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200 - ADVANCED DISCRETIZATION TECHNIQUES

Advances in Lattice Boltzmann (LBM) and Kinetic schemes

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ADVANCES IN LATTICE BOLTZMANN (LBM) AND KINETIC SCHEMES
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Key words: Lattice Boltzmann, numerical methods, kinetic schemes

ABSTRACT

The concept of LBM goes back to R. Gatignol and H. Cabanes in the early 70's, and has been popularised by Frish, d'Humières, Pommeau, Hasslacher, Lallemand and Rivet with the concept of Cellular automa. It evolved towards its current formulations, thanks to numerical interpretations of the Boltzmann equations. It has mostly been used for low Mach number flows, and the extension to compressible flows with is a timely research topics, since several families of LB methods (regularized methods, cascaded or cumulant-based methods, entropic methods) have been extended to such flows. This simplicity of the method explains its popularity both in academia and industry. Another interpretation of the BGK equation is given by Shi Jin in which the physical interpretation is forgotten. The question is: given an hyperbolic (or parabolic) system, how can we formally approximate it by a BGK type system? The stability constraints are formalised via the Whittam sub-characteristc condition. On a different, but related line of work, one can consider the work of K. Xu and collaborators, where finite volume type numerical methods are constructed directly form the BGK approximation.

The aim of this minisymposium is to gather some actors of each of these communities, and exchange experience and progresses in the numerical methods.A partial list of speakers is L.-S. Luo (Old Dominion), P. Dellar (Oxford), K. Xu (Hong-Kong), R. Natalini (Roma) and researchers from the industry.

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A CLASS OF MULTIDIMENSIONAL FULLY ADAPTIVE LATTICE-BOLTZMANN METHODS BASED ON MULTIRESOLUTION ANALYSIS

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Key Words: Lattice-Boltzmann, Multiresolution, Error control, Dynamically adaptive grid

Lattice-Boltzmann methods usually rely on uniform meshes with a strong bond between spatial and temporal discretization. This fact complicates the crucial issue of reducing the computational cost by automatically coarsening the grid where high precision is unnecessary, still ensuring the overall quality of the numerical solution through error control. This work provides a possible answer to this interesting question, by connecting, for the first time, the field of lattice-Boltzmann methods to the multiresolution approach. To this end, we employ a multiresolution transform to adapt the mesh as the solution evolves in time according to its local regularity and to evaluate the incoming and outcoming quantities in the transport phase with a given accuracy. The collision phase is not affected due to its inherent local nature and because we do not modify the speed of the sound, contrarily to most of the LBM/AMR strategies proposed in literature. We carefully test our method to conclude on its adaptability to a wide family of existing lattice-Boltzmann schemes, treating both hyperbolic and parabolic problems, then being less problem-dependent than the AMR approaches, which thus cannot grant any theoretical control on the error. We also verify an effective cost reduction, without going too deep in the study of computational cost, as far as we deal with problems involving steep solutions with a precise control on the approximation error introduced by the spatial adaptation of the mesh.

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A KINETIC SCHEME FOR A THREE-PHASE FLOW WITH PHASE TRANSITION

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Key Words: Lattice Boltzmann Method, compressible flow, phase transition.

This work is devoted to the numerical resolution of a compressible three-phase flow with phase transition by a Lattice-Boltzmann Method (LBM). The flow presents complex features and large variations of physical quantities.

The complex pressure model is build from rigorous entropy optimisation principles [3], which give to the model a clear thermodynamical meaning.

It is then possible to construct a LBM that is entropy stable under a subcharacteristic condition [1]. In addition, with usual time-splitting techniques, it can be extended to second order accuracy without additional numerical cost.

We present preliminary numerical results, which confirms the competitiveness of the entropic LBM compared to other Finite Volume methods.

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A LOW RANK TENSOR REPRESENTATION BASED ON WENO SCHEMES FOR NONLINEAR VLASOV DYNAMICS

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Key Words: Instructions, Multiphysics Problems, Applications, Computing Methods

Inspired by existing understanding of the low-rank solution structure for Vlasov dynamics (e.g. Landau damping and two-stream instabilities), as well as the observation that the differential operator in the Vlasov equation can be represented in the tensorized form, in this project we propose a novel way to (a) dynamically and adaptively build up low-rank solution basis, and (b) determine the low rank solutions in a tensor format in the context of high order WENO method. We will first demonstrate our proposed idea in a simplified 1D1V setting; then we discuss the extension to general 3D3V problems by using the hierarchical Tucker decomposition of tensors.

