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RESEARCH PAPER

Direct modeling for computational fluid dynamics

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Abstract All fluid dynamic equations are valid under their modeling scales, such as the particle mean free path and mean collision time scale of the Boltzmann equation and the hydrodynamic scale of the Navier–Stokes (NS) equations. The current computational fluid dynamics (CFD) focuses on the numerical solution of partial differential equations (PDEs), and its aim is to get the accurate solution of these governing equations. Under such a CFD practice, it is hard to develop a unified scheme that covers flow physics from kinetic to hydrodynamic scales continuously because there is no such governing equation which could make a smooth transition from the Boltzmann to the NS modeling. The study of fluid dynamics needs to go beyond the traditional numerical partial differential equations. The emerging engineering applications, such as air-vehicle design for near-space flight and flow and heat transfer in micro-devices, do require further expansion of the concept of gas dynamics to a larger domain of physical reality, rather than the traditional distinguishable governing equations. At the current stage, the non-equilibrium flow physics has not yet been well explored or clearly understood due to the lack of appropriate tools. Unfortunately, under the current numerical PDE approach, it is hard to develop such a meaningful tool due to the absence of valid PDEs. In order to construct multiscale and multiphysics simulation methods similar to the modeling process of constructing the Boltzmann or the NS governing equations, the development of a numerical algorithm should be based on the first principle of physical modeling. In this paper, instead of following the traditional numerical PDE path, we introduce direct modeling as a principle for CFD algorithm development. Since all computations are conducted in a discretized space with limited cell resolution, the flow physics to be modeled has to be done in the mesh size and time step scales. Here, the CFD is more or less a direct construction of discrete numerical evolution equations, where the mesh size and time step will play dynamic roles in the modeling process. With the variation of the ratio between mesh size and local particle mean free path, the scheme will capture flow physics from the kinetic particle transport and collision to the hydrodynamic wave propagation. Based on the direct modeling, a continuous dynamics of flow motion will be captured in the unified gas-kinetic scheme. This scheme can be faithfully used to study the unexplored non-equilibrium flow physics in the transition regime.

Keywords Direct modeling · Unified gas kinetic scheme · Boltzmann equation · Kinetic collision model · Non-equilibrium flows · Navier–Stokes equations

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1 Modeling for computational fluid dynamics

1.1 Limitation of current CFD methodology

All fluid dynamic equations are constructed by modeling flow physics with the implementation of physical laws, such as mass, momentum, and energy conservation, in different scales. With a variation of resolution to identify physical reality, different governing equations have been obtained. The two most successful ones are the Boltzmann equation and the Navier–Stokes (NS) equations. These equations are mathematical representations of the flow physics in the corresponding modeling scales. The current computational fluid

dynamics (CFD) methodology is mostly based on the direct discretization of these equations in a discretized space, i.e., the so-called numerical partial differential equations (PDEs). In the numerical discretization, there is no longer a direct account of the physical modeling scale. Even with the appearance of new scales, such as the mesh size and time step, except the truncation error, the dynamics from mesh size scale has never been seriously considered in CFD practice.

The current target of CFD is to recover the solution of the original PDEs as the mesh size and time step approach zero. Under such a CFD methodology, the best result is hopefully to get the exact solution of the governing equations. But the flow physics described by the numerical solution is still limited by the modeling physics of the original governing equations. In reality, due to the limited cell resolution, we can never get the exact solution of the original governing equations due to the truncation error. Theoretically, we never know what the exact underlying governing equation of the CFD algorithm is, especially in the regions with unresolved "discontinuities", and the uniqueness of the numerical solution becomes a luxury requirement. For example, there are many CFD algorithms for the same PDEs, such as the gigantic number of approximate Riemann solvers for the Euler equations. If the design principle of the CFD method is based on the limiting solution with vanishing mesh size, the mission of CFD can be never achieved. In addition to the assumption of the flow physics, such as the smoothness of flow variables, all PDEs are derived based on additional mathematics for simplification, such as shrinking a control volume to zero thickness in order to properly use the definition of derivatives. During this process, the peculiarity of the application of physical laws in different geometric configurations is lost. In other words, the geometric information is absent in the fluid dynamic equations. Unfortunately, a numerical scheme does need a mesh, and the lost geometric information has to be added back in the numerical discretization of the PDE, such as the implementation of geometrical conservation law.

For the Euler equations, due to the limited numerical cell resolution, it becomes impossible to capture the zero shock thickness of the equations. Theoretically, the best resolution a scheme can have is the mesh size. However, the shock thickness with numerical mesh size scale can be only recovered from the Euler equations with an additional amount of numerical dissipation. But, due to the absence of the dissipation in the Euler modeling, the lost physics, i.e., the dissipative mechanism in the mesh size scale, has to be created artificially through the numerical procedure, such as all kinds of implicit and explicit dissipation in the Euler solvers. With the possible inconsistency of this kind of artificial dissipation from a physically required one with a "physical" shock structure in the mesh size scale, it will not be surprising to observe any unfavorable numerical behavior, such as the shock instability in the Godunov method at strong shock cases, which is

