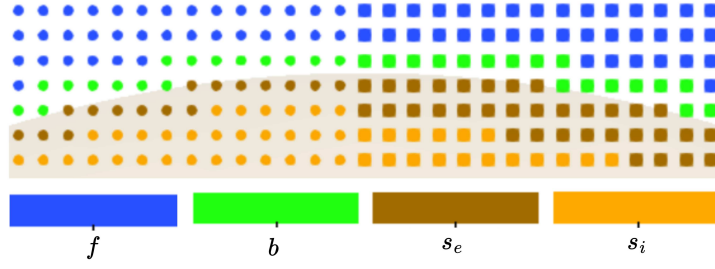


FIGURE 21. Tagging procedure in presence of a curved unfitted boundary (close-up) for $m = 4$ on the left ($\bullet$) and $m = 8$ on the right ($\blacksquare$). Fluid (f), boundary (b), solid external (s_e), and solid internal (s_i) nodes are depicted. The s_e shell, requiring the computation of the pseudopotential ψ , is widened for $m = 8$ compared to $m = 4$.

TABLE 4. Relating isotropy order m with corresponding interaction weights [132].

m	$\omega(1)$	$\omega(2)$	$\omega(3)$	$\omega(4)$	$\omega(5)$	$\omega(6)$	$\omega(8)$
4	1/6	1/12	—	—	—	—	—
6	2/15	1/15	1/60	1/120	—	—	—
8	4/45	1/21	2/105	5/504	1/315	1/630	1/5040

ranks, which cannot be achieved with a finite interaction stencil. Indeed, only a finite number L of lattice links, and thus of independent weights, is available. For this reason, the parameter m denotes the highest tensor rank up to which isotropy could be enforced for a given stencil, i.e. for all even orders $n \leq m$. Since the stencil is inversion-symmetric, odd-rank contributions vanish identically, and the attainable accuracy progresses in increments of two, $m = 2, 4, 6, \dots$, each step $m \rightarrow m + 2$ imposing the next independent constraint. Higher m requires higher values of L . In Table 4, the weights $\omega(n)$ are reported only for shells populated by at least one integer lattice link in the selected stencil [34, 132, 133].

In 3D space, the adoption of $L = q$ implies a fourth-order isotropy of the force (E4) and a sum over the x-neighborhood spanned in the streaming step.

Extending the stencil for $L > q$ allows for an increase in the isotropy order, reducing the magnitude of spurious currents [133].

Selected weights for the D3Q19 framework are provided in Table 4.

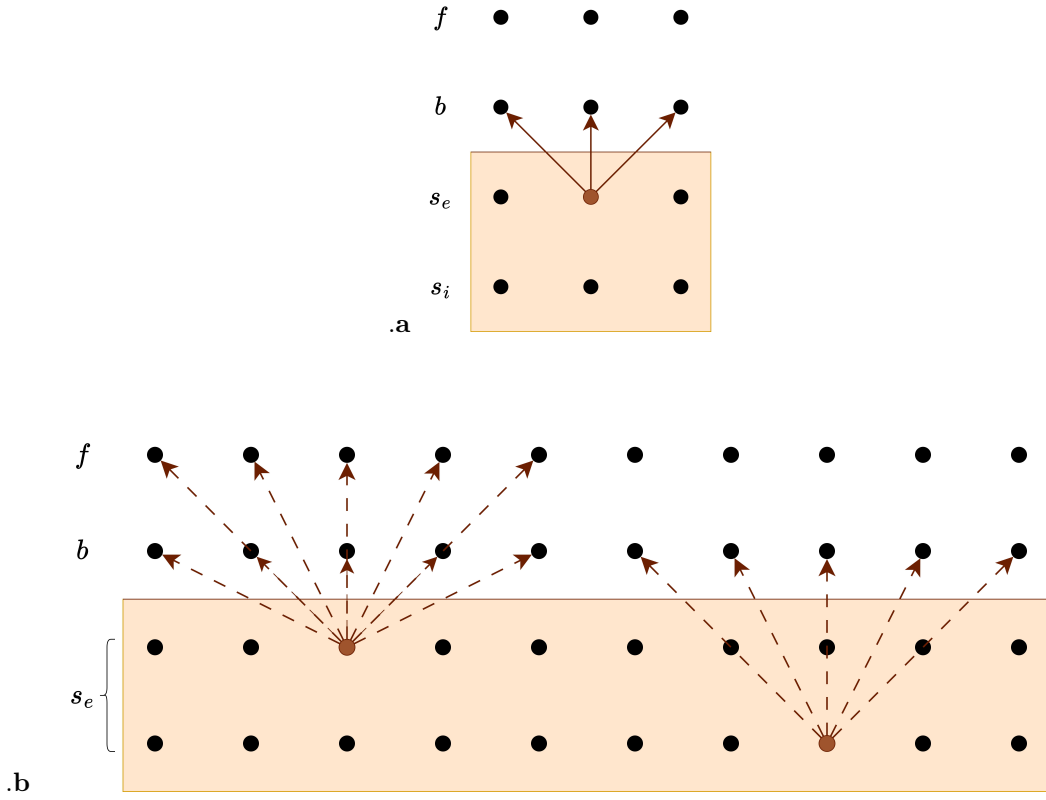


FIGURE 22. Pictorial description of the averaging procedure to evaluate the interaction force at the fluid-solid boundary. The pseudopotential ψ is constructed on solid-external nodes s_e (•). In a flat-wall configuration, adopting the compact stencil $m = 4$ ($\rightarrow$) this procedure results in a one-node thick s_e layer [.a], whereas the extended stencil $m = 8$ ($\dashrightarrow$) yields a two-nodes thick layer [.b].

Given Eq. (109), Peng averaged pseudopotential in Eq. (106) is reformulated as:

$$(113) \quad \psi_{\text{avg}}(\mathbf{x}, t) = \frac{\sum_{l=0}^{L-1} s_f(\mathbf{x} + \mathbf{e}_l) \omega(\|\mathbf{e}_l\|^2) \psi(\mathbf{x} + \mathbf{e}_l, t)}{\sum_{l=0}^{L-1} s_f(\mathbf{x} + \mathbf{e}_l) \omega(\|\mathbf{e}_l\|^2)}, \text{ with } \mathbf{x} \in \mathcal{D}_s.$$

The boundary nodes are defined as those fluid sites that have at least one solid neighbor, thus belonging to the set:

$$(114) \quad \mathcal{D}_b = \{ \mathbf{x}_b \in \mathcal{D}_f \mid \exists i \in \{1, \dots, q-1\} \text{ such that } s_s(\mathbf{x}_b + \mathbf{e}_i) = 1 \}.$$

A solid node $\mathbf{x}_s \in \mathcal{D}_s$ is hereafter labeled as *external* (e) if $\exists l \in \{0, 1, \dots, L-1\}$ such that $s_f(\mathbf{x}_s + \mathbf{e}_l) = 1$; otherwise, it is referred to as *internal* (i). Only external solid nodes are involved in the computation of a virtual ψ . Implementation details are presented in Figure 21 and Figure 22.

An extension of the Yuan approach for cohesive interactions [136] is proposed for the mentioned unified model. As such, an equivalent discretization of Eq. (43) is given by:

$$(115) \quad \mathbf{F}_u^{(k)}(\mathbf{x}, t) = -\frac{\mathcal{G}}{2} \sum_{l=0}^{L-1} \omega(\|\mathbf{e}_l\|) \psi^2(\mathbf{x} + \mathbf{e}_l, t) \mathbf{e}_l.$$

The total unified interaction force for any fluid node is thus expressed as:

$$(116) \quad \mathbf{F}_u(\mathbf{x}, t) = \beta \mathbf{F}_u^{(o)}(\mathbf{x}, t) + (1 - \beta) \mathbf{F}_u^{(k)}(\mathbf{x}, t),$$

where the original formulation in Eq. (109) is identified with the (o) superscript.

The parameter β allows tuning a linear combination between Eq. (109) and Eq. (115), which, within the cohesive interaction, has been demonstrated to mitigate the effect of spurious currents, thus enhancing the stability of the simulation [135].

2.4. The coupled boundary-wetting scheme. A coupled boundary-wettability scheme for curved geometries, ensuring both mass conservation and an accurate depiction of adhesion mechanisms, is developed here. The root of such a scheme is the Interpolated Bounce-Back [147], which does not require altering the entropic-cascaded framework on boundary nodes. A simple mass-correction scheme, which refills the rest population with the local mass leakage, would not account for the interpolation-driven momentum leakage, as the f_0 contribution in first-order raw moments is null.

Inspired by the work of Yao et al. [157] on a free-energy model, the interpolation artifacts of the Linear-IBB (L-IBB) are compensated by the directional force component, embedding the mentioned unified interaction.

Consider a boundary node $\mathbf{x}_b \in \mathcal{D}_b$, a neighboring solid node $\mathbf{x}_s = \mathbf{x}_b + \mathbf{e}_i$ in the i^{th} wall-oriented direction, and its specular fluid node $\mathbf{x}_f = \mathbf{x}_b - \mathbf{e}_i$. The curved boundary intersects the streaming direction $f_i^*(\mathbf{x}_b, t) \rightarrow f_i(\mathbf{x}_s, t + \Delta t)$ at the off-lattice wall location $\mathbf{x}_w \in \mathcal{D}$. The intersected link fraction $q_i : \mathcal{D}_b \rightarrow (0, 1]$ reads

$$(117) \quad q_i(\mathbf{x}_b) = \frac{\|\mathbf{x}_b - \mathbf{x}_w\|}{\|\mathbf{x}_b - \mathbf{x}_s\|} = \frac{\|\mathbf{x}_b - \mathbf{x}_w\|}{\|\mathbf{e}_i\|}.$$

In the linear interpolated bounce-back (L-IBB), the unknown population $f_{\bar{i}}(\mathbf{x}_b, t + \Delta t)$ is reconstructed as a linear interpolation between known populations, enforced by a body-force correction where $\mathbf{e}_{\bar{i}} = -\mathbf{e}_i$.

If $q_i(\mathbf{x}_b) \in (0, 1/2]$, such an unknown population is given by [157]:

$$(118) \quad f_{\bar{i}}(\mathbf{x}_b, t + \Delta t) = 2q(\mathbf{x}_b) f_i^*(\mathbf{x}_b, t) + [1 - 2q(\mathbf{x}_b)] f_i^*(\mathbf{x}_f, t) + [1 - 2q(\mathbf{x}_b)] R_i(\mathbf{x}_b, t).$$

Practically, $f_{\bar{i}}(\mathbf{x}_b, t + \Delta t)$ is set as the post collision population f_i^* that would stream from a fictitious point $\mathbf{x}_p \in \mathcal{D}$. it bounces off the wall in $\mathbf{x}_w$ to then reach $\mathbf{x}_b$ (see

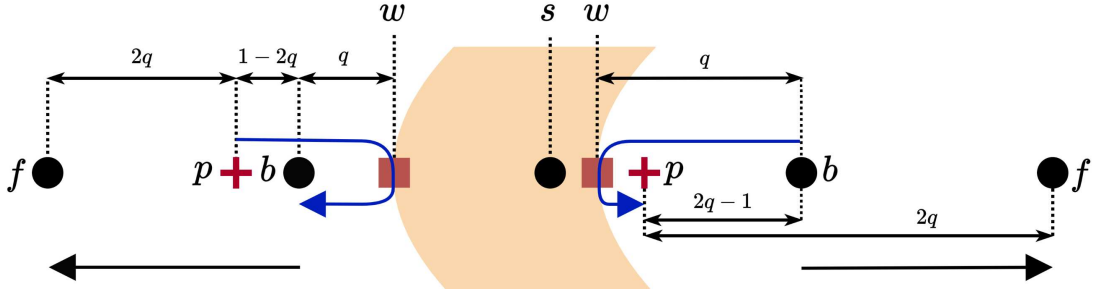


FIGURE 23. Schematic of streaming phase of a bounced-back population (from p to b and *vice-versa*) involved in the computations of the unknown populations towards the fluid node f within the L-IBB formulation. The two schemes respectively correspond to close (left) and far (right) wall configurations.

Figure 23). As $\mathbf{x}_p \notin \mathcal{D}_f$, the value of f_i^* in $\mathbf{x}_p$ is linearly interpolated from the known post-collisional boundary ($f_i^*(\mathbf{x}_b, t)$) and fluid ($f_i^*(\mathbf{x}_f, t)$) values, with a momentum correction increasing as $q(\mathbf{x}_b) \rightarrow 0$.

On the other hand, if $q_i(\mathbf{x}_b) \in (1/2, 1]$, negative values of the target population might be predicted by Eq. (118), thus it is set:

$$(119) \quad f_i(\mathbf{x}_b, t + \Delta t) = \left[\frac{1}{2q(\mathbf{x}_b)} \right] f_i^*(\mathbf{x}_b, t) + \left[\frac{2q(\mathbf{x}_b) - 1}{2q(\mathbf{x}_b)} \right] f_i^*(\mathbf{x}_f, t) + \left[\frac{2q(\mathbf{x}_b) - 1}{2q(\mathbf{x}_b)} \right] R_i(\mathbf{x}_b, t).$$

The missing population is constructed using a one-point approach, employing information at the boundary node only and including a momentum correction that mostly impacts as $q(\mathbf{x}_b) \rightarrow 1$.

A refill scheme on rest populations would compensate for the leftover mass leak by computing the difference between outgoing [$s_s(\mathbf{x}_b + \mathbf{e}_i) = 1$] and incoming [$s_s(\mathbf{x}_b + \mathbf{e}_{\bar{i}}) = 1$] f_i :

$$(120) \quad f_0(\mathbf{x}_b, t + \Delta t) = f_0^*(\mathbf{x}_b, t) + \sum_{i=0}^{q-1} [s_s(\mathbf{x}_b + \mathbf{e}_i) f_i^*(\mathbf{x}_b, t) - s_s(\mathbf{x}_b + \mathbf{e}_{\bar{i}}) f_{\bar{i}}(\mathbf{x}_b, t + \Delta t)].$$

Eq.s. (118), (119) and (120) constitute a modified IBB that pre-corrects mass leakage by embedding a body force component, including a wetting state descriptor, constituting the Unidirectional-Coupled Boundary-Wettability scheme (U-CBW). Note that if $q_i(\mathbf{x}_b) = 0.5$, the U-CBW reduces to the Halfway Bounce-Back (HBB):

$$(121) \quad f_{\bar{i}}(\mathbf{x}_b, t + \Delta t) = f_i^*(\mathbf{x}_b, t),$$

which is intrinsically mass-conserving.