A PRESSURE-BASED HYBRID REGULARIZED LATTICE-BOLTZMANN METHOD FOR NUMERICAL COMBUSTION

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Key Words: Lattice-Boltzmann method, pressure-based solver, combustion

A pressure-based Hybrid Lattice-Boltzmann method (HLBM) is proposed for combustion applications. The mass and momentum conservation are resolved by LBM, while the enthalpy and species fields are simulated with Finite Difference (FD) scheme and explicit first-order-Euler time-stepping. Unlike our previous reactive HLBM framework [1, 2], this new approach firstly models the pressure transport equation at low-Mach limit [3] in the streaming step, then recovers the correct mass equation during the regularized collision. This particular treatment enhances numerical stability. A DNS of a circular premixed flame is investigated using a grid size of 1/5 of the flame thickness. The temperature and heat release rate in figure 1(a) and 1(b) emphasize the isotropic property of the scheme and the non-reflecting characteristic boundary conditions. A LES of a 3D round jet diffusion flame corresponding to a Re number 16800 and Mach number 0.2 is performed on a mesh with a size of 1/26 of the diameter with the implicit hybrid LES sub-grid model [4]. Small flow structures in figure 1(c) from a non-reacting simulation demonstrate the low-dissipation feature of the method. Preliminary results from the reactive configuration confirm the capability of the current model for turbulent flames.

(a) Temperature (b) HRR (c) *Q*-criterion

Figure 1: Visualization of (a) Temperature field, (b) heat release rate of the circular premixed flamem and (c) *Q*-criterion iso-surface of non-reacting 3D jet.

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ARBITRARY LAGRANGIAN-EULERIAN METHOD FOR HIGH REYNOLDS NUMBER FLOWS AROUND ROTATING GEOMETRIES WITH LATTICE BOLTZMANN METHOD

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Key Words: Lattice Boltzmann Method, Arbitrary Lagrangian Eulerian, Rotating geometries, High Reynolds number flow, Chimera method

Rotating geometries in high Reynolds number flows are classical design applications, such as rotors or landing gears. In terms of numerics, one of the biggest difficulties for simulating the rotating geometries comes from the existence of fictitious forces, like centrifugal and Coriolis forces. The rise of the Lattice Boltzmann method (LBM) has successfully contributed to reducing computational cost for industrial applications. Conventionally, LBM adopts the discrete force model to take into account the fictitious forces, which may lead to discrepancy between the different models. [1, 2]

This research suggests an alternative approach called, arbitrary Lagrangian-Eulerian method (ALE). [3, 4, 5] In the conventional approach, there exists only one reference axis which is shared by both the rotating mesh and the lattice particles. It brings about the fictitious forces because velocity vectors of the lattice particles are defined with respect to the rotating axis (so called, non-inertial axis). On the contrary, the ALE approach employs two different axes, which are fixed spatial axis and moving reference axis. The fictitious forces can disappear by defining all the physical quantities in the fixed spatial axis (inertial axis), such as the velocities of the lattice particles, the velocity of the moving mesh and the gradient of the particle distribution functions. Its balance equation could be written on the arbitrary point of the moving reference axis which moves as being attached to the rotating geometries. Moreover, the ALE equation is derived using the Double-Relaxation time (DRT) collision model and its turbulence viscosity is solved by using the large eddy simulation.

The proposed ALE-LBM method is validated through several steps. First, the Poiseuille flow without any solid body is tested to check whether the mass flow rate is well conserved through the mesh interpolation procedure. Also, the simulations are conducted for the Taylor-Couette flow to assess if the ALE-LBM method can correctly capture the rotational effect. Finally, a rotating cylinder in a channel is tested to consider translation and rotational motion at the same time.