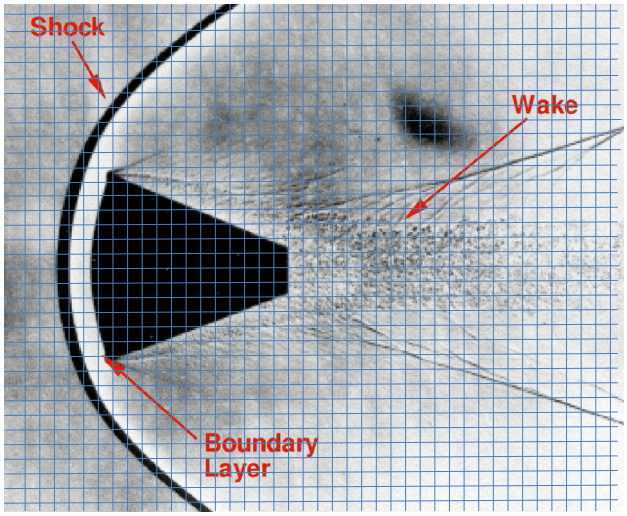

Fig. 1 Schematic of hypersonic flow over a blunted body with regions that typically exhibit non-continuum effects [1,2]

a "black cloud" hanging over the clear CFD sky. Even targeting on the inviscid Euler equations, all numerical schemes have to add a non-equilibrium dissipative effect, where new governing equations have to be solved implicitly. The incompatibility of physical modeling scale of PDEs and the mesh size scale has never been seriously studied in the current CFD methodology.

In the current CFD, due to the separation between the numerical discretization and the physical modeling, in most cases the PDEs are blindly numerically treated. For example, in the direct numerical discretization of the Fourier's law, where the heat flux is proportional to temperature gradient, the mesh size used can be from 10^{-10} m upto 1 m, 1 km, or even 1 light year! How could we believe that such a law is still valid for such a mesh size scale? The gigantic number of experiments clearly demonstrate the invalidity of Fourier's law for microscale heat transport [3]. Instead of separating numerical discretization from physical modeling, the CFD should aim to model the flow physics in the mesh size scale directly and figure out the physical law at such a scale. Figure 1 presents the experiment of a hypersonic flow passing through a blunt body. If the flow physics is to be described using a mesh size scale, at different locations different flow physics will be identified, such as the equilibrium flow in the upstream region, highly non-equilibrium flow in the shock region, the rarefied flow in the trailing edge, and turbulent flow in the wakes. In terms of mesh size resolution, different flow physics appear locally in different regions.

One example which cannot be properly treated in the current CFD methodology is the flow simulation of a flight vehicle passing through the whole atmosphere environment. With a reasonable number of mesh points around a vehicle, such as 10^9 mesh points in total, at different altitudes the number of particles and their dynamic description in the

mesh size scale will be different. At altitudes below 40 km, inside each control volume of mesh size scale, there are a gigantic number of particles, the flow can be described by the NS equations for the accumulating wave effect. At altitudes above 80 km, the mesh size may come to be compatible with the particle mean free path, the Boltzmann equation or the direct simulation Monte Carlo (DSMC) method can be used for capturing the particle movement and collision. However, in the transition regime between 40 and 80 km, the number of particles inside each numerical cell varies significantly and the corresponding physics has both particle and wave effect. There is basically no such a valid governing equation at this mesh size scale. Theoretically, we may refine the mesh size to the particle mean free path and apply the Boltzmann equation everywhere. But it just becomes a brute force approach and it is unrealistic under current computational resources. It is true that the Boltzmann equation is valid in all flow regimes from free molecular to the continuum NS solution. But this statement is based on the assumption of fully resolving the Boltzmann physics in the mean free path scale. In the continuum flow regime, we do not have the luxury of constructing a mesh in the mean free path scale. The aim of CFD is to describe the flow physics accurately in a most efficient way.

1.2 CFD modeling

Following the current CFD methodology, it becomes difficult to develop a multiple scale method if there is no such valid governing equation for all scales. A few distinct governing equations with specific modeling scales may not be adequate to present a complete picture of gas dynamics. The reason for the existence of a few distinguishable governing equations, such as the NS and the Boltzmann, is that it is relatively easy to do the modeling at these scales. The Boltzmann equation separates the particle transport and collision, which is a valid modeling in the mean free path scale for dilute gas. The NS equations describe the accumulating collisional effect of a gigantic number of particles with wave propagation in the hydrodynamic scale. The NS equations are valid in the situation that there is a linear relationship between stress and strain. In the scale between the above two limits, the non-equilibrium flow behavior appears, which encounters great difficulty in its modeling. Actually, how to describe the non-equilibrium flow and what kind of flow variables to be tracked here are not so clear.

Even without a valid governing equation for all scales, we still need to study the flow dynamics in different regimes. Fortunately, the CFD provides us an alternative way to design numerical algorithms, i.e., the so-called construction of discrete governing equations through direct modeling, see Fig. 2. The principle of direct modeling is not to solve any specific equation, but to construct a flow evolution model in the mesh size scale. With the variation of the ratio between the mesh size and the local particle mean free path, the modeling should be able to capture different flow physics from the kinetic scale particle collision and transport to the hydrodynamic scale wave propagation.

The unified gas-kinetic scheme (UGKS) has been developed under such a direct modeling principle, where a continuous description of flow physics from kinetic to hydrodynamic scale is recovered in its numerical algorithm [3–11]. The success of the UGKS is due to the automatic adoption of a crossing scale modeling of flow physics in the numerical flux construction. The specific solution used locally for the update of flow variables depends on the ratio between the local time step and the local particle collision time. With the variation of this ratio, the UGKS provides a smooth transition of different scale flow physics. In the following section, the basic idea underlying the UGKS method will be introduced, which is followed by the analysis and applications in various flow regimes.