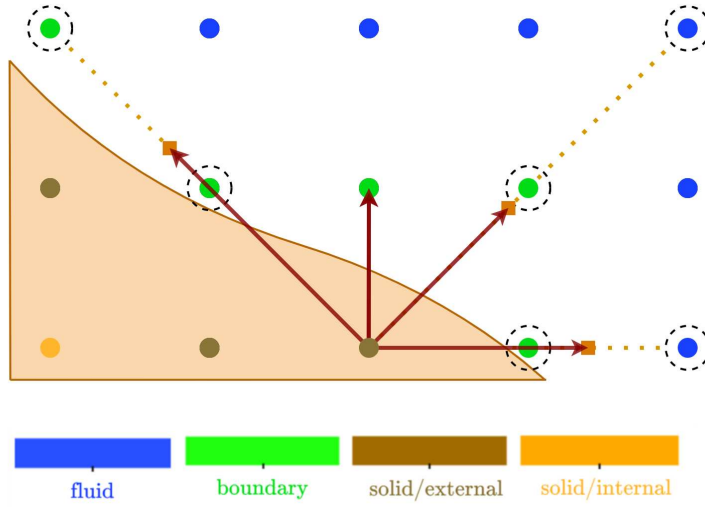


FIGURE 24. Virtual pseudopotential model averaging near an arbitrarily shaped curved boundary in a D2Q9 implementation. The averaging rays terminate on either off-lattice ($\square$) or on-lattice ($\bullet$) sites. The corresponding directional contributions are computed using Eq. (123).

An additional advancement for U-CBW involves enhancing the sensitivity of the Peng virtual pseudopotential to accurately detect the position of the real wall by adopting information related to the IBB. In the E4 case, Eq. (113) is reformulated as

$$(122) \quad \psi_{\text{avg}}(\mathbf{x}, t) = \frac{\sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) \omega(\|\mathbf{e}_i\|^2) \bar{\psi}_i(\mathbf{x}, t)}{\sum_{i=0}^{q-1} s_f(\mathbf{x} + \mathbf{e}_i) \omega(\|\mathbf{e}_i\|^2)}, \text{ with } \mathbf{x} \in \mathcal{D}_s.$$

where the $\bar{\psi}_i$ is a *fictitious pseudopotential* for the i -th direction, computed as

$$(123) \quad \bar{\psi}_i(\mathbf{x}, t) = \left[\frac{1}{2} + q_i(\mathbf{x} + \mathbf{e}_i) \right] \psi(\mathbf{x} + \mathbf{e}_i, t) + \left[\frac{1}{2} - q_i(\mathbf{x} + \mathbf{e}_i) \right] \psi(\mathbf{x} + 2\mathbf{e}_i, t), \text{ with } \mathbf{x} \in \mathcal{D}_s.$$

The $\mathbf{e}_i$ -related averaging ray points at the off-lattice site $\mathbf{x}_t \in \mathcal{D}$ which, in case of $q_i(\mathbf{x} + \mathbf{e}_i) \in (0, 1/2]$, locates on the link connecting a boundary and a fluid node, thus Eq. (123) prescribes an interpolation. Instead, if $q_i(\mathbf{x} + \mathbf{e}_i) \in (1/2, 1]$, $\mathbf{x}_t \in \mathcal{D}$ locates on the link connecting a solid and a boundary node, thus Eq. (123) prescribes an extrapolation (Figure 24).

As with Eq. (123), two-way explicit information exchange is formulated between the corrected IBB and the modified virtual pseudopotential model. This approach, termed the Bidirectional-Coupled Boundary-Wettability (B-CBW) scheme, recovers the Peng model with HBB as $\bar{\psi}_i(\mathbf{x}, t) = \psi(\mathbf{x} + \mathbf{e}_i)$, when a stair-case approximation is adopted.

Within the cascaded-entropic framework, the directional correcting term in Eqs (119) and (118) is computed in accordance with the consistent forcing scheme in Eq. (64), as:

$$(124) \quad |R_i\rangle = \mathbf{M}^{-1}\mathbf{N}^{-1}|\tilde{K}_i^R\rangle.$$

2.4.1. Note on the order of accuracy. For single-phase flows, the cascaded LBM with fixed relaxation rates and consistent forcing retains second-order accuracy under diffusive scaling ($\Delta t \propto \Delta x^2$, $\text{Ma} \ll 1$), as verified through mesh-refinement studies on canonical flows [158]. To the best of our knowledge, explicit convergence data are not available for entropic-CLBM formulations, although near equilibrium they reduce to their fixed-relaxation counterparts. Concerning boundaries, the interpolated bounce-back scheme of Bouzidi et al. imposes no-slip conditions on off-lattice walls with second-order spatial accuracy [147]. Considering diffuse-interface pseudopotential LBM, however, the observed convergence depends on how the interfacial thickness and interaction parameters are rescaled with grid refinement; in practice, discretization and modeling errors in the interface and contact-line regions may dominate the asymptotic behavior [159]. Consequently, in multiphase wetting simulations, the global convergence rate is expected to be at most second order and may be effectively reduced by interfacial and boundary coupling effects, which motivates validation through established physical benchmarks rather than an asymptotic order assessment.

3. The computational approach

The governing equations are sequenced in a fully-parallel algorithm and implemented in modern Fortran, adopting the Message Passing Interface (MPI).

3.1. Bites of parallel computing. Parallel computing comprises paradigms that enable the simultaneous execution of multiple operations. Practically, this ensures faster simulations or, at fixed wall time, larger physical domains, higher accuracy, and higher-fidelity modeling of physical phenomena. Parallelism is expressed hierarchically at three main levels:

- i **CPU:** In-core vectorization via Single Instruction, Multiple Data (SIMD) units. Regular, contiguous memory access patterns from loops trigger automatic vectorization, thus enabling the simultaneous application of one instruction to multiple data elements.
- ii **Shared Memory:** On a single node, individual cores share the same memory address space and handle different loop chunks independently, with tools such as OpenMP.

- iii **Distributed Memory:** On High Performance Computing (HPC) clusters, each process owns a portion of the domain and exchange data at the boundary using point-to-point or neighborhood collective *halo/ghost* communications. At this level, MPI is the de facto standard.

The shared-memory parallelization suffers from limited total memory bandwidth, which is highly detrimental to the parallel efficiency of memory-intensive algorithms, such as LBM. The most effective strategy for such applications is to leverage solely CPU-level vectorization and distributed memory decomposition, the top and bottom levels of the hierarchy.

The combination of Fortran and MPI dates back to the mid-1990s, e.g. with the reimplement of a standard HPC test suite, the NAS Parallel Benchmarks [160].

Fortran perfectly fits the requirements for scientific calculus workloads, as it efficiently handles dense, multi-dimensional column-major arrays and, by default, enforces no-aliasing semantics: distinct dummy arguments do not alias unless explicitly declared with `pointer/target`. This enables aggressive loop transformations—fusion, tiling, vectorization, and prefetching, key for stencil codes with regular memory access [161].

MPI offers explicit message passing, Cartesian process topologies, and mature, vendor-optimized, standards-backed scalability on distributed-memory systems. The sustained use of Fortran+MPI for LBM at scale is well documented in scientific and technical literature [162].

3.2. Code Implementation. In the Fortran-MPI implementation of the LBM code, the 3D cartesian communicator is built by adopting the command `MPI_Cart_create`.

The computational domain of size xg, yg, zg , respectively the number of grid points on the x, y, z axes, is partitioned by prescribing the number of processes in each direction, as `dims=(nx,ny,nz)`. To reduce the communication overhead, one should prefer nearly-cubic subdomains to minimize the surface-to-volume ratio, thus reducing the number of ghost nodes per unit volume. Local coordinates `xBMin:xBMax`, `yBMin:yBMax`, `zBMin:zBMax` are computed for each rank and gathered to rank 0 for bookkeeping and coordinate I/O. Periodicity flags `x_per, y_per, z_per` activate toroidal or bounded topologies. The neighboring relationship between processes is queried by means of `MPI_Cart_shift`. In the case of non-periodic boundaries, the corresponding surfaces are set to `MPI_PROC_NULL`. Fields are allocated as integer and double precision, in column-major arrays, with up to two ghost point layers in every direction (e.g. `...xBMin-2:xBMax+2, ...`).

The halo-exchange follows a synchronous just-in-time (JIT) policy, which is a demand-driven approach: ghost data are communicated immediately before the kernels that consume them. The term 'synchronous' reflects the use of `MPI_Sendrecv`, a single, blocking call that both sends and receives data logically at the same time. Such a command avoids classic deadlocks from the separate implementation of `MPI_Send` and `MPI_Recv` and ensures deterministic behavior in the code.

Non-local, domain-wide quantities are handled by `MPI_Gather`, which collects data from all ranks and locates it contiguously on a root one, and `MPI_Allreduce`, which performs a reduction operation (e.g. sum, min, max, ...) across all ranks and returns the results to all of them, providing information about global quantities.

Below is a concise pseudocode in which ghost communications are assumed to be implicit and respect the mentioned JIT policy.

A. Setup of the MPI environment and LBM structure

-build 3D cartesian topology and get rank coordinates;
 -allocate $f_i, \rho, \mathbf{u}, \psi, p, \dots$ and other fields;
 -construct the geometry and prepare .stl files;
 -tag fluid, boundary and solid nodes and cut-link distance q ;
 -select $\{\mathbf{e}_i, w_i\}$, force stencil, matrices $\mathbf{M}$ and $\mathbf{M}^{-1}$

B. Initialization

for $i=0:n_points$ [compute $|f_i^{eq}\rangle$ by $\rho_0, \mathbf{u}_0$, assign $|f_i\rangle \leftarrow |f_i^{eq}\rangle$,
 compute $\mathbf{F}_u$, write variables to disk]

C. Time-stepping loop

while $t < t_{max}$ or *condition* is satisfied

C1. Computation of macroscopic variables

for $i=0:n_points$ [compute $\mathbf{F}_u, \rho, \mathbf{u}, p, \psi$ and save to disk]

C2. Collision

for $i=0:n_points$ [compute $\mathbf{N}, \mathbf{N}^{-1}, |\tilde{K}_i^R\rangle, |\tilde{K}_i^{eq}\rangle, \gamma^*$, thus $|f_i^*\rangle$]

C3. Streaming and imposition of BCs

for $i=0:n_points$ [impose $|f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t)\rangle \leftarrow |f_i(\mathbf{x}, t)\rangle$ and
 construct missing f_i by the CBW scheme

$t \leftarrow t + \Delta t$

end while

-Deallocate fields;

CHAPTER 4

Testing and results

Both cohesive and adhesive phenomena are validated through dedicated tests within a discrete cubic domain $\mathcal{D}_f$, by investigating the behavior of a single droplet of liquid immersed in its own vapor.

The initial density field is prescribed as

$$(125) \quad \rho(\mathbf{x}, 0) = \frac{\rho_l + \rho_v}{2} - \frac{\rho_l - \rho_v}{2} \tanh \left[\frac{d(\mathbf{x})}{W} \right],$$

where the hyperbolic tangent profile ensures a smooth transition from ρ_l to ρ_v within a diffused interface of thickness $W > 0$ to prevent numerical instabilities due to a steep $\nabla \psi$, and $d(\mathbf{x})$ is defined depending on the intended shape of the droplet at $t = 0$.

In the case of a diffuse spherical/hemispherical droplet:

$$(126) \quad d(\mathbf{x}) = 2(|\mathbf{x} - \mathbf{x}_0| - r_0)$$

being $\mathbf{x}_0 \in \mathcal{D}_d$ and $r_0 > 0$ the location of the center of the droplet and the initial droplet radius, respectively.

The kinematic viscosity $\nu : \mathcal{D}_f \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is defined locally as a density-dependent linear interpolation between vapor and liquid values:

$$(127) \quad \nu(\mathbf{x}, t) = \nu_v + (\nu_l - \nu_v) \frac{\rho(\mathbf{x}, t) - \rho_v}{\rho_l - \rho_v},$$

where $\nu_v = 1/6 \approx 0.1666$, $\nu_l = 1/30 \approx 0.0333$. These values ensure dynamic viscosity matching across interfaces.

The maximum spurious currents module is defined, for a quiescent fluid, as:

$$(128) \quad u_{sp} = \max_{\mathbf{x} \in \mathcal{D}_f} |\mathbf{u}(\mathbf{x})|.$$

1. Validation of the cohesion physics

The test results discussed in this section stem from the article *On the effect of force isotropy in a multiphase cascaded lattice Boltzmann scheme with entropic stabilization*, coauthored by Marco Desiderio Loffredo Senesi, Prof. Alessandro Coclite, and Prof. Eng. Michele Dassisi, published on *Computers & Mathematics with Applications* [163].

The entropic inner product is computed by Eq. (92).

TABLE 5. Equilibrium properties of water at selected temperatures

T_r	$\rho_{l,r}$	$\rho_{v,r}$	DR
0.97	1.725	$3.904 \cdot 10^{-1}$	4.417
0.95	1.880	$2.969 \cdot 10^{-1}$	6.333
0.90	2.150	$1.672 \cdot 10^{-1}$	12.86
0.85	2.347	$9.780 \cdot 10^{-2}$	24.00
0.80	2.506	$5.635 \cdot 10^{-2}$	44.47
0.75	2.644	$3.047 \cdot 10^{-2}$	86.78
0.70	2.755	$1.596 \cdot 10^{-2}$	172.7
0.65	2.855	$7.419 \cdot 10^{-3}$	384.8
0.60	2.941	$3.002 \cdot 10^{-3}$	979.6
0.55	3.013	$1.011 \cdot 10^{-3}$	2979

Both static and dynamic tests are performed on a discrete cubic domain set with periodic boundary conditions.

Parameters of the equation of state are set as $\theta_v = 0.64c_s^2$, $\theta_m = -0.02c_s^2$, $\theta_l = c_s^2$.

All tests are conducted by employing E4, E6 and E8 force weights and stencils, each case being henceforth denoted as Em, with $m = 4, 6, 8$.

The coexistence curve of water is reconstructed; its reduced thermodynamic properties [164] are reported in Table 5, where $T_r = T/T_c$ and $\rho_r = \rho/\rho_c$ are the critical temperature and density, respectively, being T_c and ρ_c .

1.1. Static droplet test. A static droplet test is performed on $\mathcal{D}_f$ with a size of $N = 100$ to assess both the effect of spurious currents and the thermodynamic consistency of the model.