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DISCRETE VELOCITY BOLTZMANN MODELS AS RELAXATION SYSTEMS FOR SCALAR ADVECTION–DIFFUSION EQUATIONS

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Key Words: Lattice Boltzmann methods, discrete velocity model, relaxation system, partial differential equations

The connection of relaxation systems (RS) and discrete velocity Boltzmann models (DVBM) was and is essential to the progress of stability as well as convergence results for lattice Boltzmann methods (LBM). In the present study we propose a formal perturbation ansatz for the construction of an RS on the basis of a given scalar one-dimensional partial differential equation. Subsequently, equivalence to a DVBM is found. Via this procedure, a 3×3 RS as a link to a generalized $D1Q3$ DVBM [1] with the corresponding equilibria formally derived from—and pertaining to—the targeted partial differential equation is obtained. The inclusion of a null velocity, which distinguishes e.g. $D1Q3$ from $D1Q2$, is an essential feature of many DVBM used in LBM. Hence, the study serves as an extension of the commonly found notes (e.g. [2]) on the relation of $D1Q2$ DVBM to the classical 2×2 RS [4, 3]. Further, the specification of stability structures [5] of the obtained DVBM allows for algebraic characterizations of the equilibrium and collision operator. The introduced methodology for scalar linear advection–diffusion equations can be used as a foundation for the constructive design of DVBM approximating different types of partial differential equations.

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HYBRID REGULARIZED LATTICE BOLTZMANN MODEL FOR COMPRESSIBLE FLOWS : INTERACTION OF KOVÁSZNAY MODES WITH A SHOCK WAVE.

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Key Words: Compressible flows, Thermal lattice Boltzmann model, Kovásznay modes, Shock wave.

Recent studies demonstrated the applicability of the Hybrid Lattice-Boltzmann Method (HLBM) to a wide range of physical phenomena such as combustion [1] and compressible flows [2].

Here, a pressure-based Hybrid Lattice-Boltzmann solver is used to simulate the propagation and interaction of Kovásznay modes [3] with a shock wave. The mass and momentum conservation are solved by a Lattice-Boltzmann algorithm coupled with an explicit Finite-Difference solver for the energy equation.

Stationary and non-stationary shock solutions are presented along with Vortical, Entropic and Acoustic modes propagation to demonstrate the capability of the current model for compressible flows. Shock-vortex interaction results are then compared with the literature [4, 5].

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A KINETIC FLUX DIFFERENCE SPLITTING METHOD WITH DISCRETE VELOCITIES IN IMMERSED BOUNDARY FRAMEWORK

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Key Words: Discrete Velocity Boltzmann scheme, Kinetic Flux Difference Splitting, Mahalanobis Distance, Exact Discontinuity Capturing, Immersed Boundary

The discrete velocity based kinetic schemes are simpler than the the continuous molecular velocity based kinetic schemes, as the integrals are replaced by summations and the equilibrium distributions are simple algebraic functions of conserved variables and fluxes. While some of the discrete velocity kinetic schemes are quite efficient, none of the kinetic or discrete kinetic schemes can capture steady grid-aligned discontinuities exactly, a feature well-established in some of the macroscopic schemes. In the present work, A flux difference splitting based kinetic scheme is developed based on three discrete velocities, starting from a discrete velocity Boltzmann equation. While the minimal design of this exact discontinuity capturing kinetic scheme requires just two discrete velocities, the third component is utilized to prevent entropy condition violation, which is typical of low diffusive algorithms, by utilizing the Mahalanobis distance (directed divergence or D^2-distance, see Kullback [1]). Raghavendra *et al.* [2] utilized the D^2-Distance successfully as a tool for mesh adaptation. Here we use Mahalnobis distance and entropy to distinguish expansion regions from discontinuities so that additional numerical diffusion can be added without disturbing exact discontinuity capturing.

The new Boltzmann scheme is coupled with ghost-cell based immersed boundary method so that effort in meshing can be simplified. The resulting scheme has been tested on several 2-D bench-mark problems for both inviscid and viscous compressible flows.

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Lattice Boltzmann Method for the numerical simulation of multiphasic flows

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Key Words: *Lattice Boltzmann Methods, Multiphasic flows, colour gradient methods, mean field.*

Motivated by the reduction of the environmental impactof aviation, fuel and air injections in turbo-jets are intensively investigated as they are essential to optimize the combustion process. Among others, a current challenge is to understand the coupling between the injection system, the flame and the chamber acoustics, in order to predict and possibly avoid thermo-acoustic combustion instabilities. Such a goal needs a realistic description of the physics of atomization, which is highly sensitive to the gas flow hydrodynamics and acoustics.