2 Unified gas kinetic scheme

2.1 General methodology

Physically, different flow regimes are defined through the Knudsen number, which is defined as the ratio of the particle mean free path to the characteristic length scale, such as the continuum ($Kn \leqslant 10^{-3}$), transition ($10^{-3} < Kn < 10$), and free molecular ones ($Kn \geqslant 10$). Numerically, the computation takes place in a discretized space. With the current computer power, the mesh size used in an engineering application is limited, such as $10^3 \times 10^3 \times 10^3$ grid points in the physical space. With such a mesh distribution around a flying vehicle, the flow dynamics to be identified inside each control volume depends on the local mesh resolution and the particle mean free path. With a large variation of the mesh size over the particle mean free path, a unified scheme aims to capture the corresponding flow physics in different flow regime.

The construction of the unified scheme is similar to the modeling process in the derivation of theoretical fluid dynamic equations, but without shrinking the control volume to zero. Different mesh size scale in terms of local particle mean free path will notify different transport phenomena. The accuracy requirement in a physical modeling depends on the information needed for a practical engineering application, and the availability of computational resources. If the cell size comes to a scale of particle mean free path everywhere, the Boltzmann modeling physics, such as transport and collision, can be directly used to construct the scheme [12,13]. If the cell size and time step are much larger than the particle mean free path and particle collision time, the corresponding physics due to the accumulation of particles transport and collision needs to be modeled.

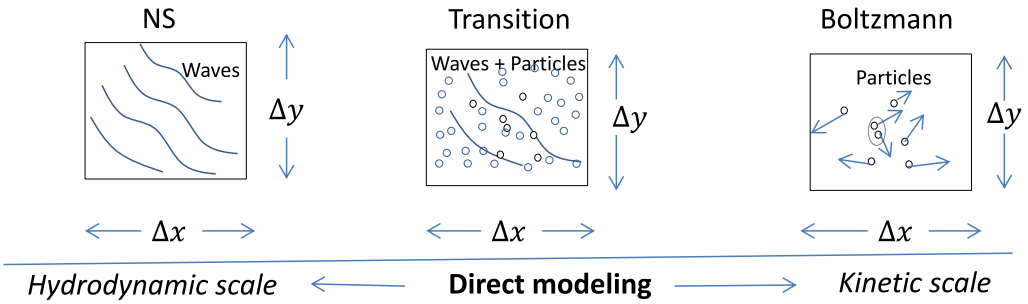

Fig. 2 Direct CFD modeling in mesh size scale

The main ingredients in the unified scheme are the modeling of flow transport across a cell interface and inner cell collision. The modeling solution covers the evolution process from the initial free transport to the final hydrodynamics wave propagation. More specifically, the time evolution solution modeling in the algorithm includes the non-equilibrium particle transport and the equilibrium NS solution within a single formulation. The weights of the contribution from the kinetic and hydrodynamic parts in the flux transport depend on the ratio of time step to the local particle collision time. Therefore, the numerical governing equation underlying the unified scheme depends on the space and time resolution. The Boltzmann equation is recovered in the kinetic scale. The evolution solution with the accumulation of particle collisions captures the flow physics in the transition regime.

2.2 Numerical evolution equations

The unified scheme is a direct modeling in a discretized space. The "governing" equation is the numerical algorithm itself. Since the modeling is on the mesh size and time step scale, there is no reason to "get" the so-called PDEs.

The discretized space is divided into control volume, i.e., $\boldsymbol{\Omega}_{i,j,k}(\boldsymbol{x}) = \Delta x\Delta y\Delta z$ with the cell sizes $(\Delta x) = x_{i+1/2,j,k} - x_{i-1/2,j,k}$, $\Delta y = y_{i,j+1/2,k} - y_{i,j-1/2,k}$, and $\Delta z = z_{i,i,k+1/2} - z_{i,j,k-1/2}$ in a physical space. The temporal discretization is denoted by t^n for the n-th time step. The particle velocity space is discretized by Cartesian mesh points with velocity spacing Δu, Δv, and Δw with a volume $\boldsymbol{\Omega}_{l,m,n}(\boldsymbol{u})$, around the center of the (l, m, n)-velocity interval at (u_l, v_m, w_n). The fundamental flow variable in a discretized space is the cell-averaged gas distribution function in a control volume (i, j, k), at time step t^n, and around particle velocity (u_l, v_m, w_n),

$$f(x_i, y_j, z_k, t^n, u_l, v_m, w_n) = f^n_{i,j,k,l,m,n} = \frac{1}{\Omega_{i,j,k}(\boldsymbol{x})\Omega_{l,m,n}(\boldsymbol{u})}\int_{\Omega_{i,j,k}}\int_{\Omega_{l,m,n}} f(x, y, z, t^n, u, v, w)\,\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{u},$$

where $\mathrm{d}\boldsymbol{x} = \mathrm{d}x\mathrm{d}y\mathrm{d}z$ and $\mathrm{d}\boldsymbol{u} = \mathrm{d}u\mathrm{d}v\mathrm{d}w$.