A spherical droplet is initialized by adopting Eq.s (125)-(126), setting $\mathbf{x}_0$ as the center of the discrete domain, also $r_0 = N/4$ and $W = 5$ with $\lambda = 0$.

The influence of the force tuning coefficient β on the spurious current magnitude u_{sp} is investigated.

An initial parametric study is performed at $m = 8$, as analytical evidence suggests this configuration to be the most favorable for ensuring stability down to the lowest T_r within the range of interest [132, 133]. The set $\beta \in \{0, 1, 2, 3, 4\}$ is investigated, thus extending the literature results [135, 137, 165, 166].

β	0	1	2	3	4
$T_{r,min}$	0.85	0.75	0.55	0.55	0.55
u_{sp}	8.79E-4	4.00E-3	9.97E-4	5.88E-2	8.22E-2

TABLE 6. Minimum stable T_r and related u_{sp} for selected β at $m = 8$.

Notably, the individual effects of $\mathbf{F}^{(k)}$ and $\mathbf{F}^{(o)}$ are isolated and analyzable for $\beta = 0$ and $\beta = 1$, respectively. The results presented in Table 6 reveal a convex trend, with the most promising performance for $\beta = 2$.

A subsequent golden section search is performed around this value at $T_r = 0.55$, showing that u_{sp} is minimized at $\beta \approx 2$, making this setting highly relevant and thus considered in further analyses.

A qualitative analysis of spurious currents is proposed at $\beta = 2$ and $T_r = 0.8$.

A cross-section of the droplet, cut by a plane normal to the z-axis and containing $\mathbf{x}_0$, is displayed in Figure 25. The symmetry of the system allows us to represent, respectively, the density profile (Figure 25a) and the $\mathbf{u}$ projection at E4 (Figure 25b), E6 (Figure 25c), and E8 (Figure 25d) on distinct quadrants. Independently of the selected Em, multiple sets of counter-rotating structures are observed, manifesting circular or elliptical patterns. In E4, intense spurious currents manifest on the internal side of the diffuse interface, reducing towards the first and second sets of external structures, the latter covering a wider area. In the E6 case, both internal and external sets of vortices are observed, which are spread out and less pronounced compared to the critical ones in E4. Finally, E8 results in similar but scaled down current structures compared to E6.

A quantitative analysis is now proposed (Figure 26) over $\beta \in \{0, 1, 2\}$ and the entire T_r set for $m = 4, 6, 8$.

Focusing on E4 (Figure 26a), both $\beta = 0$ and $\beta = 1$ result in unsatisfactory performances, displaying stable behavior only down to $T_r = 0.85$, with the second option resulting in a scaled down u_{sp} trend. Spurious currents are severely reduced at $\beta = 2$, enabling to reach $T_r = 0.6$, its u_{sp} being close to the $\beta = 1$ result at $T_r = 0.85$. Furthermore, u_{sp} shows limited sensitivity to T_r in the wide range between $T_r = 0.9$ and $T_r = 0.65$.

The E6 results (Figure 26b) at $\beta = 0$ and $\beta = 1$ manifest the same trend hierarchy as in the E4 case, though $\beta = 1$ enables the achievement of a lower stable reduced temperature ($T_r = 0.75$).

The u_{sp} trend at optimal β presents a steady increase down to $T_r = 0.55$, differing from the corresponding E4 results.

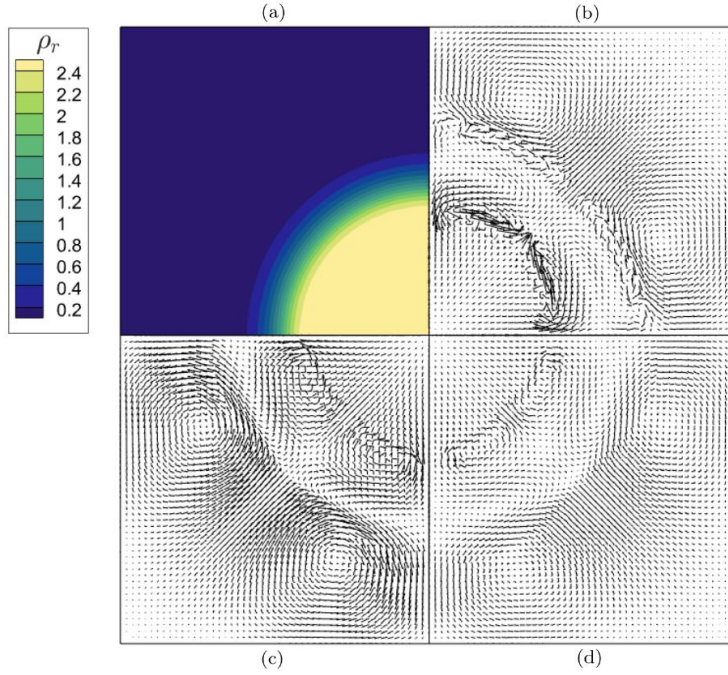


FIGURE 25. Cross section of the droplet at $\beta = 2$ and $T_r = 0.8$ displaying (a) the density profile and the spurious currents projection in the (b) E4, (c) E6 and (d) E8 case.

The implementation of the E8 stencil and weights (Figure 26c) results in a similar but scaled down u_{sp} trend pattern compared to the E6 case.

Regardless of the selected Em, at high T_r , the u_{sp} values at $\beta = 1$ are comparable to those at the more computationally demanding $\beta = 2$. However, at intermediate and low T_r , increasing β in the selected range results in a significant reduction in u_{sp} .

At $\beta = 0$ and $\beta = 1$, spurious currents are reduced by increasing the isotropy order. Spurious current data are compared at $\beta = 2$ (Figure 26d).

From the critical point down to $T_r = 0.8$, E4 performs visibly worse than E6 and E8; the latter two present almost overlapping values of u_{sp} . Towards intermediate T_r , the E6 curve presents a steep increment, resulting in the highest u_{sp} values from $T_r = 0.7$ downward.

The E8 curve displays the most satisfactory results, minimizing u_{sp} over the entire T_r set, achieving $u_{sp} \approx 9.97 \cdot 10^{-4}$ l.u. at $T_r = 0.55$.

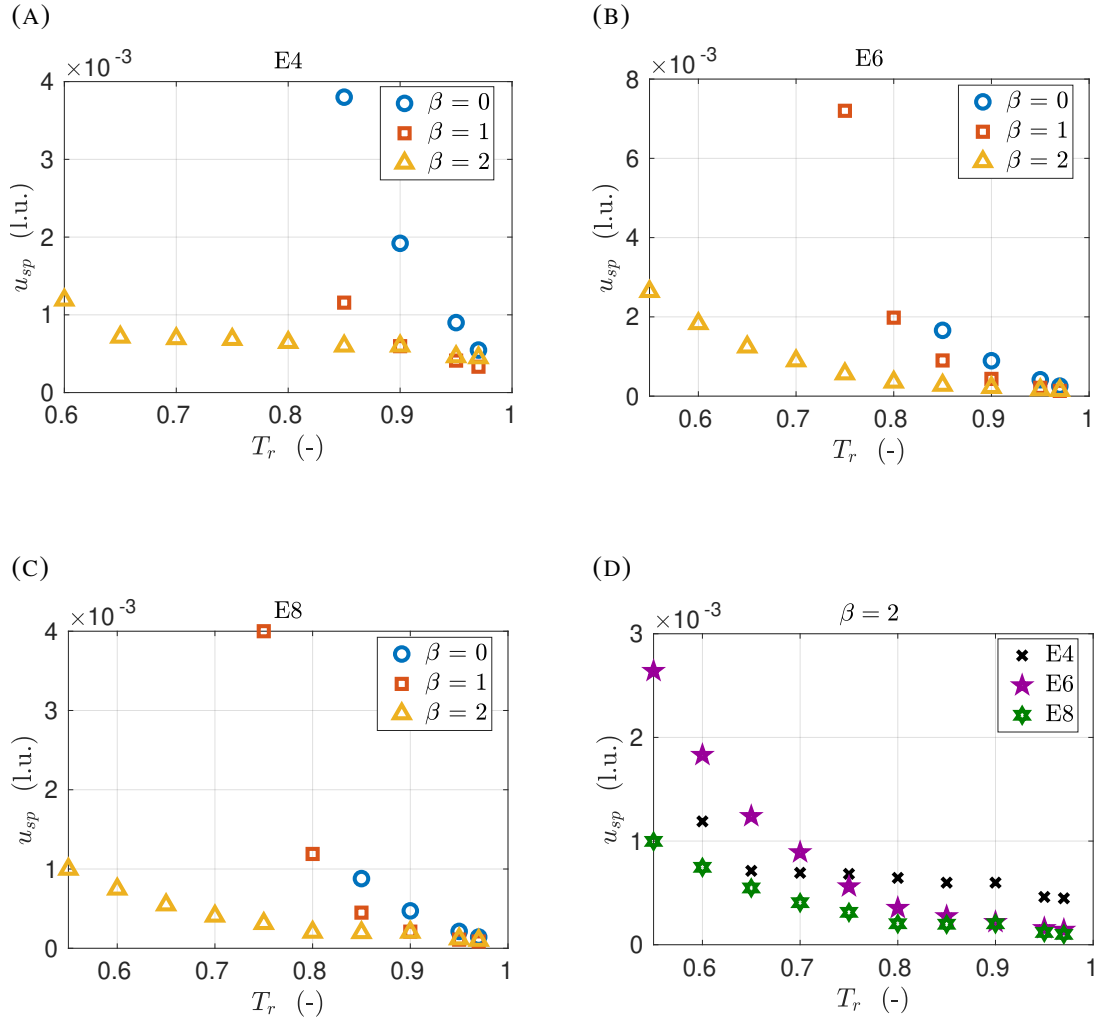


FIGURE 26. Maximum spurious current magnitude vs reduced temperature for (a) E4, (b) E6, (c) E8 cases at different β and (d) comparison among Em at $\beta = 2$.

Thermodynamic consistency is assessed for $\beta = 2$ (Figure 27) by comparing theoretical data (Table 5) and numerical results. An inspection of both vapor and liquid branches (Figure 27a) suggests highly consistent results down to the lowest stable T_r .

From intermediate to low T_r , the high steepness of the theoretical vapor branch results in tightly clustered data close to $\rho_r = 0$. A focused representation is thus provided in Figure 27b, supporting the claim of high thermodynamic consistency at different Em cases.

1.2. Laplace test. In the pseudopotential method, the surface tension $\sigma \in \mathbb{R}_+$ spontaneously emerges as a result of the peculiarities of the interaction force.

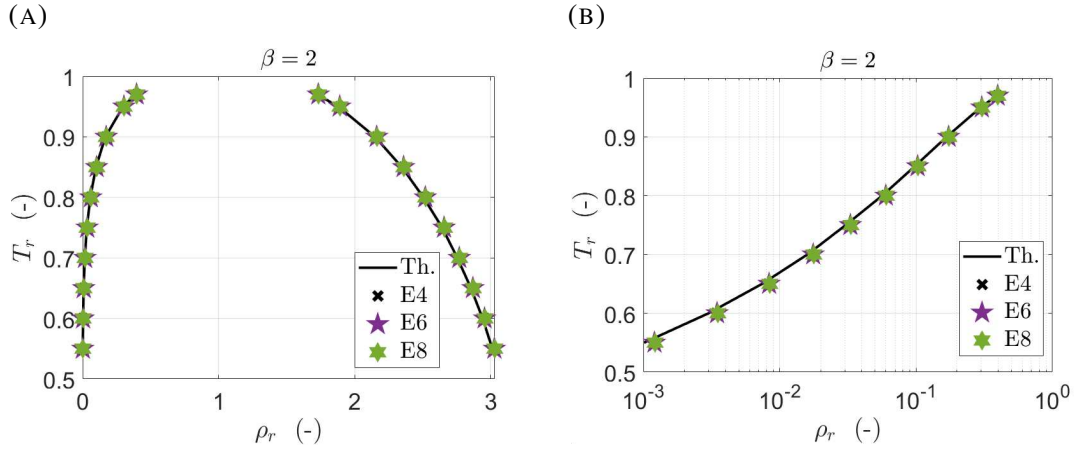


FIGURE 27. Verification of thermodynamic consistency by (a) coexistence curves comparison between theoretical values and E4, E6, E8 cases and (b) a focus on their vapor branch at optimal $\beta = 2$.

The Young-Laplace law in Eq. (27) holds for a zero-thickness interface, where a discontinuity in normal stress is present. The pseudopotential method, however, is characterized by a diffuse interface between phases, resulting in a smooth transition in physical properties across the interface width. The radius $r = |\hat{\mathbf{x}} - \mathbf{x}_0|$ is hence computed such that

$$(129) \quad \rho(\hat{\mathbf{x}}) = \frac{\rho_l^{eq} + \rho_v^{eq}}{2},$$

where $\hat{\mathbf{x}} \in \mathcal{D}$ is a linearly interpolated point that satisfies the equation above.

Both p_{in} and p_{out} are measured far enough from the diffuse interface, where $|\nabla p| \approx 0$.

Figure 28 displays σ ($r_0 = N/4$, $N = 100$, $\beta = 2$, $\lambda = 0$) as a monotonically decreasing function of T_r for all the Em cases, in accordance with experimental and theoretical predictions [167].

Surface tension increases with m across the entire range of reduced temperatures.

Higher σ leads to a steeper $\nabla \psi$, resulting in increased u_{sp} at fixed m and T_r .

Notably, the E8 implementation minimizes u_{sp} despite exhibiting the highest σ values; this corroborates its superiority over the E4 and E6 cases, particularly at low T_r .

A Laplace test is performed on selected r_0 and T_r , imposing $\beta = 2$ (Figure 29).

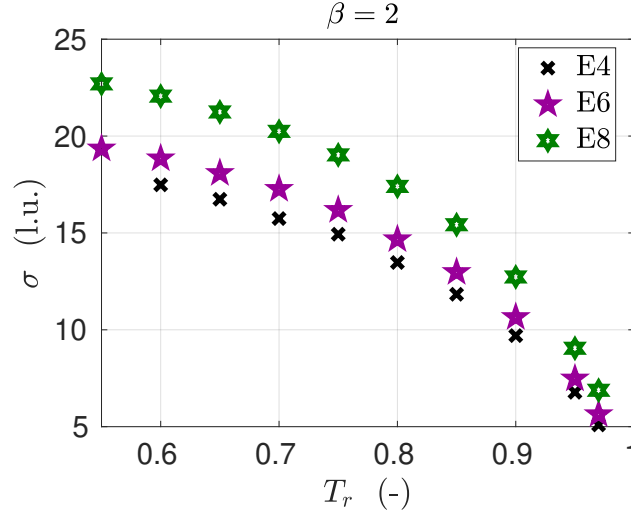


FIGURE 28. Numerical results of surface tension spanning selected T_r values for E4, E6 and E8 cases

A linear dependence between Δp and $2/r$ could be qualitatively appreciated for the E4 (Figure 29a), E6 (Figure 29b), and E8 (Figure 29c) cases by examining the corresponding plots.