Although atomization of liquid jets and sheets has been the subject of intense research, its modeling and simulation is still a challenge. Most works use surface tracking approaches like Level-Set [1], Volume Of Fluid [2] or Ghost Fluid methods [3]. Those methods proved to be efficient and able to predict various configurations of multiphase flows but are still facing difficulties when it comes to simulate primary atomization, and require considerable computing time which make them hardly applicable to real complex cases. Another class of approach is based on the "diffuse interface" concept, where a thermodynamic closure allows to describe the liquid-gas equilibrium without resolving the interface. However, such methods still require high mesh resolution. In this context the Lattice-Boltzmann Method (LBM), which relies on a mesoscopic description of the fluids, offers an interesting numerical alternative. Its easy implementation and its highly-parallelizable nature make it competitive with standard CFD approaches. The high potential of LBM to simulate diffuse interface problems has been recently demonstrated [4], in particular in the case of high density and/or velocity ratios between the phases, which is relevant for the study of atomization which corresponds to those conditions.

In this work, we describe a new method inspired by both color gradient method [5] and mean field method [6]. This method offers many advantages compare with popular ones (Shan-Chen, Mean Field, Free energy and RK). The use of a pressure-based method allows the possibility to choose the equation of state in a stable way, and the recoloration step from color gradient method offers a simple way to thicken artificially the interface between the two phases. The ability to produce realistic results, and the stability at high density ratio is evaluated and the advantages of this new method is assessed by a comparison with classical ones. From these results future research directions are finally proposed.

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LATTICE-BOLTZMANN MODELLING OF PARTICLE SOLIDIFICATION UNDER FLOW

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Key Words: Lattice-Boltzmann method, boundary conditions, advection-diffusion, solidification, suspension

Nanoparticles have wide potential for present and future applications, from drug delivery to surface coatings. Control over (e.g. silica) nanoparticle morphology, size, porosity and dispersity is crucial for realisation of their use [1]. The physics of growth of such particles in flow relies on various effects and time scales (such as advection, diffusion, and deposition rates) and is therefore not well understood. Industrial scale-up, which remains challenging, relies on predictability that can only be developed with novel numerical methods.

We present a lattice Boltzmann (LB) algorithm [2] that models growth of particles under particle-resolved flow conditions via chemical species deposition. The method combines fluid LB for hydrodynamics, advection-diffusion LB for species transport, resolved suspended particle dynamics, and a novel mesoscale sub-grid adsorption boundary condition for particle growth. The algorithm has been benchmarked for different 2D cases, such as isotropic particle growth in a purely diffusive reservoir and growth of moving particles in a simple shear flow at different Péclet and Hatta numbers.

Our method enables the study of flow effects on particle growth, morphology and size distribution of particle suspensions. The method will be further extended to nanoscale particle growth where it will advance the field of nanoscale particle synthesis.

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NUMERICAL SIMULATION OF THERMAL PLUMES USING LATTICE BOLTZMANN METHOD

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Key Words: *Thermal plumes, Buoyancy force, Turbulent flow, CFD, Lattice Boltzmann method, ProLB.*

Thermal plumes are involved in many aspects of fire safety including wildfires, fire detection, and fire suppression. Consequently, the accurate prediction of those turbulent plumes is fundamental and indispensable. In the literature many works on thermal plumes were reported, from the early correlative approaches from experiments to more recent numerical simulations. Most of numerical studies have considered numerical simulations based on **Navier-Stokes** equations from direct numerical simulation, **DNS**, large eddy simulation, **LES**, reaching Reynolds Averaged Navier Stokes, **RANS** [4-5]. In this work, a new promising technique is investigated, utilizing a whole different set of equations called the **Lattice Boltzmann** equations. The speed of the LBM makes it attractive nowadays compared to classical Navier-Stokes solvers. The need of such a low cost method rises from the huge computational resources required for LES in large–scale plumes. Hybrid LBM-NS [1-2-3] will be used in this study where the LBM will be used for mass and momentum conservations while the usual Navier-Stokes formulation will be considered for the energy equation. This hybrid technique is chosen because it is easily extendable afterwards for fire plume simulations where combustion will be required. Free inlet/outlet boundary conditions are considered along the sides and at the top boundary of the computational domain, a no slip boundary condition is applied on the ground, as for the inlet a velocity profile is imposed in addition to a constant heat input or temperature. Different collision models and sub-grid models are assessed and different levels of refinements are exploited for mesh convergence study. Comparisons and validations with other numerical simulations are held to demonstrate the potential inherited in the LBM from both accuracy and cost points of view. Experimental results and analytical solutions from the literature will be used for validation as well.

