DG methods for the Galerkin-Boltzmann equations in *Nektar++*

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1 Outline

Nektar++ is an open-source software for scientific computations based on spectral/*hp* element methods, which is designed to simplify the task of applying high-order finite element methods in a variety of application areas and support the development of high-performance scalable solvers for partial differential equations, typically for fluid mechanics simulations. The focus on this project is to implement an alternative to the lattice-Boltzmann equations, which is the so-called Galerkin-Boltzmann equations — a first-order PDEs system. For this system, there exists a freedom in choice of the numerical methods which gives the possibility to use implicit or semi-implicit schemes and unstructured meshes. At the same time, one has a possibility to use absorbing boundary layers and improve time step restriction to achieve better stability in solving high Reynolds number flows. It is needed to mention that around the theoretical part of the work, we are going to explore potential joint interest with Prof. Christopher Pains group.

2 Project objectives

The Boltzmann equations based on kinetic theory describe fluids at the microscopic level. In the low Mach limit, it has been shown that the Boltzmann equations recover the Navier-Stokes equations. In order to circumvent the complex nonlinear integral nature of the collision term in the Boltzmann equations, the collision term is often replaced by relaxation models. The Bhatnaggar-Gross-Krook (BGK) scheme is broadly adopted based on single time relaxation approximation. Recently, for weakly-compressible flows, lattice Boltzmann methods are widely used to discretize the BGK-Boltzmann equations, which is a first order, explicit, upwind finite difference scheme for the discrete Boltzmann equation by using a finite number of velocities to approach the continuous velocity space. Although lattice Boltzmann method has achieved a great success in simulating low-Mach flows and aeroacoustics, lattice Boltzmann method is based on structured meshes and suffers numerical instability at high Reynolds numbers due to small relaxation time. Implicit-Explicit (IMEX) methods are popular schemes to relax the time step restriction in stiff ODEs such as the discrete Boltzmann equations. For this project, we are going to apply these schemes to the Galerkin-Boltzmann equations. The continuous velocity space is discretized by a Galerkin procedure with Hermite polynomials. The Hermite expansion coefficients are corresponding to macroscopic variables, which are governed by a first order conservation law. These first-order partial differential equations can be solved by discontinuous Galerkin discretizations. Therefore, the classical methodologies for the first order conservation law can be applied to enhance stability of numerical schemes. Meanwhile, the perfectly matching layer (PML) formulation is implemented for the Galerkin-Boltzmann equations for removing the wave reflection from boundaries of computational domain. The purpose of this project is to support the development of a new solver to compute the Galerkin-Boltzmann equations by IMEX time integration (or implicit time integration) and discontinuous Galerkin discretizations for low-Mach vehicle flows and aeroacoustics.

One of the key tasks before finishing the discontinuous Galerkin discretizations for Galerkin-Boltzmann equations such that the 2D or 3D system is solved in *Nektar++*. Once the basic solvers have been validated, the PML will be coupled with the system. I have been working on both the code development and numerical computations, such that I am in an excellent position to continuously achieve the above outline project goals in a fast and efficient manner. This can be a very valuable contribution to *Nektar++* and will open up the opportunity to use the Galerkin-Boltzmann equations to efficiently simulate low-Mach flows and aeroacoustics in a simple manner. At the same time, the final solver can be employed to implement complex computations for complex industrial flows under the framework of *Nektar++*.

3 Alignment with PRISM strategy

Development of key staff: I have a strong background in computational mathematics and physics, and will be closely working with Dr. Hui Xu who is one of the developers of *Nektar++*. At present, I am actively seeking a permanent academic position, in which *Nektar++* forms a central part of my research activities. This will be beneficial for the dissemination of *Nektar++* into other fields and institutions. My expertise will allow me to finish the goals of the proposal in the 6-month timeframe.
Collaboration with other PRISM projects: The project will allow the PRISM group to use the new generation Unstructured mesh Galerkin-Boltzmann Solvers (UGBS) for other related applications. An additional goal of this project is to resolve complex low-Mach flows with minimal computational performance. For this goal, I plan to collaborate with other members of PRISM group such as Prof. Christopher Pain.
Longer-term research: This project provides me an opportunity to get back into research after having a baby. At the same time, the project is intended to lay the basis of an application for a fellowship, in which some new methodologies will be implemented and some fundamental applications will also be studied. However, this project will provide initial evidence to use the unstructured Galerkin-Boltzmann method to understand low-Mach complex flows.

4 Brief workplan

The framework of the solver has been created. The class “GalerkinBoltzmann” was created. Now, the work is focused on finishing the classes of “BoltzmannSolver” and “UpwindSolver” and handling the boundary condition. In implementing the DG discretizations , I will try to find out a solution for rotational invariance. The follow-up work will be focused on implementing PML for acoustic problems. Finally, a manuscript will be drafted.