The time evolution of a gas distribution function in the computational space is due to the particle transport through cell interface and the particle collisions inside each cell, which re-distributes particles in the velocity space. The direct modeling in such a space gives

$$f^{n+1}_{i,j,k,l,n,m} = f^n_{i,j,k,l,m,n} + \frac{1}{\Omega_{i,j,k}}\int_{t^n}^{t^{n+1}}\sum_{r=1} u_r \hat{f}_r(t)\Delta S_r\mathrm{d}t + \frac{1}{\Omega_{i,j,k}}\int_{t^n}^{t^{n+1}}\int_{\Omega_{i,j,k}} Q(f)\mathrm{d}\boldsymbol{x}\mathrm{d}t, \quad (1)$$

where $\hat{f}_r$ is the time-dependent gas distribution function at a cell boundary, which is integrated along the surfaces of the control volume $\Omega_{i,j,k}$, u_r is the particle velocity component normal to the cell interface, ΔS_r is the r-th cell interface area, and $Q(f)$ is the particle collision term, which redistributes the particle in the velocity space due to collision. The above equation is the fundamental governing equation in a discretized space. It is an evolution equation in the mesh size scale. The dynamics underlying the above equation depends on the size of the control volume, where the modeling of the interface flux and collision term inside each cell depends on the scale of control volume.

Equation (1) can be considered an integral form of the Boltzmann equation, but it is beyond the validity regime of the Boltzmann equation on the kinetic scale if the interface flux is properly modeled instead of direct streaming of particles. On the other hand, if Eq. (1) is considered a direct modeling; the Boltzmann equation can be derived from it with a specific modeling scale on the size of control volume. The Boltzmann equation is a consequence of the physical modeling in the particle mean free path and collision time scale. Under such a scale, the particle free transport and collision can be separated in the Boltzmann equation. However, in the above equation, the mesh size and time step can go much beyond the kinetic scale. Under a much enlarged scale, such as tens of particles mean free path, the time evolution of a gas distribution function at a cell interface will not take free transport, and the collision effect inside each cell could be an accumulation of multiple particle collisions. Therefore, in terms of physical modeling

the above equation is more general than the Boltzmann equation, such as the continuity assumption is not needed for flow variables in Eq. (1). Instead of using the integral equation, a direct discretization of the Boltzmann equation will use the upwind or particle free transport for the flux evaluation. But the interface flux in the above equation has to go beyond the kinetic scale transport if the NS solution in the hydrodynamic limit needs to be recovered. Equation (1) is a representation of physical law in the mesh size scale, which could include different scale flow physics in comparison with the Boltzmann modeling. The quality of the scheme depends on the modeling of interface flux and the inner cell collision term, which are closely related to the mesh size.

If we take conservative moments ψ_α on Eq. (1), i.e.,

$$\boldsymbol{\psi} = \left(\psi_1, \psi_2, \psi_3, \psi_4, \psi_5\right)^\top = \left(1, u, v, w, \frac{1}{2}(u^2+v^2+w^2)\right)^\top,$$

where $\mathrm{d}\boldsymbol{u} = \mathrm{d}u\mathrm{d}v\mathrm{d}w$ is the volume element in the phase space. Due to the conservation of conservative variables during particle collisions, the update of conservative variables becomes

$$\boldsymbol{W}_{i,j,k}^{n+1} = \boldsymbol{W}_{i,j,k}^{n} + \frac{1}{\Omega_{i,j,k}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \boldsymbol{S}_r \cdot \boldsymbol{F}_r(t)\mathrm{d}t, \tag{2}$$

where $\boldsymbol{W}$ is the volume averaged conservative mass, momentum, and energy densities inside each control volume, and $\boldsymbol{F}$ is the flux for the corresponding macroscopic flow variables across the cell interface. These fluxes for macroscopic flow variables can be obtained from a time-dependent gas distribution function as well. Now the fundamental governing equations of the unified scheme are the Eqs. (1) and (2). These two equations are the governing equations for the description of flow motion in all flow regimes, where the flow physics solely depends on the time evolution of the gas distribution function at a cell interface and the particle collision inside each control volume. Equations (1) and (2) are the direct modeling equations; physically there is no any error introduced. The updates of the gas distribution function and the conservative flow variables depend on the modeling of interface flux and the inner cell particle collision term. In general, no conservative moments can be taken as well on Eq. (1), such as the rotational or vibrational energy, and the corresponding macroscopic equations will have additional source terms.

The central task of the unified scheme is to model a time-dependent gas distribution function at a cell interface, which is to recover gas evolution process in the mesh size scale, with a variation of the ratio between the time step and the particle collision time. In order to model the gas evolution process for the flux construction and collision term, the gas-kinetic Bhatnagar–Gross–Krook (BGK) model, the Shakhov model, the ellipsoid statistical BGK (ES-BGK) model, the Rykov model for diatomic gases, and even the full Boltzmann equation, can be used to do the modeling. Basically, a local time evolution solution of the gas distribution function at a cell interface and the particle collision inside each cell need to be supplied to the above numerical governing equations.

2.3 Physical modeling for interface flux and inner cell collision

In order to construct the interface gas distribution function and the inner cell collision in the mesh size and time step scales, we need to understand the kinetic equation first, and model the flow physics in other scales. The Boltzmann equation describes the time evolution of the density distribution of a dilute monatomic gas with binary elastic collisions. For space variable $\boldsymbol{x} \in \mathbb{R}^3$, particle velocity $\boldsymbol{u} = (u, v, w)^t \in \mathbb{R}^3$, the Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + \boldsymbol{u} \cdot \nabla_{\boldsymbol{x}} f = Q(f, f), \tag{3}$$

where $f := f(\boldsymbol{x}, t, \boldsymbol{u})$ is the time-dependent particles distribution function in the phase space. The collision operator $Q(f, f)$ is a quadratic operator consisting of a gain term and a loss term,