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Random Batch Methods for classical and quantum interacting particle systems

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Key Words: *interacting particle systems, N-body Schrodinger equation, random batch methods*

We develop random batch methods for interacting particle systems with large number of particles. These methods use small but random batches for particle interactions, thus the computational cost is reduced from O(N^2) per time step to O(N), for a system with N particles with binary interactions.

For one of the methods, we give a particle number independent error estimate under some special interactions.

For quantum N-body Schrodinger equation, we obtain, for pair-wise random interactions, a convergence estimate for the Wigner transform of the single-particle reduced density matrix of the particle system at time t that is uniform in N > 1 and independent of the Planck constant \hbar. To this goal we need to introduce a new metric specially tailored to handle at the same time the difficulties pertaining to the small \hbar regime (classical limit), and those pertaining to the large N regime (mean-field limit).

The classical part was a joint work with Lei Li and Jian-Guo Liu, while the quantum part was with Francois Golse and Thierry Paul.

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SOME PRELIMINARY RESULTS ON A KINETIC SCHEME THAT HAS AN LATTICE BOLTZMANN METHOD FLAVOUR TRACK NUMBER : 200

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Key words: LBM, kinetic schemes

ABSTRACT

In this talk we intend to describe one way to construct explicit arbitrarily high order kinetic schemes on regular meshes. The method can be arbitrarily high order in space and time, and run at CFL one. This is a common feature with the Lattice Boltzmann Methods. However, the type of Maxwellian we use here are different. This results in very simple and CPU efficient methods.

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STUDY OF A PRESSURE-BASED HYBRID LATTICE BOLTZMANN METHOD FOR THE SIMULATION OF COMPRESSIBLE FLOWS

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Key Words: Lattice Boltzmann Method, Compressible flows, Hybrid method, Recursive regularized

The Lattice Boltzmann Method (LBM) is an alternative technique for the simulation and modelling of fluid flows based on the Boltzmann equation. One of its advantages is its ability to handle very complex geometries with massively parallel computing. The LBM has achieved great success in simulating nearly incompressible and isothermal fluid flows, but it restricts its application range. A particularly active topic of investigation is its extension to more complex flows (e.g. multi-phase, thermal, compressible). We propose a pressure-based prediction-correction [1, 2] hybrid LBM model compatible with nearest-neighbor lattices (D2Q9 and D3Q19) with a single time relaxation process, to simulate subsonic and transonic compressible flows without shock.

The approach is hybrid [3]: mass and momentum conservation equations are computed using a LBM solver while an entropy conservation equation is solved via a finite difference approach. Following [3], an adequate forcing term is added to reproduce a correct viscous stress tensor and hybrid recursive regularized approach [4] is used to stabilize the solution. Discretization of the entropy equation with viscous heat dissipation, in the finite difference part of the solver, is studied to improve accuracy of the scheme and to reduce the cost of calculations.

Validation of this new method is carried out on a number of canonical cases, systematically challenging the coupling between velocity, pressure and temperature, including pressure wave propagation, and thermal Couette flows.

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The worm-LBM

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Key Words: *lattice Boltzmann method, high Knudsen number, phonon transport*

The lattice Boltzmann method (LBM) is widely used in fluid dynamics, radiation transfer, neutron transport, and more recently to study diffusive-ballistic phonon heat transport [1]. The LBM has the advantage that it naturally avoids numerical smearing and angular false scattering in the ballistic regime. Nonetheless, the ray effect hinders the application of the LBM in the limit of high Knudsen numbers, i.e. the diffusive-ballistic regime [2]. The ray effect is caused by the use of a limited number of propagation directions, to discretize the angular space, which leads also to an artificially anisotropic propagation. We propose the worm-lattice Boltzmann method (worm-LBM), which allows an arbitrary number of propagation directions, by decomposing them into the basic directions (along grid and diagonal) of a standard LBM grid, and alternating these directions over time [3]. Moreover, applying a time adaptive scheme it is possible to impose a close to isotropic propagation (or in fact any angular distribution of lattice velocities). We demonstrate the method for ballistic-diffusive phonon transport. However, the applicability of the method goes beyond this particular example, and can be used for numerical simulations of any transport problem in the high Knudsen number regime, which can be described by the Boltzmann transport equation.