Quantitative results are summarized in Table 7, showing satisfactory coefficients of determination (R^2) at each m investigated, with the highest R^2 occurring at $T_r = 0.65$ for E6.

An analysis of the fitted surface tension (σ_f), derived as the slope of the linear regression, confirms a scale up in σ trends as m increases.

An additional test is conducted on E8 at $T_r = 0.55$ setting $\lambda \neq 0$ (Figure 29d).

The tuning capability of the forcing term $\mathbf{F}^{(l)}$ allows for both increasing and decreasing σ at high DR while complying with the Young-Laplace law, from $\sigma_f = 22$ l.u. ($\lambda = 0$) to $\sigma_f = 27.2$ l.u. ($\lambda = -1$) with $R^2 = 0.9998$ and $\sigma_f = 17.56$ l.u. ($\lambda = 1$) with $R^2 = 0.9988$.

TABLE 7. Laplace test linear fitting data at $\beta = 2$.

T_r	0.95			0.8			0.65		
m	4	6	8	4	6	8	4	6	8
σ_f (l.u.)	6.469	7.1353	8.5291	13.033	14.223	16.74	16.144	17.588	20.579
R^2	0.999	0.9989	0.9984	0.9993	0.9993	0.9991	0.9991	0.9994	0.9991

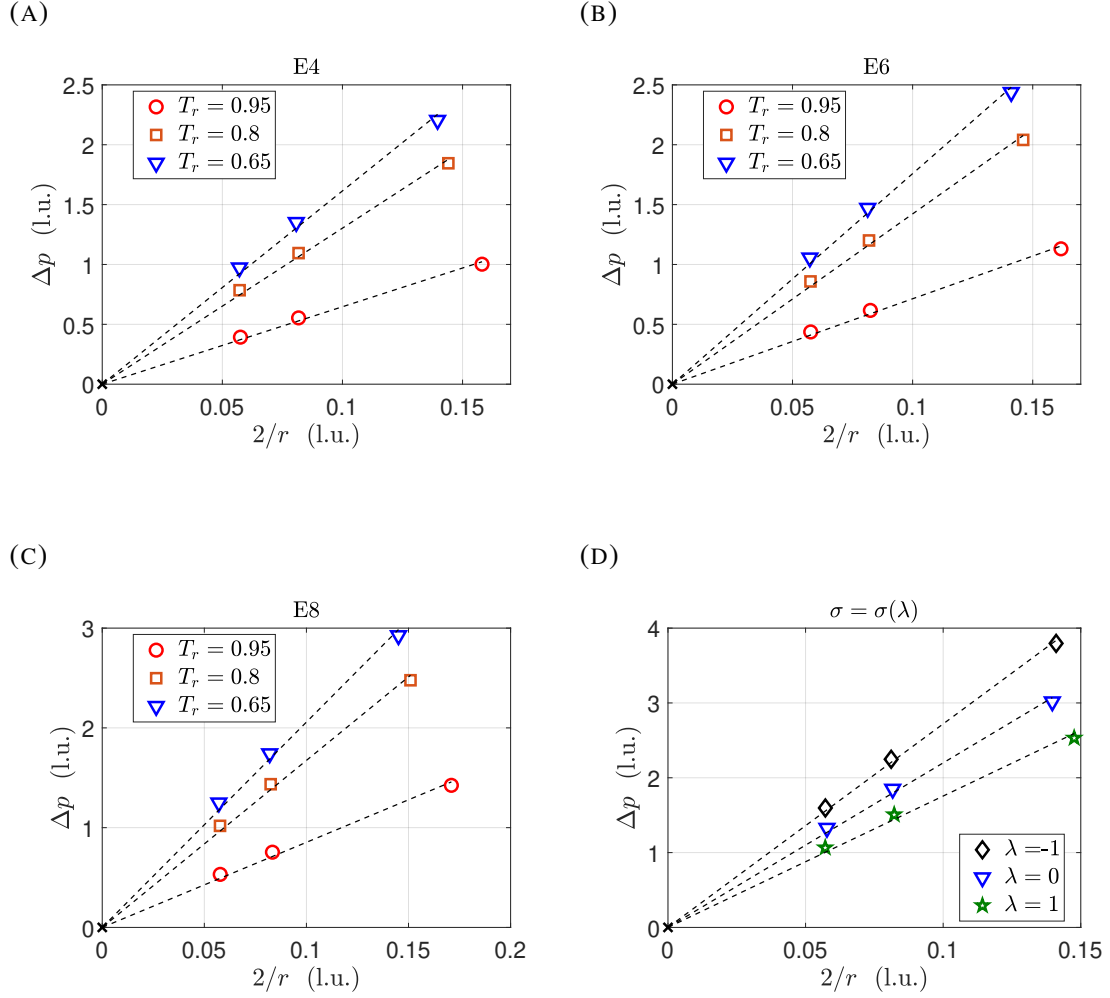


FIGURE 29. Laplace test at (a) E4, (b) E6, (c) E8 setting $\beta = 2$ and (d) focus on σ tuning by λ at E8, $T_r = 0.55$

1.3. Droplet oscillation test. The phenomenon of a liquid droplet freely oscillating in its own vapor is investigated as a dynamic test. Considering an initially deformed configuration, the surface tension between phases acts as a restoring force towards the droplet spherical shape, while the viscosity of both the internal and external fluids dampens the oscillations.

In the case of small amplitudes, its free-surface shape deviation from equilibrium is expressed as a linear combination of independent normal modes. For $n = 2$, the droplet is a spheroid oscillating between prolate and oblate configurations (Figure 30).

The transient behavior of the interface could be approximated by a damped harmonic oscillator. In the most general case, though, the oscillation frequency is time dependent, shifting from an initial (ω_{n0}) to an asymptotic value ($\omega_{n,\infty}$).

An expression for ω_{n0} is adopted as a reference, accounting for the dynamic effects of both inner and outer fluids. For the n^{th} oscillation mode [168]:

$$(130) \quad \omega_{n0}^2 = \frac{n(n+1)(n-1)(n+2)}{n\rho_v + (n+1)\rho_l} \frac{\sigma}{r_d^3},$$

being r_d the rest radius of the droplet.

In the damped harmonic oscillator approximation, one finds its natural frequency by [169]

$$(131) \quad \omega_n = \omega_{n0} - \frac{1}{2}\alpha(\omega_{n0})^{\frac{1}{2}} + \frac{1}{4}\alpha^2,$$

$$(132) \quad \alpha = \frac{(2n+1)^2(\mu_l\rho_l\mu_v\rho_v)^{\frac{1}{2}}}{\sqrt{2}r_d[n\rho_v + (n+1)\rho_l] [\sqrt{\mu_l\rho_l} + \sqrt{\mu_v\rho_v}]}.$$

The case $n = 2$ is considered; a diffuse interface spheroid is initialized by imposing:

$$(133) \quad d(\mathbf{x}) = 2 \left[\frac{(x-x_0)^2}{a_x} + \frac{(y-y_0)^2}{a_y} + \frac{(z-z_0)^2}{a_z} - 1 \right] r_0,$$

being z the symmetry axis, $a_x = a_y$, and r_0 the radius of an equal volume sphere.

The normalized droplet radius is defined as

$$(134) \quad \tilde{r}_\alpha(t) = \frac{r_\alpha(t) - r_d}{r_d},$$

α being h or v respectively for horizontal (xy plane) and vertical (z axis) radii of the spheroid. Tests are conducted at $a_x = 0.8a_z$, $N = 200$, $r_0 = N/8$ at E4, E6 and E8 for

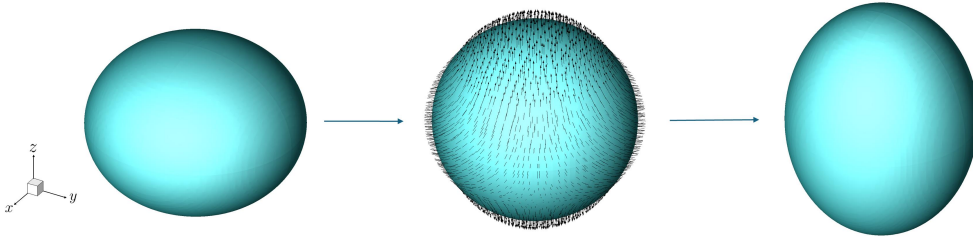


FIGURE 30. Droplet relaxation towards equilibrium at $n = 2$ in the prolate to oblate half-period.

The elastic potential energy is converted in kinetic energy, with local maxima in the spherical configuration. Test case at $m = 8$, $T_r = 0.55$ and $\lambda = -1$.

$T_r = 0.65$ and at E8, $T_r = 0.55$ for $\lambda \in \{-1, 0, 1\}$.

A qualitative analysis of the numerical results suggests that both radii evolve over time with a damped oscillatory behavior for $m = 4, 6, 8$ (Figure 31a-c).

The conservation of droplet volume implies both a quadratic relationship between vertical and horizontal radii and that the intersection between $\tilde{r}_h$ and $\tilde{r}_v$ occurs at their null values. Both conditions are verified at E4 and E6, while the slight initial offset present at E8 is recovered in its second oscillation period.

The impact of surface tension on the oscillation frequency is observed through visual inspection, increasing with m . At fixed $m = 8$ and $T_r = 0.55$, a test on σ tuning by λ proves compliance with theoretical trends even at high DR (Figure 31d).

A quantitative analysis is also conducted (Table 8), comparing theoretical ω_{n0} and ω_n with the corresponding numerical results $\hat{\omega}_{n0}$ and $\hat{\omega}_n$, the latter computed as an averaged quantity over the first two periods.

The relative errors, respectively $\varepsilon_{\omega_{n0}}$ and ε_{ω_n} , both decrease with m , corroborating the superiority of E8, its maximum relative error being below 2% on ω_{n0} .

From λ tuning, it appears that accuracy is improved at low surface tension values, reaching a minimum below 0.4% on ω_{n0} .

The deviation from theoretical results is interpreted as a result of the oscillation amplitude being not negligible compared to r_d ; additionally, both the adoption of linear interpolation to reconstruct the surface radii and the effect of the periodic boundary conditions could play a role in determining the error. Regarding the last point, pressure waves would travel across the boundaries, interfering with the free oscillation of the droplet and acting as an external force.

Nonetheless, the experimental results are considered compliant with theoretical predictions, both qualitatively and quantitatively.

TABLE 8. Theoretical and numerical values of droplet oscillation frequencies (in 10^{-3} l.u.)

T_r	case	σ	ω_{n0}	ω_n	$\hat{\omega}_{n0}$	$\hat{\omega}_n$	$\varepsilon_{\omega_{n0}} \%$	$\varepsilon_{\omega_n} \%$
0.65	E4	16.14	2.991	2.989	2.879	2.879	3.740	3.648
	E6	17.59	3.122	3.119	3.056	3.006	2.109	3.608
	E8	20.58	3.376	3.372	3.430	3.377	1.607	0.1544
0.55	$\lambda=-1$	27.20	3.778	3.776	3.644	3.631	3.527	3.859
	$\lambda=0$	21.99	3.968	3.958	3.312	3.278	2.496	3.456
	$\lambda=1$	17.56	3.056	3.052	3.025	3.007	0.3484	0.9314

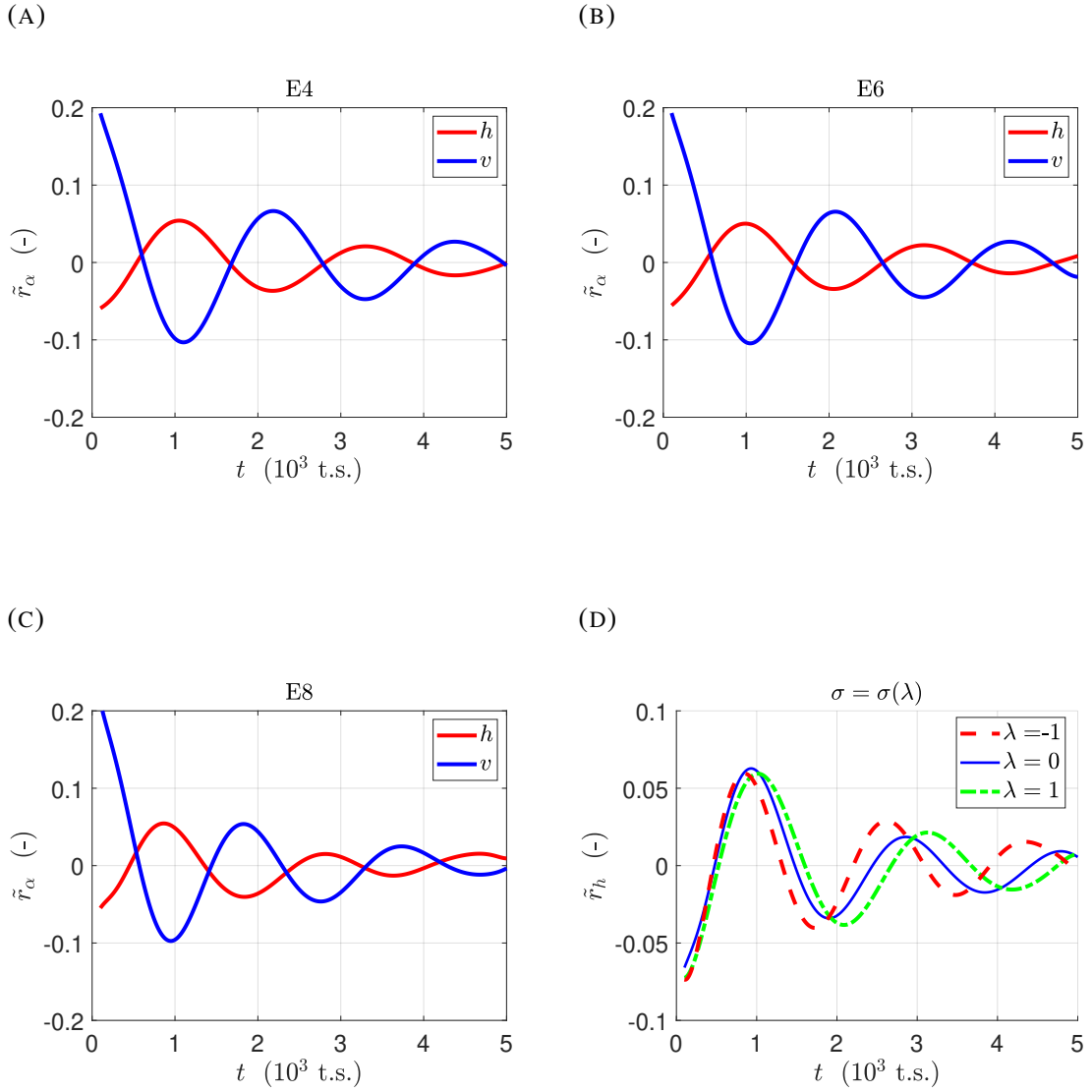


FIGURE 31. Evolution of droplet normalized radii over time at $T_r = 0.65$ in the (a) E4, (b) E6 and (c) E8 cases and (d) focus on σ tuning by λ at E8, $T_r = 0.55$

2. Validation of the wetting physics

The assessment is now extended to the unified adhesive-cohesive formulation through a comprehensive testing campaign. The entropic inner product is computed by Eq. (93). In the piecewise equation of state, $\theta_v = 0.64c_s^2$ and $\theta_l = c_s^2$. For $m = 4$, the choice $\theta_m = -0.02c_s^2$ induces a reference surface tension σ_0 . For $m = 8$, θ_m is iteratively adjusted to match σ_0 .