$$Q(f, f) = \underbrace{\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(\cos\theta, |\boldsymbol{u} - \boldsymbol{u}_*|) f(\boldsymbol{u}'_*) f(\boldsymbol{u}') \mathrm{d}\Omega \mathrm{d}\boldsymbol{u}_*}_{Q^+} - \underbrace{\nu(\boldsymbol{u}) f(\boldsymbol{u})}_{Q^-},$$

where

$$\nu(\boldsymbol{u}) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(\cos\theta, |\boldsymbol{u} - \boldsymbol{u}_*|) f(\boldsymbol{u}_*) \mathrm{d}\Omega \mathrm{d}\boldsymbol{u}_*,$$

is the collision frequency. Here, $\boldsymbol{u}$ and $\boldsymbol{u}_*$ are the pre-collision particle velocities, while $\boldsymbol{u}'$ and $\boldsymbol{u}'_*$ are the corresponding post-collision velocities. Conservation of momentum and energy yield the follow relations

$$\boldsymbol{u}' = \frac{\boldsymbol{u} + \boldsymbol{u}_*}{2} + \frac{|\boldsymbol{u} - \boldsymbol{u}_*|}{2}\Omega = \boldsymbol{u} + \frac{|_r|\Omega - \boldsymbol{u}_\mathrm{r}}{2},$$
$$\boldsymbol{u}'_* = \frac{\boldsymbol{u} + \boldsymbol{u}_*}{2} - \frac{|\boldsymbol{u} - \boldsymbol{u}_*|}{2}\Omega = \boldsymbol{u}_* - \frac{|\boldsymbol{u}_\mathrm{r}|\Omega - \boldsymbol{u}_\mathrm{r}}{2},$$

where $\boldsymbol{u}_\mathrm{r} = \boldsymbol{u} - \boldsymbol{u}_*$ is the relative pre-collision velocity and Ω is a unit vector in $\mathbb{S}^2$ along the relative post-collision velocity $\boldsymbol{u}' - \boldsymbol{u}'_*$. The collision kernel $B(\cos\theta, |\boldsymbol{u} - \boldsymbol{u}_*|)$ is nonnegative and depends on the strength of the relative velocity and deflection angle. For hard sphere molecules,

the collision kernel $B = |\boldsymbol{u}_r|\sigma = |\boldsymbol{u}_r|d^2/4$, where d is the molecular diameter. For $(\eta - 1)$-th inverse power-law, the collision kernel is a power-law function of the relative velocity

$$B = |\boldsymbol{u}_r|\sigma = c_\alpha(\theta)|\boldsymbol{u}_r|^\alpha, \quad \alpha = \frac{\eta - 5}{\eta - 1},$$

and according to the Chapman–Enskog expansion [12], the viscosity coefficient follows

$$\mu = \frac{5m(RT/\pi)^{1/2}(2mRT/\kappa)^{2/(\eta-1)}}{8A_2(\eta)\Gamma\left(4 - \frac{2}{\eta-1}\right)},$$
$$A_2(\eta) = \int_0^\infty \sin^2\chi W_0 \mathrm{d}W_0.$$

Most kinetic model equations replace the Boltzmann collision term in Eq. (3) with a relaxation-type source term $S(f)$,

$$S(f) = \frac{\tilde{M}(f) - f}{\tau_s},$$

where $\tilde{M}(f)$ maps f to the corresponding modified equilibrium state, where the ES-BGK [14] and Shakhov [15] are two popular ones, which can be combined as well [16]. Here, we will concentrate on the full Boltzmann and Shakhov model equations to construct UGKS.

The Shakhov model can be written as,

$$f_t + \boldsymbol{u}\cdot\nabla_{\boldsymbol{x}} f = \frac{\tilde{M}(f) - f}{\tau_s}, \tag{4}$$

where

$$\begin{aligned}\tilde{M}(f) =& M(f)\left[1 + (1 - Pr)\boldsymbol{c}\cdot\boldsymbol{q}\left(\frac{\boldsymbol{c}^2}{RT} - 5\right)/(5pRT)\right],\\ =& M(f) + \tau_s g^1(f),\end{aligned}$$

where $M(f)$ is the Maxwellian distribution function, $\boldsymbol{c}$ is the peculiar velocity, and $\boldsymbol{q}$ is the heat flux. Although the kinetic models are much simpler than the full Boltzmann equation, they share the similar asymptotic property [12] in the hydrodynamic regime, which means both equations recover the Euler and NS equations when the Knudsen number is small.

In UGKS, the interface flux plays a dominant role to capture the flow evolution in different scales from kinetic up to the NS ones. For example, in the 1D case, depending on the scale of Δx and Δt, the solution at the interface $f_{j+1/2,k}$ is constructed from an evolution solution of the kinetic model (Eq. (4)). Without loss of generality, the cell interface is assumed to be at $x_{j+1/2} = 0$ and t_n is assumed to be 0,

$$f(0,t,u_k,\xi) = \frac{1}{\tau_s}\int_0^t \tilde{M}(x',t',u_k,\xi)\mathrm{e}^{-(t-t')/\tau_s}\mathrm{d}t'$$
$$+ \mathrm{e}^{-t/\tau_s} f_0(-u_k t, u_k, \xi), \tag{5}$$