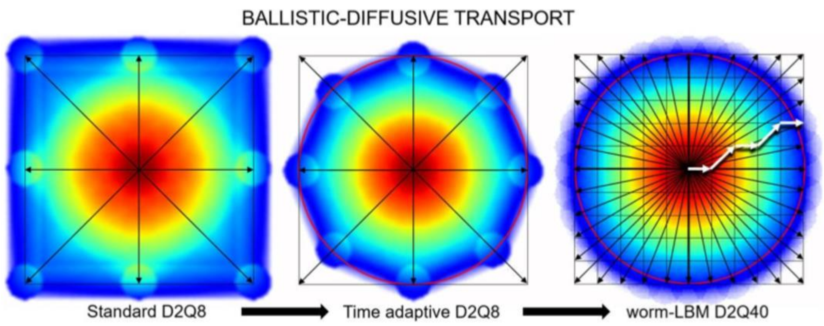

Figure 1: Ballistic-diffusive phonon transport, shown for conventional D2Q8 scheme, the time adaptive D2Q8 and the worm-LBM-D2Q40. The initial temperature of the domain, was set to 299.5 K, except for a central region of radius 1/30 of the domain length, which was initialized at 300.5. The Knudsen number is ~0.05.

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TOWARDS AN IMPROVED MODELING OF SOLID WALL BOUNDARY CONDITION IN A LBM THERMAL MODEL FOR FULL SCALE INDUSTRIAL FLOW SIMULATION

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Key Words: LBM, Thermal model, Wall boundary condition, Industrial flow simulation

Lattice Boltzmann method presents a good potential in the simulation of fluids mechanics, in particular for isothermal incompressible flows with its properties of high accuracy, parallel calculation and easy implementation to predict the complex flow in the realistic conditions [1]. More recently, in the team the extension to compressible thermal flows has been conducted successfully [2].

In this context, a hybrid Lattice Boltzmann based finite volume method is introduced [2] in which the continuity and momentum equations are solved by the traditional Lattice Boltzmann solver and an additional energy or entropy equation solved under the classical finite volume solver. In addition, a hybrid recursive regularization (HRR) collision operator is developed on standard lattices [3] which improves the stability and accuracy so that we could capture the turbulent flow in high Reynolds numbers.

The combination of uniform grids and cut-cell method [4, 5] still raise some open numerical issues that we propose to address in this work. It's probably true in nonisothermal simulations in which the heat flux must be accurately predicted at the solid wall. The impact of the interpolation schemes and of a turbulent wall model will be analysed in terms of mass leakage and heat flux accuracy.

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TOWARDS LATTICE-BOLTZMANN SIMULATIONS OF LOW-REYNOLDS-NUMBER FLOW-STRUCTURE INTERACTIONS USING IMMERSED BOUNDARIES

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Key Words: lattice-Boltzmann method, immersed-boundary method, low-*Re* flows, flow-structure interactions

Flow-structure interactions (FSI) can occur at the microscale. In living organisms for instance, microscale FSI are determinant for several critical processes as cell locomotion, mechanotransduction and fluid transport involving cilia, flagella or other types of slender bodies. At such scale, the Reynolds number (*Re*) tends to be small and adapted numerical methods have to be developed. In this work, we address the development of efficient numerical methods, based on the lattice-Boltzmann (LB) and immersed-boundary (IB) methods, for the simulation of such systems.

Considering a given geometry, two parameters can be varied in order to decrease the value of *Re* in LB simulations: the flow velocity and the fluid viscosity. However, explicit immersed-boundary methods exhibit a major boundary slip at large viscosities. An analysis of this numerical error allows to derive a new IB scheme that drastically extends the range of viscosities that can be employed using the IB-LB method [1], avoiding any additional computational cost. As this range remains finite, further decrease of the Reynolds number can only be achieved by decreasing the flow velocity, which can dramatically increase the computational cost of unsteady simulations. To overcome this problem, a dual-time-stepping (DTS) algorithm is proposed, allowing to freely vary the value of the time step [2]. The DTS is coupled to a multigrid method that ensures high computational efficiency.

The reliability of these methods is illustrated for two standard physical configurations: the pipe flow and the flow past a circular cylinder. The latter setup is considered in various forms including fixed, towed, oscillating and impulsively started cylinders. The proposed methods are efficient, accurate and exhibit features that may be beneficial in a variety of engineering contexts. Their implementation in three-dimensions is straightforward and they are suitable for addressing complex flow dynamics as non-Newtonian behaviors often encountered in biological systems.

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