TABLE 9. Neutral wetting test results at $q_z = 0.5$ and $DR = 25$.

m	β	$\Delta M_{\sigma\%}$	$\varepsilon_{s\sigma\%}$	$u_{sp} [10^{-3} \text{ l.u.}]$
4	1	0.009	-0.62	1.3
	2	-0.004	-0.002	0.67
8	1	0.003	0.56	0.41
	2	0.017	0.05	0.37

The test results discussed in this section stem from the manuscript *A cascaded-entropic lattice Boltzmann method for wettability control on off-grid surfaces via coupled boundary-force interpolation*, coauthored by Marco Desiderio Loffredo Senesi, Prof. Alessandro Coclite, Prof. Dr. Ingenuin Gasser and Prof. Eng. Michele Dassisti, currently under review in *Computers & Mathematics with Applications* [170].

2.1. Wetting on flat walls. As a first case, the wetting behavior of a liquid droplet, surrounded by its vapor, on a flat surface under zero-gravity conditions is examined. As such, a cubic domain is set with $N = 100$ nodes per side; periodic boundary conditions are imposed along the x and y axes. The domain is bounded by flat walls set normal to the z axis. Their location is parameterized by the link fraction $q_z \in (0, 1]$ such that $q_i(x, y, 0) = q_z$ when $e_{iz} = -1$ (bottom lid) and $q_i(x, y, N - 1) = q_z$ when $e_{iz} = 1$ (top lid). The droplet is initialized as a diffuse-interface hemisphere by Eq.s (125)-(126). The base of the half-droplet lies on the off-lattice bottom wall, thus (Figure 32):

$$(135) \quad \mathbf{x}_0 = (N/2, N/2, -q_z).$$

Two additional performance indicators are introduced:

(1) Relative mass leakage:

$$(136) \quad \Delta M_{\sigma\%} = 100 \cdot \frac{M_f - M_i}{M_i},$$

where $M_i = \sum_{\mathbf{x} \in \mathcal{D}_f} \rho(\mathbf{x}, 0)$ and $M_f = \sum_{\mathbf{x} \in \mathcal{D}_f} \rho(\mathbf{x}, t_{eq})$. $M_i = M(0)$ is the initial mass of the system and $M_f = M(t_{eq})$ is its settling value.

(2) Shape deviation:

$$(137) \quad \varepsilon_{s\sigma\%} = 100 \cdot \left| \frac{r_v - r_h}{r_0} \right|,$$

where r_v and r_h are the pseudo-vertical and pseudo-horizontal radii at equilibrium, estimated by linear interpolation at the location where $\rho = (\rho_v + \rho_l)/2$.

Initially, $q_z = 0.5$ (corresponding to the well-known HBB configuration) is considered for $DR = 25$, $\theta = 90^\circ$, and $m \in \{4, 8\}$. The parameter β is set equal to 1 and 2,

minimum u_{sp} shifts to $\theta = 135^\circ$. Increasing stencil size m reduces u_{sp} across the θ - R_σ parameter space, at the expense of slightly worsened mass conservation.

In Figure 33, the density field, as well as the magnitude and orientation of the interaction force, are displayed for $DR = 25$, under different stencils $m \in \{4, 8\}$ and wetting states $\theta \in \{45^\circ, 90^\circ, 135^\circ\}$. In each case, the liquid-vapour interface appears diffuse, particularly so for $m = 8$. The intensity of the force is proportional to the density gradient, reaching its highest value close to the mean-density region and fading to zero towards the bulk of each phase. Increasing the isotropy order ($m = 8$) broadens the annular region of significant $\|\mathbf{F}_u\|$ and lowers its peak value. This behavior is a direct consequence of the E8 smoother ρ field. Far from the contact region, force vectors direct towards the droplet center, balancing the Laplace pressure and ensuring mechanical equilibrium. Close to the contact region, however, the orientation reflects the wetting regime. For a hydrophilic wall, adhesion exceeds cohesion, resulting in a net attraction towards the surface. In the case of neutral wetting, adhesive and cohesive effects are balanced; the wall-normal force component vanishes, and vectors become tangential. This, combined with the no-slip halfway bounce-back, induces the wall surface to act as a symmetry plane. For a hydrophobic wall, cohesion prevails over adhesion, resulting in a net repulsive force. Here, the normal component at the wall is instead oriented towards the liquid phase.

The mass-corrected schemes (U-/B-CBW) are compared to the bare linear-IBB implementation for $DR = 25$, $\theta \in \{45^\circ, 90^\circ, 135^\circ\}$ and $q_z \in \{0.01, 0.3, 0.7, 0.99\}$. The linear-IBB manifests a severe violation of mass conservation in all the considered cases (Figure 34). The mass leakage profile for the hydrophilic ($\theta = 45^\circ$) wetting regime suggests a progressive and complete vanishing of the liquid phase. Under neutral wetting conditions, a short initial numerical transient manifests. This may possibly be related to a stabilization of the ψ -profile at the interface. Subsequently, mass steadily increases, following linear trends, with steeper slopes for $m = 4$. The mass violation is amplified at extreme q_z values. The wetting of off-grid hydrophobic surfaces ($\theta = 135^\circ$) induces a more severe mass increase, with distinct trends for intermediate and extreme values of q_z . The raw linear-IBB implementation is therefore unsuitable for accurate simulations, regardless of the wetting state of interest. Activating a simple refill on the rest population (hereafter f_{0r}) or the U-/B-CBW schemes would instead ensure mass conservation.

While controlling mass leakage is necessary to ensure physical consistency, it alone is not sufficient; the spatial distribution of phases within the system must also be

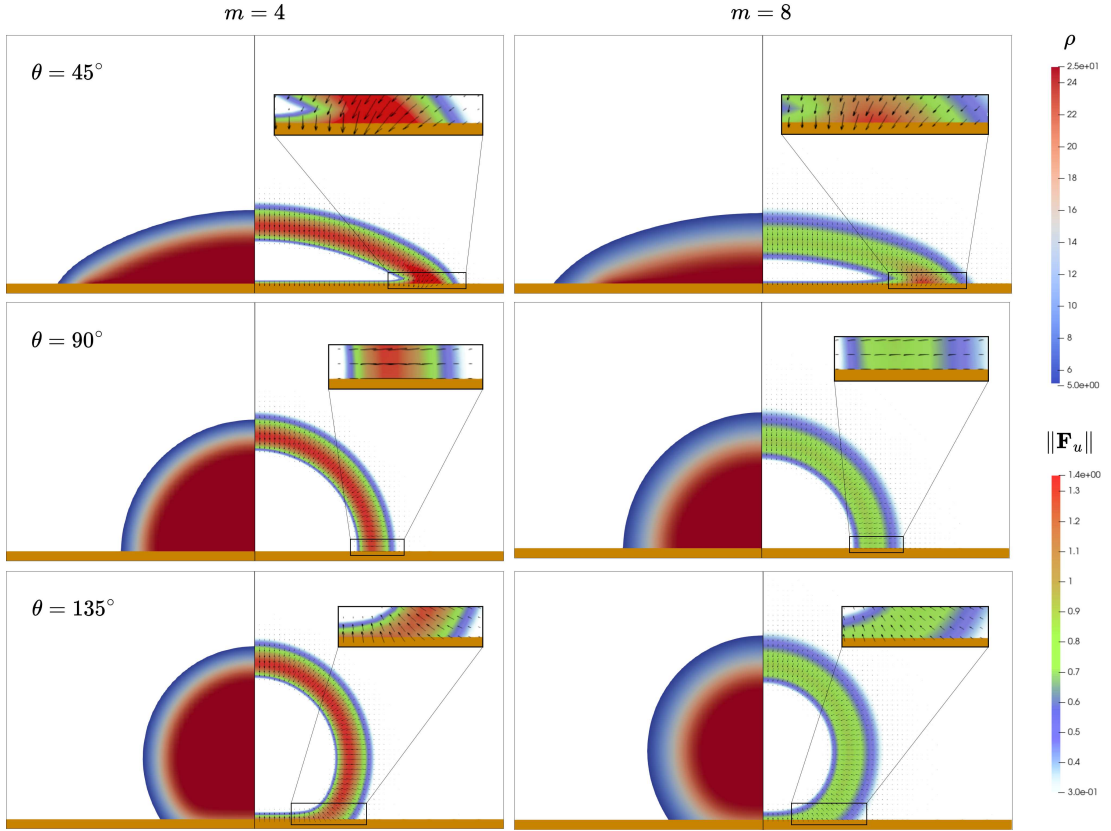


FIGURE 33. Contour plots of the density field and interaction force for different wetting states $\theta = 45^\circ$ (upper row), 90° (central row), and 135° (lower row), $DR = 25$, $m = 4$ (left), $m = 8$ (right) within the halfway bounce-back formulation.

carefully considered. Figure 35 shows the time evolution of droplet half-density iso-surfaces under different wetting conditions at moderate and extreme offsets from the HBB wall location, specifically for $q_z = 0.7$ and $q_z = 0.01$. For the latter case, the long-term behavior under the f_0r and B-CBW schemes is also presented. In the hydrophilic IBB case, rapid mass loss corresponds to a swift deflation of the initially hemispherical droplet, a phenomenon that worsens as the wall position deviates from the HBB condition. The f_0r scheme significantly overestimates surface wettability, causing the droplet to flatten into a liquid slab formed by coalescence induced by periodic boundary conditions. In contrast, the CBW schemes accurately reproduce the intended wetting behavior. On neutral wetting surfaces modeled with IBB, increasing deviation of q_z from the HBB condition leads to more pronounced shape distortions: the droplet expands and the contact angle increases over time. The equilibrium droplet shape predicted by the f_0r scheme diverges markedly from the physically correct hemisphere,

TABLE 10. Static test varying σ and θ in HBB wetting at $DR = 25$.

m	R_σ	θ [°]	$\Delta M_{\%}$	u_{sp} [10^{-3} l.u.]
4	0.75	45	-0.036	4.27
		90	-0.004	0.72
		135	0.012	2.39
	1	45	-0.014	2.20
		90	-0.004	0.67
		135	0.069	0.69
	1.5	45	-0.021	7.47
		90	-0.004	2.04
		135	0.143	4.68
8	0.75	45	0.055	1.25
		90	-0.010	0.19
		135	0.101	0.83
	1	45	0.092	2.07
		90	-0.017	0.37
		135	-0.159	0.75
	1.5	45	0.665	3.30
		90	-0.031	0.86
		135	-0.297	0.79

while CBW schemes capture this shape with high fidelity. For hydrophobic surfaces, distinct behaviors emerge between the two IBB cases. At $q_z = 0.7$, the droplet inflates until it coalesces with its periodic images, resulting in domain flooding. At $q_z = 0.01$, the droplet initially detaches from the bottom wall and adheres to the top surface, where it eventually grows until flooding occurs. The f_0r scheme drastically overestimates wall hydrophobicity: the elastic potential energy stored in the initial droplet configuration suffices to expel it from the bottom, causing an oscillatory bouncing motion between the walls. Conversely, CBW schemes maintain high physical accuracy and stable droplet behavior.