where $x' = -u_k(t - t')$ is the particle trajectory and $f_0(-u_k t, u_k, \xi)$ is the gas distribution function at time $t = 0$. In order to determine fully the evolution solution, the initial condition and the equilibrium states around the cell interface have to be modeled. The basic ingredient in the above equation is that the initial non-equilibrium state decays exponentially due to particle collision, which presents a gas evolution process from the kinetic scale, such as particle free transport, to the hydrodynamical scale evolution, with the emerging of equilibrium solution due to intensive particle collisions. In the hydrodynamic limit, the NS solutions can be recovered from the integration of the above equilibrium state. Besides the above two limits, the above modeling also presents the physics in the whole transition regime, which depends on the ratio of t/τ. Equation (5) is the direct modeling for the interface gas distribution function, which can be used to evaluate the interface fluxes for the update of Eqs. (1) and (2). Theoretically, we may integrate the flux based on the solution equation (5) over a local time step $\Delta t_{\mathrm{local}}$, then divide it by $\Delta t_{\mathrm{local}}$ to get an average flux. This averaged flux represents the dynamics of the local mesh size scale. Then, this local averaged flux can be used explicitly for the update of flow variables with a uniform time step Δt over the whole domain for an unsteady flow computation. In this way, the constraint on the local flow physics equation (5) due to the direct adoption of a global uniform small time step, which is determined by the Courant–Friedrichs–Lewy (CFL) condition on the smallest cell size, can be released.

Now we have two choices for the collision term modeling inside each control volume, which can be the full Boltzmann collision term $Q(f^n, f^n)$ and the model equation $(\tilde{M}(f^{n+1}) - f^{n+1})/\tau_s^{n+1}$. Depending on the flow regime, the UGKS uses a time step Δt which varies significantly relative to the local particle collision time. Starting from a general initial distribution function, for the account of particle collision only inside each control volume, the evolution solutions from the full Boltzmann collision term and the kinetic model equation will become identical after a few collision times. In other words, for a single binary collision, there are differences between the solutions from the full Boltzmann collision term and the model equation. However, when many collisions take place within a time step inside each control volume, these differences diminish. Therefore, the real place where the full Boltzmann collision term is useful is the region of highly non-equilibrium flow and with a time step being at or less than the local particle collision time [17,18]. This is reasonable because when a few collision are taken into account within a time step, the solution will not be sensitive to the individual particle collision [19]. As a result, we can model the collision term in Eq. (1) from the combination of the full Boltzmann collision term [17,18] and Shakhov model [15],

$$Q(f) = AQ(f_j^n, f_j^n)_k + B\frac{\tilde{M}(f_j^{n+1})_k - f_{j,k}^{n+1}}{\tau_s^{n+1}}, \tag{6}$$

where the coefficients A and B in the above modeling needs to satisfy the following constraints,

(1) $A + B = 1$ in order to have a consistent collision term treatment.
(2) The scheme is stable in the whole flow regime.
(3) In the rarefied flow regime, the scheme gives the Boltzmann solution.
(4) In the continuum regime, the scheme can efficiently recover the NS solutions.

One of the choices can be $A = 1$ if $\Delta t \leqslant \tau$; otherwise $A = 0$. The unified scheme does not require that the time step to be less than the particle collision time. Therefore, the unified scheme can use a scale-dependent collision term. The full Boltzmann collision term plays a role only in a small subset of the collision process. Even with the choice of Shakhov collision model only ($A = 0, B = 1$), the unified scheme can still present reasonable and accurate results in the whole flow regime. Based on the above constraints, we may also use the following choice

$$A = \beta, B = (1 - \beta), \tag{7}$$

with

$$\beta = \mathrm{e}^{-\frac{\Delta t}{\tau_r}} \min\left(1, \frac{1}{\tau_r \sup_{\mathbf{u}\in\boldsymbol{\Upsilon}} \left|\frac{Q(f,f)}{f-M}\right|}\right), \tag{8}$$

where $\boldsymbol{\Upsilon} := \{\boldsymbol{u} \in \mathcal{R}^3 | (f - M(f))(\boldsymbol{u}) \neq 0\}$. The above choice presents a smooth transition from the Boltzmann collision term to the kinetic model equation. The transition parameter β is chosen based on the following two reasons [29]:

(1) Based on the numerical experiments, we find when the ratio $\Delta t/\tau_r$ becomes large, the Shakhov model performs similarly as the Boltzmann collision term. It is reasonable to use the Shakhov model to approximate the Boltzmann operator when the time step is large. Thus, β contains an exponential term $\mathrm{e}^{-\Delta t/\tau_r}$.
(2) Both the Boltzmann collision term and Shakhov model are stiff operators. An implicit part must be included to stabilize the scheme, especially when the distribution function is highly non-equilibrium. Therefore, β contains the term $\sup_{\boldsymbol{u}\in\boldsymbol{\Upsilon}} \left|\frac{Q(f,f)}{f-M}\right|$ which indicates the deviation of the local distribution from the corresponding equilibrium. For highly non-equilibrium f, the term $\sup_{\boldsymbol{u}\in\boldsymbol{\Upsilon}} \left|\frac{Q(f,f)}{f-M}\right|$ is large such that more weight is put on the implicit part to stabilize the scheme.

Practically, many other simplified models for the determination of A and B can be used as well in the numerical computations. Even with $A = 0$ and $B = 1$, all simulations are still acceptable [5,6]. The choice of ($A = 1, B = 0$) is not applicable due to the following reasons. Firstly, the calculation of the full Boltzmann collision term is too time consuming and it is hard to make it implicit. Fortunately, the explicit form can be faithfully used in the rarefied regime with the time step being less than the particle collision time. Secondly, it is not needed physically to use the full Boltzmann collision term when the time step is larger than the particle collision time.

