High-order gas evolution model for computational fluid dynamics

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The foundation for the development of modern computational fluid dynamics (CFD) is based on the Riemann solution of the Euler equations. The high-order schemes are basically related to high-order spatial reconstruction. In order to overcome the low-order wave interaction mechanism due to the Riemann solution, the temporal accuracy of the scheme is improved through the Runge-Kutta time stepping method. The close coupling between the spatial and temporal evolution in the original nonlinear governing equations seems weakened due to its spatial and temporal decoupling. For the viscous flow, the piece-wise discontinuous initial data and the hyperbolic-parabolic nature of the Navier-Stokes equations seem inconsistent mathematically, such as the divergence of the viscous and heat conducting terms due to initial discontinuity. Therefore, in order to alleviate this difficulty, the inviscid and viscous terms in the NS equations are numerically treated differently in most CFD methods.

Based on the Boltzmann equation, we are going to present a high-order gas dynamic model, the so-called time-dependent flux function at a cell interface, from a high-order discontinuous initial reconstruction. The theoretical basis for such an approach is due to the fact that the Boltzmann equation has no specific requirement on the smoothness of the initial data and the kinetic equation has dynamic mechanism to construct a dissipative wave structure starting from an initially discontinuous flow condition on a time scale of particle collision time. More specifically, the gas-kinetic scheme covers a whole spectrum of scales, from the kinetic to the hydrodynamic ones. This talk will present a hierarchy to construct high-order gas-kinetic scheme (GKS).

In comparison with the Riemann solver, the GKS provides a valid physical evolution process from a discontinuity. The GKS first presents particle free transport process, then through the particle collision it generates the dissipative wave structure. With intensive particle collisions within a time step, such as in the hydrodynamic scale, a Navier-Stokes gas distribution function can be obtained from the GKS. The Euler solution is considered as a limiting case when intensive particle collisions take palce. Numerically, the GKS formulation makes a smooth transition from the upwind to the central difference scheme in the process of gas evolution. It is a unification of two different algorithm development methodologies in the traditional CFD methods. This kind of mechanism can be hardly described using any macroscopic governing equation. Theoretically, the gas-kinetic equation provides a mechanism for the transport in all scales from kinetic to hydrodynamic. On the other hand, the macroscopic governing equations, such as the NS equations, describe the flow evolution in the hydrodynamic one only. How to handle the discontinuity becomes a fundamental problem in

CFD. Even though the Riemann solution of the Euler equations can mathematically handle the initial discontinuity, the validity of using such a solution in the description of a numerical shock in a discretized space is questionable from a physical modeling point of view.

A numerical shock layer on the scale of a few mesh points needs to be considered as an enlarged physical shock structure. Since a physical shock has the thickness on the order of particle mean free path, an enlarged numerical shock layer means the size to become the length scale of numerical particle mean free path. Therefore, on the scale of cell size, the non-equilibrium flow physics has to be taken into account in the gas evolution process in the shock region. As we know, as a particle moves across a physical shock layer, there is only limited number of particle collisions. The non-equilibrium shock structure is constructed through the competition between particle free transport and collision. This non-equilibrium process provides the appropriate dissipation for the smooth transition from one equilibrium state at upstream to another equilibrium one at downstream. But, inside the numerical shock layer, the exact Riemann solver replaces the non-equilibrium physical reality by an equilibrium one with the assumption of infinite number of particle collisions and the generation of distinguishable waves. As a result, the numerical process of the Riemann solution has no a dynamic dissipative mechanism, especially in multi-dimensional case. Therefore, the use of the Euler equations in the flux modeling must have problem in the non-equilibrium region, such as the triggering of shock instability in Godunov method in high Mach number flow simulation. The GKS follows closely the flow physics. The initial free transport, which provides numerical dissipation, depends closely on the jump of the discontinuity. For the contact discontinuity wave, the exact Euler solution assumes infinite number of particle collisions which prevent the penetration of particles crossing each other. For the GKS, the particle penetration exists all the time in its underlying modeling.

In a discretized space, any physical discontinuity is enlarged to the cell size scale due to the limited resolution. Since the Riemann problem is truthfully solving the Euler equations, the absence of non-equilibrium mechanism indicates that the Euler solution cannot be properly used as dynamic evolution model for the enlarged dissipative region. One may think of using the NS equations with dissipative terms to capture the corresponding non-equilibrium layer. But, this cannot be fully valid, because the NS equations have only the physical dissipation on the hydrodynamic scale, which cannot be used to describe the flow behavior in the kinetic scale, such as the initial particle free transport process from an discontinuity.

The main idea we would like to deliver is that for a shock capturing scheme we need a correct physical mechanism to model the gas evolution from a discontinuity in the discretized space. There is no valid macroscopic governing equations to describe such a physical mechanism yet. The value of gas-kinetic scheme is that it provides a new way for the CFD algorithm development. A valid physical process will become more important in the construction of high-order CFD methods. The numerical examples will demonstrate the importance of high-order gas evolution model.