In Table 11, the CBW schemes are compared in terms of relative mass leakage $\Delta M_{\%}$, shape deviation $\varepsilon_{s\%}$, and peak velocity magnitude u_{sp} over $DR \in \{25, 100, 500, 1000, 1500, 3000\}$ and $q_z \in \{0.01, 0.3, 0.7, 0.99\}$. Mass leakage is negligible, particularly for $m = 4$. The B-CBW scheme significantly reduces $\varepsilon_{s\%}$ by up to an order of magnitude across the full range of q_z and DR values. Additionally, B-CBW tends to dampen u_{sp} compared to the $m = 4$ U-CBW configuration, especially at high density

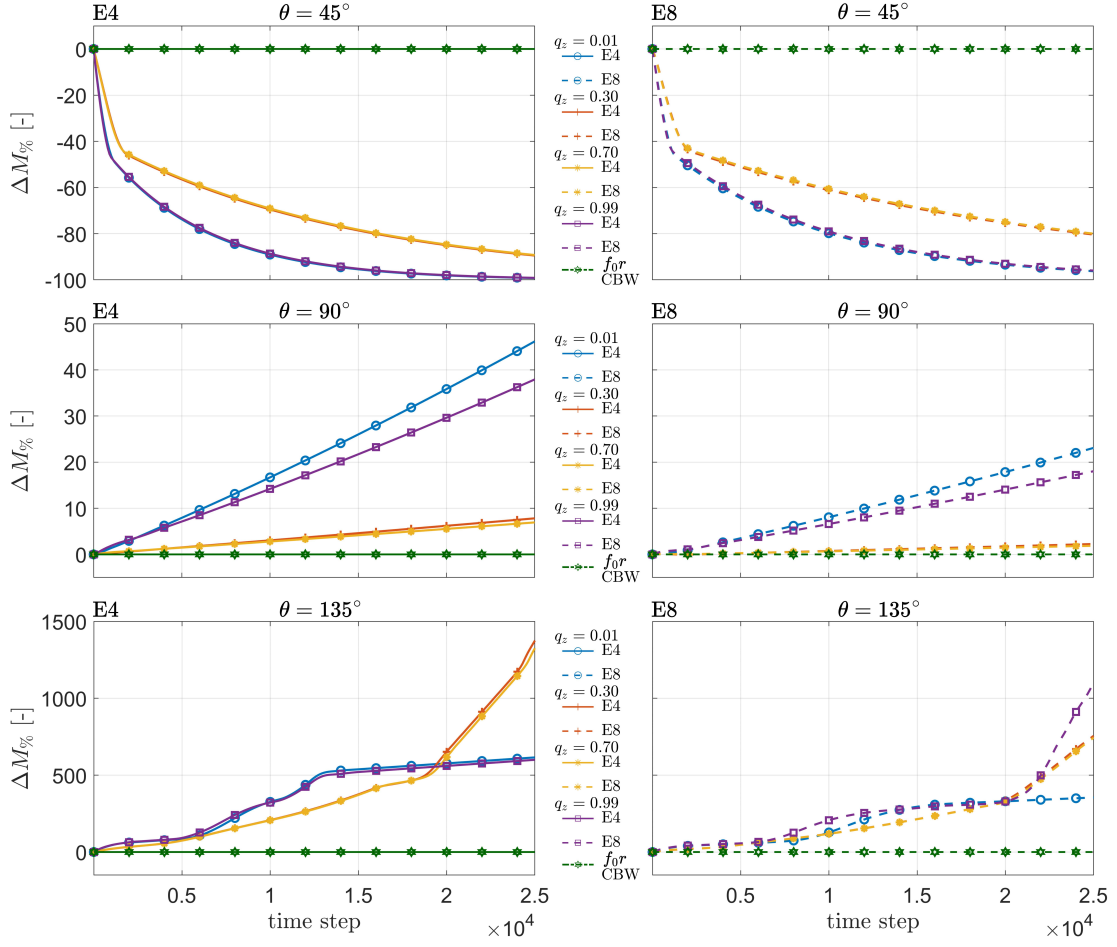


FIGURE 34. Evolution of mass leakage in a wetting test. The classic linear IBB, the rest-population refill method (f_0r) and the proposed CBW schemes are compared for $DR = 25$, wetting angles $\theta \in \{45^\circ, 90^\circ, 135^\circ\}$ and off-lattice wall positions $q_z \in \{0.01, 0.3, 0.7, 0.99\}$. Experiments are performed for $m = 4$ (left) and $m = 8$ (right).

ratios. Overall, u_{sp} slightly increases with DR within each scheme. The E8 U-CBW minimizes u_{sp} , enabling stable simulations even for $DR = 3000$, though this comes at the cost of slightly less perfect mass conservation and more pronounced deviations in droplet shape.

An investigation of the distribution of spurious currents at equilibrium is conducted for $DR \in \{25, 1500\}$ and $q_z \in \{0.01, 0.7\}$. In Figure 36, each panel displays an inset map of $\|\mathbf{u}\|$ at the bottom wall, with an average-density iso-surface overlaid. In each inset map, one observes four distinct $\mathcal{D}$ -shaped lobes characterized by high $\|\mathbf{u}\|$. This qualitative layout appears regardless of the sub-case of interest due to a confinement

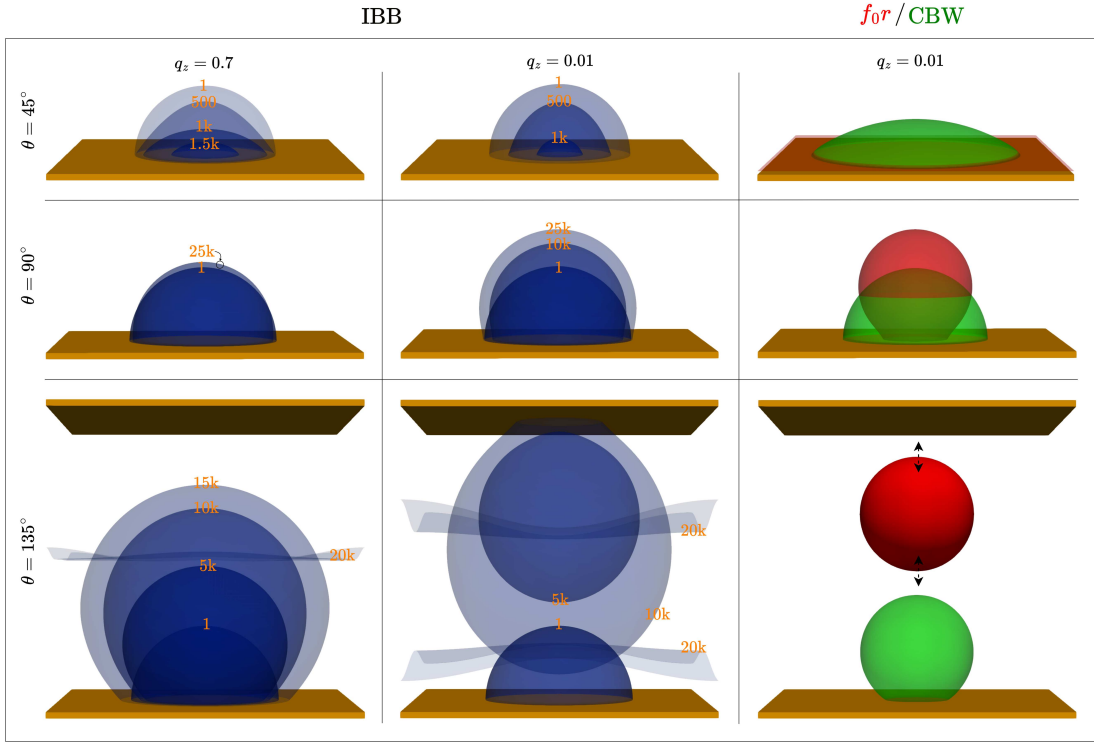


FIGURE 35. Average-density iso-surfaces ($DR = 25$) of droplets wetting flat walls for $\theta \in \{45^\circ, 90^\circ, 135^\circ\}$, respectively in the top, central and bottom panels. The droplet is initialized as hemispherical, its envelope is tracked at different time steps $t \in \{t_1, \dots, t_n\}$ for a linear IBB boundary condition on the top and bottom off-lattice walls, at $q_z = 0.7$ and $q_z = 0.01$. The long-term behavior of the mass-conserving schemes f_0r (●) and CBW (●) is also investigated at $q_z = 0.01$.

effect, namely the interaction between the cubic shape of the domain and the hemispherical shape of the droplet. At fixed DR , E4-U and E4-B cases yield similar results, with B-CBW ensuring slightly lower peaks. In the E8-U case, the lobes appear less intense and more diffused. Raising DR amplifies maxima, sharpens the edges of the lobes, and shifts their centroids marginally farther from the mid-density contour, most noticeably at $q_z = 0.01$. As the position pattern of the lobes is consistent, a section of a vertical and diagonal slice is presented in each panel, displaying the spurious current vector field. Near-wall recirculation cells are observed around the contact regions. A stagnation locus lies close to the average-density iso-surface for $m = 4$. For $m = 8$ sub-cases, such a locus rises to higher z . A weak updraft persists close to the droplet apex, indicating a broad, low-intensity circulation modulated by the aforementioned confinement effect. Such features are common for both DR .

TABLE 11. Comparison between E4 U/B-CBW and E8 U-CBW schemes in a static neutral wetting test.

		$\Delta M_{\%}[10^{-2}]$			$\varepsilon_s\%$			$u_{sp}[10^{-3} \text{ l.u.}]$		
$\beta = 2$		E4		E8	E4		E8	E4		E8
DR	q_z	U	B	U	U	B	U	U	B	U
25	0.01	-0.46	-0.36	3.67	1.022	0.331	1.085	1.08	1.09	0.36
	0.3	-0.39	-0.38	3.54	-0.523	0.066	0.472	0.93	0.80	0.36
	0.5	-0.37	-0.37	1.71	-0.002	-0.002	0.051	0.67	0.67	0.37
	0.7	-0.37	-0.38	3.53	-0.528	0.073	-0.395	0.74	0.67	0.38
	0.99	-0.39	-0.39	3.59	-1.026	0.733	-1.017	0.93	0.63	0.42
100	0.01	-0.62	-0.52	5.98	0.987	0.254	1.040	2.30	2.27	0.68
	0.3	-0.46	-0.47	5.21	0.390	0.041	0.436	1.60	1.66	0.71
	0.5	-0.43	-0.43	0.11	-0.006	-0.006	0.017	1.22	1.22	0.74
	0.7	-0.51	-0.45	5.08	-0.419	0.059	-0.409	1.52	1.39	0.75
	0.99	-0.60	-0.24	5.33	-1.034	0.707	-1.015	1.88	1.30	0.78
500	0.01	-0.52	-0.64	15.71	0.923	0.207	1.011	4.18	4.06	1.24
	0.3	-0.43	-0.58	14.03	0.398	0.024	0.412	2.85	2.99	1.30
	0.5	-0.54	-0.54	13.70	-0.006	-0.006	-0.010	2.53	2.53	1.33
	0.7	-0.67	-0.48	13.64	-0.423	0.099	-0.419	2.69	2.47	1.36
	0.99	-0.87	-0.09	14.01	-1.022	0.686	-1.028	3.27	2.32	1.40
1000	0.01	-0.18	-0.25	14.09	0.922	0.221	1.012	5.13	4.95	1.52
	0.3	-0.03	-0.21	12.44	0.377	0.016	0.399	3.45	3.69	1.58
	0.5	-0.17	-0.17	12.17	0.000	0.000	-0.010	2.80	2.80	1.62
	0.7	-0.31	-0.06	12.06	-0.460	0.091	-0.461	3.88	2.95	1.66
	0.99	-0.50	0.25	12.42	-1.248	0.677	-1.029	3.88	2.77	1.71
1500	0.01	0.21	0.14	12.72	0.902	0.205	1.020	5.69	5.47	1.89
	0.3	0.36	0.17	11.08	0.373	0.014	0.401	3.78	4.07	1.87
	0.5	0.20	0.20	4.73	-0.010	-0.010	-0.010	3.40	3.40	1.88
	0.7	0.22	0.33	10.78	-0.473	0.091	-0.430	5.69	3.21	1.88
	0.99	0.22	0.61	11.15	-1.023	-0.476	-1.032	5.69	3.21	1.91
3000	0.01	x	x	10.79	x	x	1.090	x	x	9.42
	0.3	x	x	9.06	x	x	0.455	x	x	8.65
	0.5	x	x	4.14	x	x	0.040	x	x	8.13
	0.7	x	x	8.70	x	x	-0.387	x	x	7.59
	0.99	x	x	9.08	x	x	-0.999	x	x	6.85

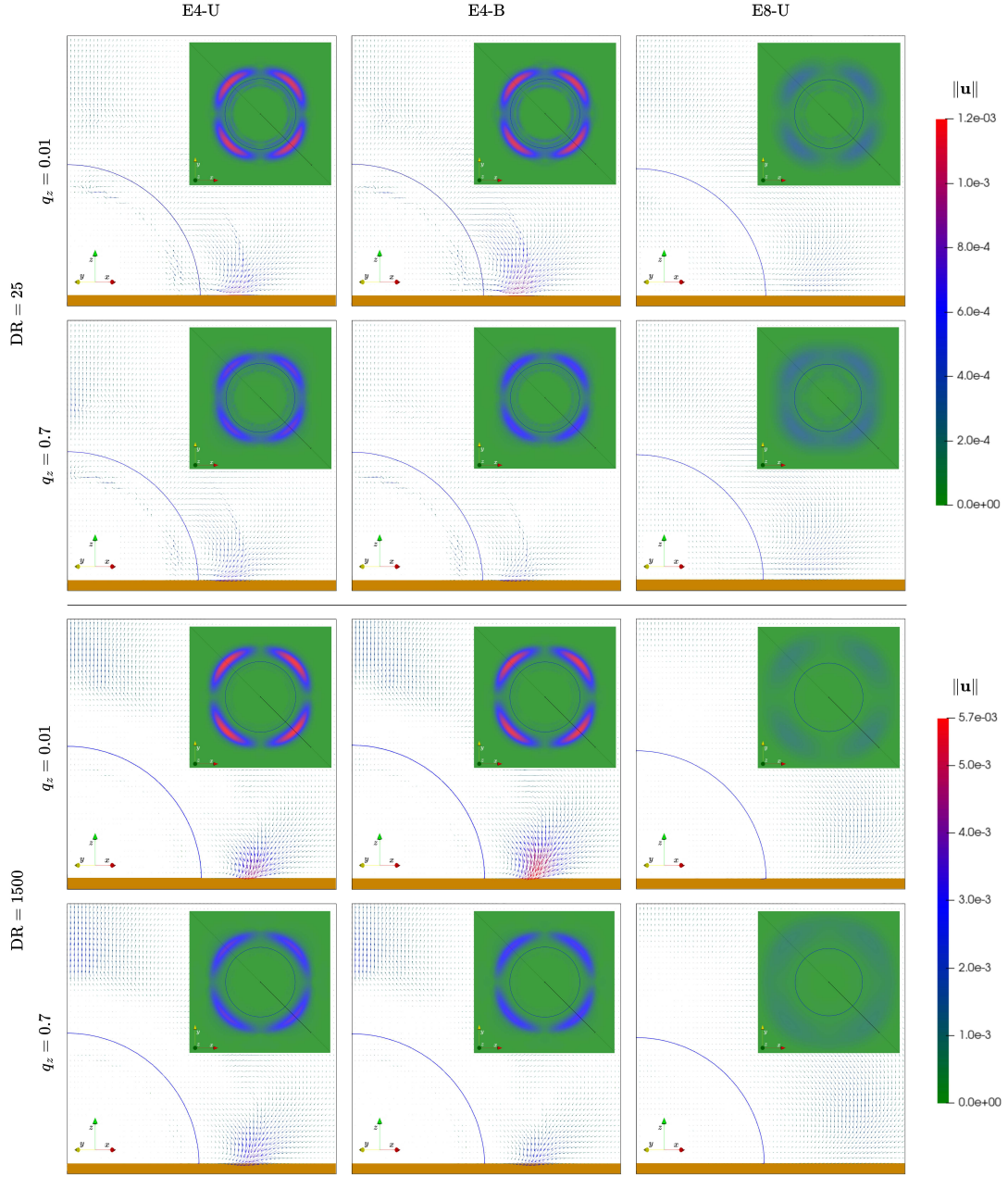


FIGURE 36. Spurious velocity field obtained in a droplet wetting test for $DR = 25$ and 1500 , $q_z = 0.01$ and 0.7 . Results are displayed for $m = 4$ (employing both stencils U- and B-CBW) and $m = 8$ (only U-CBW). Each panel displays a diagonal slice of the velocity vector field, with an inset showing the corresponding top view of the velocity magnitude distribution at the bottom wall.