After determining coefficients A and B, the collision term in Eq. (6) can be supplied to Eq. (1) for the evaluation of the inner cell collision term. With the modeling of both interface gas distribution function equation (5) and inner cell collision equation (6), the numerical procedure for UGKS is the following,

(1) Update the conservative flow variables through Eq. (2) and evaluate the equilibrium inside each cell at the next time step;
(2) Update the gas distribution function in Eq. (1), where the collision term can be treated implicitly.

3 Analysis of unified scheme

The traditional continuum and rarefied flow simulations are based on solving different governing equations, such as the NS and direct Boltzmann solver. The UGKS provides a smooth transition for gas dynamics from the kinetic to the hydrodynamic scales. The solutions obtained from UGKS depend on the ratio of the time step (or local time step) to the local particle collision time. In the following, we are going to analyze properties of the UGKS.

3.1 Dynamic coupling between different scales

The UGKS is a multiscale method to simulate both rarefied and continuum flow with the update of both macroscopic flow variables equation (2) and the microscopic gas distribution function equation (1). Instead of solving different governing equations, the UGKS captures the flow physics through the direct modeling of a scale dependent evolution solution for the flux evaluation. In the continuum flow regime, intensive particle collision with $\Delta t \gg \tau$ will drive the gas system close to the equilibrium state. Therefore, the part based on the integration of the equilibrium state in Eq. (5) will automatically

play a dominant role. It can be shown that the integration of the equilibrium state presents precisely an NS gas distribution function when $\Delta t \gg \tau$. Because there is one-to-one correspondence between macroscopic flow variables and the equilibrium state, the integration of the equilibrium state can be also fairly considered as a macroscopic component of the scheme to capture the flow physics in hydrodynamic scale. In the free molecule limit with inadequate particle collisions, the integral solution at the cell interface will automatically present a purely upwind scheme, where the particle free transport f_0 in Eq. (5) will give the main contribution when $\Delta t \leqslant \tau$. This is precisely the modeling used in the derivation of the Boltzmann equation. Therefore, the UGKS captures the flow physics in the rarefied regime as well.

In UGKS simulation, the ratio between the time step Δt to the local particle collision time τ can cover a wide range of values. Here, the time step is determined by the maximum particle velocity, such as $\Delta x/\max(|\boldsymbol{u}|)$, which is equivalent to

$$\Delta t = \mathrm{CFL}\frac{\Delta x}{|U| + c},$$

where CFL is the CFL number, c is the sound speed, and Δx is the local mesh size. On the other hand, the particle collision time is defined by

$$\tau = \frac{\mu}{p} = \frac{\rho |U| \Delta x}{p Re},$$

where $Re = \rho \Delta x |U|/\mu$ is the cell's Reynolds number. With the approximation,

$$|U| + c \simeq c,$$

which is true for low speed flow and is approximately correct even for hypersonic flow because the flow velocity is on the same order as sound speed; we have

$$\frac{\Delta t}{\tau} = \frac{Re}{M},$$

where M is the Mach number. So, in the region close to equilibrium, even for a modest cell Reynolds number, such as 10, the local time step for the UGKS can be much larger than the local particle collision time. The above equation can be written in the following form

$$\Delta t = \frac{\tau}{Kn},$$

where $Kn = M/Re$ is the local cell Knudsen number. So, in a computation which covers both continuum and rarefied regimes, the ratio of time step over local particle collision time can be changed significantly. For steady state calculation, the use of local time step will enhance the efficiency of the scheme further for the steady state calculations.

3.2 Asymptotic preserving property

The numerical scheme, which is capable of capturing the characteristic behavior in different scales with a fixed discretization in both space and time, is called an asymptotic preserving (AP) scheme [20,21]. Specifically, for a gas system, it requires the scheme to recover the NS limit in a fixed time step and mesh size as the Knudsen number goes to zero. A standard explicit scheme for kinetic equation always requires the space and time discretizations to resolve the smallest scale in the system, such as the particle mean free path and collision time. It causes the scheme to be extremely expensive when the system is close to the continuum limit. In recent years, many studies contributed to the development of AP schemes. It has been shown that the delicate time and space discretizations should be adopted in order to achieve AP property [22]. From a physical point of view, the continuum limit is achieved through intensive particle collisions. The local velocity distribution function evolves rapidly to an equilibrium state. Based on this fact, it is clear that any plausible approximation to the collision process must project the nonequilibrium data to the local equilibrium one in the continuum limit. Previous results show that an effective condition for recovering the correct continuum limit is that the numerical scheme projects the distribution function to the local equilibrium, which has a discrete analogue of the asymptotic expansion for the continuous equations. In these studies, implicit time discretization is implemented to meet requirement of the numerical stability and AP property.