2.2. Wetting on curved surfaces. Curved solid targets of both spherical and cylindrical shapes are immersed in a cubic domain with $N = 100$ nodes per side. The equilibrium neutral wetting behavior of a droplet contacting such targets is investigated. A study involving curved surfaces enables the assessment of the concurrent effect on the performance of CBW schemes over a wide range of values $q_i \in (0, 1]$. Different curvature radii are explored: $r_c \in \{25, 50, 75, 100\}$. Closing bottom and top flat walls are located normal to the z axis at $q_z = 0.5$. The E4 stencil on both U- and B-CBW schemes and the E8 stencil on the U-CBW scheme are implemented. The study is conducted over a wide range of density ratios, $DR \in \{100, 500, 1000, 1500\}$. A droplet is initialized by adopting Eq.s (125)-(126), with $r_0 = N/4$, $W = 5$ and $\mathbf{x}_0$ set as:

$$(139) \quad \mathbf{x}_0 = (N/2, N/2, z^*), \text{ with } z^* = z_c + \sqrt{r_c^2 + r_0^2}.$$

Equilibrium iso-surfaces at average density are displayed in Figure 37 for $m = 8$, $DR = 1500$. The droplet minimizes the liquid-vapor interface area while ensuring an angle $\theta = 90^\circ$ with the local normal to the boundary surface. While on a flat substrate, this effect leads to a hemispherical cap; on curved surfaces, the equilibrium shape is affected by different geometric constraints, yielding distinct symmetry classes. Considering a spherical target, the constant positive curvature r_c in all directions induces an axisymmetric capillary problem. The three-phase contact line, therefore, forms a circle that lies in a plane of constant z for both radii. Given the relatively small size of the liquid droplet, the symmetry is preserved even in the presence of artifacts induced by the cubic shape of the domain. The cylindrical target is characterized by one finite principal curvature ($1/r_c$) and a null curvature along its axis. The system develops a mirror symmetry with respect to the vertical xz -plane containing such an axis. The contact line spans a finite interval in z to comply with the imposed neutral wetting. As r_c increases, such a range shrinks down to a point, in the limit of a planar wall.

A quantitative analysis of the distribution of u_{sp} is reported for spherical and cylindrical targets in Figures 38 and 39. For both geometries and all selected DR, E8-U exhibits a clean, monotonic decrease in u_{sp} as r_c increases, due to the competition between reconstruction accuracy and locality. The E8 approach outperforms E4 for cohesive interactions [163] and in wetting modeling on flat surfaces. Increasing the curvature of the target leads to higher u_{sp} as the extension of the E8 averaging stencil, adopted to compute the virtual ψ , becomes comparable in size to r_c ; by contrast, the E4 stencil is more compact and better suited to depict fluid-solid interaction at high r_c . The detrimental behavior of E8 appears to be negligible at larger r_c . The E4-U and E4-B implementations display non-monotonic trends of u_{sp} in r_c , with extrema at

intermediate radii. Increasing DR amplifies u_{sp} for every scheme and geometry; amplifying the E8-decay primarily in the moderate to large r_c range, while penalizing E8 at high curvatures, as the extended averaging stencil encloses steeper gradients. The performances of E4-U and E4-B are comparable. At low DR, the unidirectional scheme results are slightly superior, whereas at high DR, the two curves nearly collapse. At fixed DR and r_c , u_{sp} on the cylinder is comparable to the sphere, while it is notably higher for small r_c . As r_c increases, the u_{sp} values would be primarily attributable to finite-box confinement and discretization effects. Overall, the results support E8-U as a robust choice for curved-geometry wetting at high DR when r_c is not extreme, yielding lower peaks in many, though not all, cases and a regular, predictable dependence on r_c , while E4 remains a cost-driven option, less sensitive to curvature-induced averaging bias at high surface curvature but exhibiting non-monotonic behavior in r_c .

Finally, regions of the domain characterized by intense spurious currents are displayed in Figure 40 for $m = 8$, DR = 1500, and $r_c \in \{25, 100\}$ l.u., considering both spherical and cylindrical solid geometries. The location and shape of such regions, here complying with the criterion $0.5 \leq \|\mathbf{u}\|/u_{sp} \leq 1$, denote how the fluid-solid interactions dictate the discretization artifacts, as seen in the flat-wall test cases, which are severely dependent on the geometry and curvature of the target. Considering the spherical substrate with a small curvature radius ($r_c = 25$ l.u.), a single region appears in an axisymmetric band shape, tight and close to the contact line between the average-density iso-surface and the curved wall. At low curvature ($r_c = 100$ l.u.), instead, two distinct regions appear, both close to the curved wall. The farthest one extends toward the corners of the domain, manifesting a clear confinement effect. A different pattern emerges for the cylindrical substrate: low r_c induces pairs of both confinement-driven structures and elongated lobes extending along the cylinder length. These latter are absent when high r_c is considered.

2.2.1. Notes on locality and geometry effects. In the L-IBB closure, the post-streaming reconstruction of $f_i(\mathbf{x}_b, t + \Delta t)$ is nonlocal only for $q_i(\mathbf{x}_b) \in (0, 1/2]$, where it involves the boundary node $\mathbf{x}_b$ and a single fluid neighbor $\mathbf{x}_f$ through linear interpolation, whereas for $q_i(\mathbf{x}_b) \in (1/2, 1]$ it is fully local at $\mathbf{x}_b$. The CBW additional forcing correction is applied pointwise to the reconstructed populations; thus, it does not involve additional neighbors. The rest-population refill step is also local, although it can affect subsequent force evaluations indirectly through the pre-existing pseudopotential stencil via the updated $\rho(\mathbf{x}_b, t + \Delta t)$ and $\psi(\mathbf{x}_b, t + \Delta t)$. Consequently, for sufficiently resolved smooth concave surfaces, one expects the same qualitative behavior observed on convex targets, with errors mainly controlled by local curvature and by the

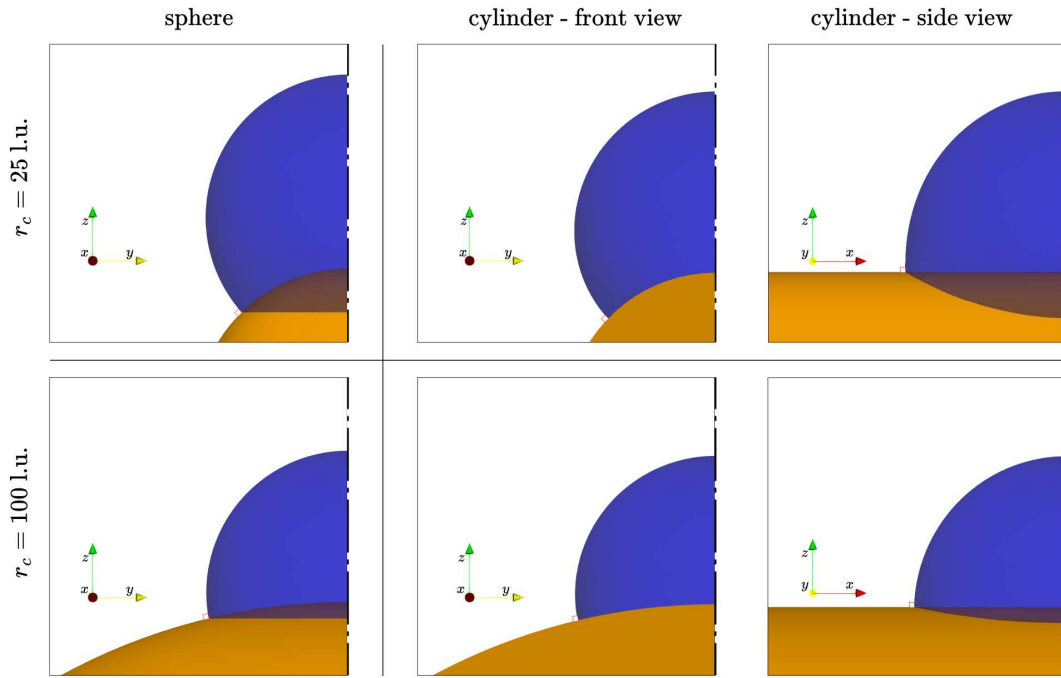


FIGURE 37. Equilibrium average-density iso-surfaces ($DR = 1500$) of droplets neutrally wetting spherical and cylindrical targets for $m = 8$ within the U-CBW scheme.

ratio between geometric length scales and the diffuse-interface thickness. For strongly re-entrant concavities, or when adopting the less local B-CBW variant, reconstruction/averaging rays may intersect the solid boundary more than once; in this case, grid refinement is advised.

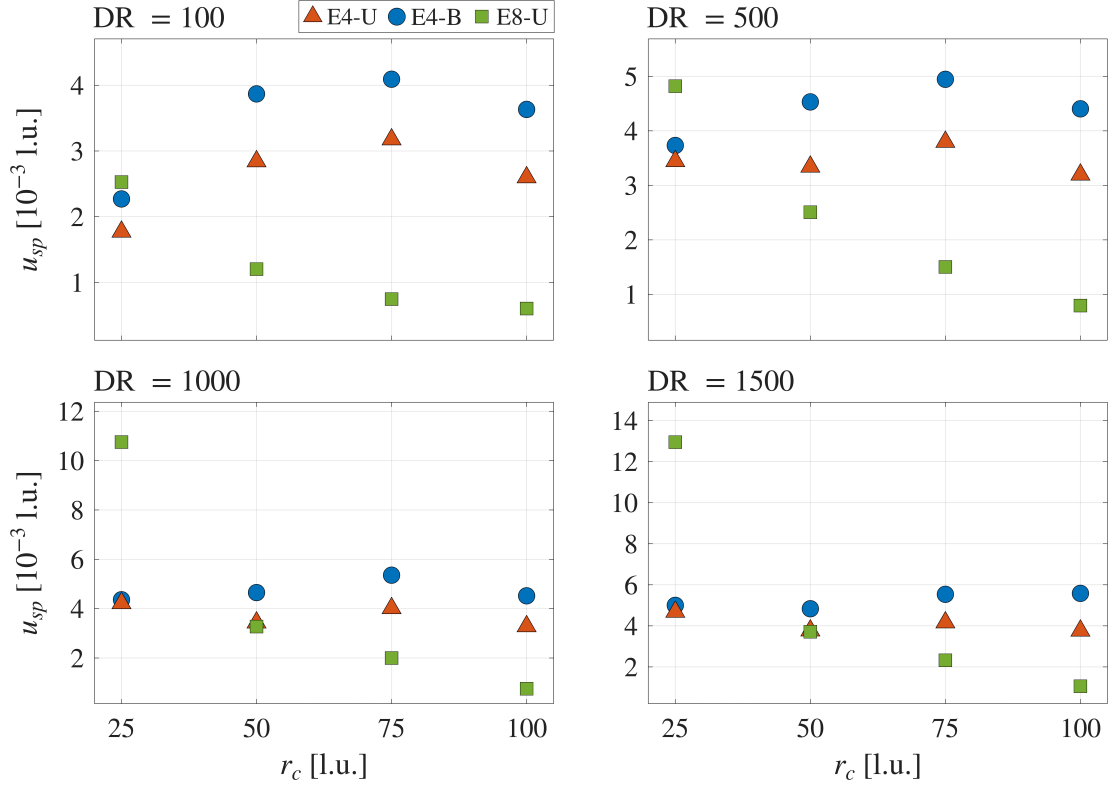


FIGURE 38. Plot of the peak spurious current magnitude (u_{sp}) against the target's curvature radius (r_c) for a droplet wetting a sphere when employing the compact stencil ($m = 4$) with the U- and B-BCW schemes and for the extended stencil ($m = 8$) with the U-CBW scheme. Results are displayed for a wide range of density ratios (DR).

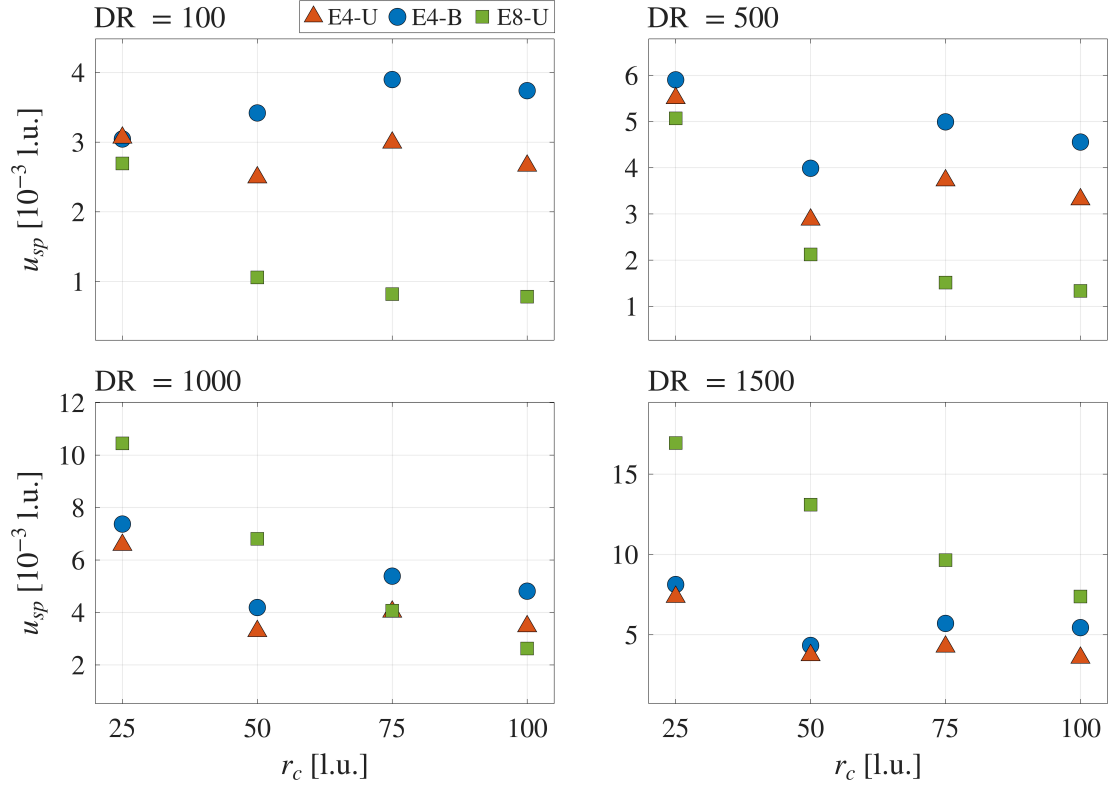


FIGURE 39. Plot of the peak spurious current magnitude (u_{sp}) against the target's curvature radius (r_c) for a droplet wetting a cylinder when employing the compact stencil ($m = 4$) with the U- and B-BCW schemes and for the extended stencil ($m = 8$) with the U-CBW scheme. Results are displayed for a wide range of density ratios (DR).

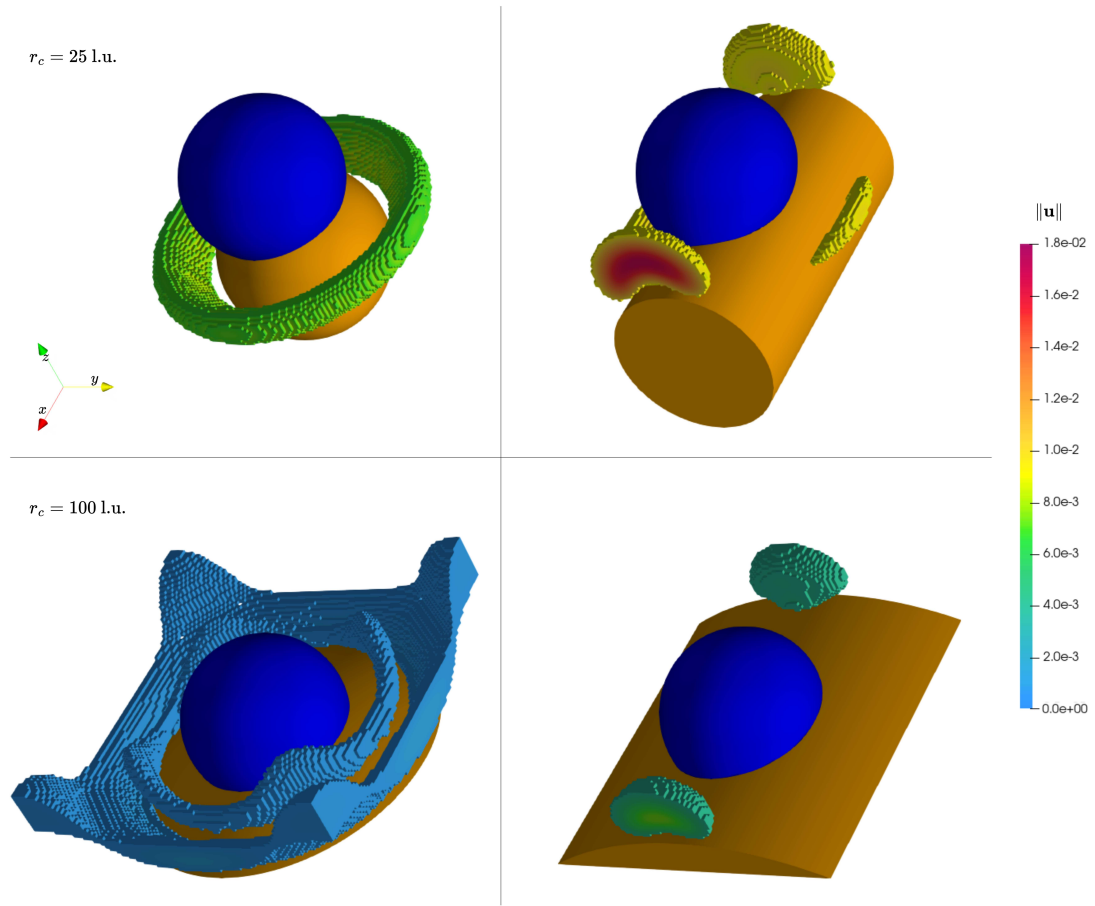


FIGURE 40. Spatial distribution of spurious currents obtained with $m = 8$ within the range $0.5u_{sp} \leq \|\mathbf{u}\| \leq u_{sp}$ for a droplet neutrally wetting spherical (left) and cylindrical (right) targets.

Conclusions and future work

The efforts presented in this thesis are motivated by the broad and complex challenge of sustainable mobility. Achieving long-term European and global climate targets requires a substantial reduction in CO₂ and pollutants emissions from a transport sector that still depends heavily on fossil-fuels. Renewable-energy-driven electrification cannot rely exclusively on battery electric vehicles, whose deployment is constrained by long charging times, heavy infrastructure requirements, and the economic and socio-political impacts of lithium-ion technologies. Thus, a complementary pathway is offered by Fuel Cell (Hybrid) Electric Vehicles, whose powertrains integrate Proton Exchange Membrane Fuel Cells (PEMFCs). When supplied with green hydrogen, these electrochemical converters can guarantee low-emission electrical power with high efficiency, long driving range, and short refueling times. Nevertheless, high system and stack costs remain major barriers to widespread deployment.

In this context, this thesis presents: (i) the design, fabrication, and testing of a modular PEMFC power system; and (ii) the development of a high-fidelity numerical framework for multiphase flows and wetting, ultimately targeted at water management in PEMFC porous electrodes.

The first point was addressed within the core activities of the project *Hydrogen Mobility Made in Italy*. A modular PEMFC power system was designed, built, and extensively tested to promote the scalability and easy maintainability of fuel-cell powertrains for mobility applications. The underlying rationale is that mass-produced standardized stacks could be combined to cover a broad power range without redesigning the entire system architecture. The prototype consists of a twin PEMFC stack operable with both air/H₂ and O₂/H₂ feeds, comprising two base units supplied by a symmetric piping system that promotes uniform reactant distribution. Each 16-cell stack integrates distributed liquid cooling and tailored reactant flow fields at the single-cell level. Experimental testing under both air/H₂ and O₂/H₂ feeds confirmed stable operation across the investigated current-density range, with the twin-stack efficiency closely matching that of the single units, revealing negligible coupling losses. These results proved the effectiveness of the modular design in preserving electrochemical performance while enabling power scaling through the straightforward stacking of base units.

The experimental campaign, however, also confirmed a critical aspect widely reported in the literature: the management of liquid water within the stack, particularly at high current loads, represents a key design and operating constraint, primarily governed by multiphase transport within each cell.

This insight motivated the effort in mathematical modeling and simulation, as the experimental tests, while providing meaningful global metrics, cannot predict the local distribution of liquid water within the porous electrodes. Modeling approaches reported in the literature, although valuable, still lack an accurate representation of the underlying multiphase physics and typically rely on overly simplified wetting schemes.

A numerical method has therefore been developed: a novel three-dimensional entropic Lattice Boltzmann framework for the modeling and simulation of multiphase flow and wetting phenomena at pore-scale, featuring a cascaded collision operator with entropic stabilization, a unified non-ideal force formulation, and extended sensitivity to curved immersed geometries. The cascaded approach relies on the relaxation of central moments, which improves accuracy and stability by introducing higher Galilean invariance and avoiding crosstalk, while the entropic stabilization enhances physical consistency by constraining the free relaxation parameters. The multiphase and wetting features are introduced by an extended Shan-Chen pseudopotential method embedding an exogenous linear piecewise equation of state, which allows for direct control over equilibrium thermodynamic properties. The cohesive and adhesive interactions are blended in a unified force formulation, which contributes to the development of the Coupled Boundary-Wettability (CBW) scheme. This latter enhances the interpolated bounce-back boundary conditions by incorporating local force data to ensure mass conservation and an accurate imposition of the wetting state.

At first, the experimental campaign focused on the sole cohesive interaction, with the imposition of triply periodic boundary conditions. Different values of the interaction force isotropy order were explored, achieving density and viscosity ratios of up to $DR = 3000$ and $VR = 600$, respectively.

In static droplet tests, spurious currents exhibit distinct spatial distributions and magnitudes depending on the interplay between the force isotropy order and model parameters, displaying non-trivial results as the density ratio between the phases increases. Thermodynamic consistency of the model was also demonstrated on both the liquid and vapor branches, alongside compliance of the model with the Young-Laplace law. Furthermore, a dynamic test was performed to investigate the transient response of the fluid system: an initially spheroidal droplet is allowed to relax towards the equilibrium spherical shape, manifesting a damped oscillating behavior between prolate

and oblate configurations. The interface oscillation period is strongly influenced by the surface tension. The accuracy with respect to analytic solutions is also maximized when extended interaction stencils are implemented, proving that including additional neighboring shells within the computation of the discrete force does not compromise the consistency with analytical models that assume a zero-thickness interface.

The peculiarities of the adhesive interaction were subsequently investigated by immersing solid structures in the computational domain.

At first, an extensive hemispherical droplet test conducted on a flat wall with diverse wetting properties and set at different off-grid locations confirmed the need for fine-tuned mass-conservative boundary schemes. Finally, wetting tests on spheres and fibers characterized by different curvature radii have been conducted. Given the test results, the proposed framework applies to arbitrarily positioned and shaped boundaries and supports both low and high density and viscosity ratios regimes, reaching up to $DR = 3000$ and $VR = 600$. The U-CBW and B-CBW variants exhibit complementary features. While the unidirectional formulation maintains minimal computational complexity, the bidirectional scheme enhances shape fidelity and contact-angle robustness by incorporating directional pseudopotential corrections. Both schemes significantly outperform traditional bounce-back implementations, particularly in preserving mass across off-lattice boundary intersections and in suppressing spurious currents through higher-order isotropic force stencils. The integration with entropic stabilization ensures compliance with a discrete H-theorem, enhancing numerical stability even at high density ratios. The modularity of the CBW strategy makes it compatible with a broad class of LBM collision models and boundary treatments, paving the way for its integration into general-purpose entropic multiphase solvers.

Future developments could include deploying the proposed framework to resolve wetting phenomena in realistic PEMFC porous electrodes, particularly within the Gas Diffusion Layer, by exploiting three-dimensional tomographic reconstructions. This would enable the computation of percolation thresholds, breakthrough pressures, local saturation fields, and preferential flow paths under prescribed boundary flow conditions, as well as their correlation with material descriptors such as porosity, anisotropy, and pore-size distributions, along with the performance of an entire PEMFC stack, supported by experimental test data.

More generally, the model could be embedded within fluid–structure interaction solvers to investigate capillary-driven erosion phenomena in biological systems and microfluidic devices.

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Appendix A

Explicit forms of the transformation matrices $\mathbf{M}$ and $\mathbf{N}$ are displayed to allow for their fast implementation in one's algorithm.

It must be stressed that, while the elements of the D3Q19 velocity sets are standardized, their order within the set is not. These explicit matrices can be directly adopted only if the specific ordering given in Eq. (17) is followed; otherwise, one must compute their elements using Eq. (61) and Eq. (54).

The matrix $\mathbf{N}$ is represented by means of two submatrices for layout constraints and clarity, such that $\mathbf{N} = (\mathbf{N}_{:,0:7}, \mathbf{N}_{:,8:18})$.

$$\mathbf{M} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & -1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 \\ 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 1 & 1 & 0 & 0 & -1 & -1 & 1 & 1 & 0 & 0 & -1 & -1 & 1 & 1 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

$$\mathbf{N}_{:,0:7} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -u_x & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -u_y & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -u_z & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ u_x u_y & -u_y & -u_x & 0 & 1 & 0 & 0 & 0 \\ u_x u_z & -u_z & 0 & -u_x & 0 & 1 & 0 & 0 \\ u_y u_z & 0 & -u_z & -u_y & 0 & 0 & 1 & 0 \\ u_x^2 + u_y^2 + u_z^2 & -2u_x & -2u_y & -2u_z & 0 & 0 & 0 & 1 \\ u_x^2 - u_y^2 & -2u_x & 2u_y & 0 & 0 & 0 & 0 & 0 \\ u_x^2 - u_z^2 & -2u_x & 0 & 2u_z & 0 & 0 & 0 & 0 \\ -u_x u_y^2 & u_y^2 & 2u_x u_y & 0 & -2u_y & 0 & 0 & -u_x/3 \\ -u_x u_z^2 & u_z^2 & 0 & 2u_x u_z & 0 & -2u_z & 0 & -u_x/3 \\ -u_x^2 u_y & 2u_x u_y & u_x^2 & 0 & -2u_x & 0 & 0 & -u_y/3 \\ -u_x^2 u_z & 2u_x u_z & 0 & u_x^2 & 0 & -2u_x & 0 & -u_z/3 \\ -u_y u_z^2 & 0 & u_z^2 & 2u_y u_z & 0 & 0 & -2u_z & -u_y/3 \\ -u_y^2 u_z & 0 & 2u_y u_z & u_y^2 & 0 & 0 & -2u_y & -u_z/3 \\ u_x^2 u_y^2 & -2u_x u_y^2 & -2u_x^2 u_y & 0 & 4u_x u_y & 0 & 0 & (u_y^2 + u_x^2)/3 \\ u_x^2 u_z^2 & -2u_x u_z^2 & 0 & -2u_x^2 u_z & 0 & 4u_x u_z & 0 & (u_z^2 + u_x^2)/3 \\ u_y^2 u_z^2 & 0 & -2u_y u_z^2 & -2u_y^2 u_z & 0 & 0 & 4u_y u_z & (u_z^2 + u_y^2)/3 \end{bmatrix}$$

$$\mathbf{N}_{:,8:18} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (2u_x)/3 & -u_x/3 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -u_x/3 & (2u_x)/3 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -u_y/3 & -u_y/3 & -u_y/3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -u_z/3 & -u_z/3 & -u_z/3 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -u_y/3 & (2u_y)/3 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (2u_z)/3 & -u_z/3 & -u_z/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ (u_y^2 - 2u_x^2)/3 & (u_y^2 + u_x^2)/3 & -2u_x & 0 & -2u_y & 0 & 0 & 0 & 0 & 0 & 1 \\ (u_z^2 - 2u_x^2)/3 & (u_z^2 + u_x^2)/3 & 0 & -2u_x & 0 & -2u_z & 0 & 0 & 0 & 0 & 1 \\ (-2u_z^2 + u_y^2)/3 & (u_z^2 + u_y^2)/3 & 0 & 0 & -2u_y & -2u_z & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$