Asymptotic preserving for the NS solution in the continuum limit is a preferred property for all kinetic schemes. Before designing such an AP method, we have to realize that the continuum and non-continuum flow behavior depends closely on our numerical cell resolution. Specifically, it depends on the ratio of numerical cell size to the particle mean free path. It is basically meaningless to talk about AP method without sticking to the discretized space resolution. The Boltzmann equation itself is a dynamical model in particle mean free path and mean collision time scale. The direct upwind discretization of the transport part of the kinetic equation can not go beyond such a modeling scale, where Δx needs to be on the same order as the particle mean free path. If Δx is on the scale of hundreds of particle mean free path, this free transport discretization is problematic. Certainly, the flow physics from the kinetic to the hydrodynamic scale can be still captured by solving the kinetic equation through a brute force approach. Then,

the efficiency will become a problem because in many cases the brute force approach with the resolution up to mean free path everywhere is unnecessary and too expensive. In most applications, we may not need to get such detailed information of a flow system. Practically, the cell size with respect to the mean free path varies significantly in different regions around a flying vehicle at different altitudes. As a result, with the variation of the ratio between the cell size and particle mean free path, the corresponding physical behavior needs to be captured. The free transport for the interface flux has to be avoided for a valid AP method. Unfortunately, it seems that most current kinetic AP solvers use the free transport mechanism without doubt. More analysis about these kind of AP schemes can be found in Ref. [23].

The distinguishable feature of the UGKS is that a time-dependent solution of the kinetic model equation with the inclusion of collision effect is used for the flux evaluation at a cell interface. This solution itself covers different flow regimes from the initial free molecular transport to the NS formulation. The real solution used depends on the ratio of time step to the particle mean collision time. In the continuum flow limit, due to the massive particle collision, the contribution from the free transport part f_0 disappears. The UGKS will pick up the NS solution automatically. For the update of the conservative flow variables, the unified scheme recovers the GKS for the NS solution in the hydrodynamic limit [24,25].

In the region with comparable values of time step and local particle collision time such as in the transitional flow regime, both the kinetic scale free transport and the hydrodynamic NS evolution will contribute to its dynamical evolution. The UGKS provides a continuous transition with the variation of the ratio $\Delta t/\tau$. The UGKS has been validated through extensive benchmark tests [11].

4 Extension of unified framework to other transport process

The multiscale modeling in the unified scheme can be applied to many other transport equations, such as radiation and neutron transports, plasma simulation, and the electron and phonon transport process in semiconductors. In radiation transport, the governing equation is a linear kinetic equation. Similar to the Boltzmann equation, the dynamics of the radiation equation is driven by a balance between photon free transport and interaction with material medium. Since the collision frequencies vary by several orders of magnitude through the optical thin or thick material, equations of this type will exhibit multiscale phenomena, such as those in the rarefied and continuum flow regimes. For the neutron and radiation transport, many AP schemes have been proposed. The UGKS provides a framework for the construction of schemes covering multiple scale transport mechanism. Recently, Mieussens applied the methodology of the UGKS to the radiative transfer equation [26]. While such a problem exhibits purely diffusive behavior in the optically thick (or small Knudsen) regime, it is proven that the UGKS is still asymptotic preserving in this regime, and captures the free transport regime as well. Moreover, he modified the scheme to include a time implicit discretization of the limit diffusion equation, and to correctly capture the solution in case of boundary layers. Contrary to many AP schemes, the UGKS-type AP method for radiative transfer is based on a standard finite volume approach, and it does not use any decomposition of the solution or staggered grids. It provides a general framework for the solution of transport equation. Along the same line, recently the UGKS has been extended to solve gray radiative transfer equations [27]. The recent applications of the UGKS for phonon heat transfer and multiple frequency radiative transport are very successful as well.

The UGKS presents a modeling for the transition from free molecular transport to the NS solutions. This NS solution is the same as the direct numerical simulation (DNS) approach for the turbulence, where all scales in the hydrodynamic regime are well resolved. As the mesh size becomes even larger, the flow structures with eddy will appear inside each numerical cell, which cannot be fully resolved by the mesh size resolution. As shown in Fig. 3, there are both laminar and turbulent flows in the order of mesh size scale. Therefore, instead of averaging on the NS equations, such as the most approaches for turbulent modeling [28], we would like to propose a continuous extension of the UGKS from the NS up to the unresolved turbulent modeling,

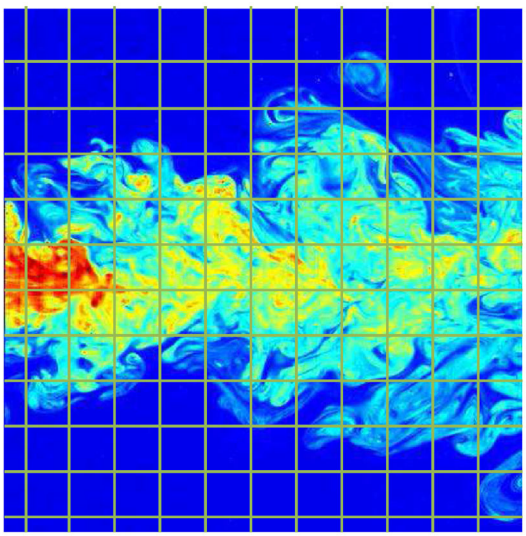

Fig. 3 The representation of turbulent flow numerically with mesh size scale [28]

$$f(\boldsymbol{x},t,\boldsymbol{u},\xi) = \frac{1}{\tau_t}\int_0^t \mathrm{e}^{-(t-t')/\tau_t} P^{\mathrm{pdf}}(\boldsymbol{x}',t',\boldsymbol{u}',\xi)\mathrm{d}t' + \mathrm{e}^{t/\tau_t}\left[\frac{1}{\tau}\int_0^t \mathrm{e}^{-(t-t')/\tau} g(\boldsymbol{x}',t',\boldsymbol{u}',\xi)\mathrm{d}t' + \mathrm{e}^{-t/\tau} f_0(\boldsymbol{x}-\boldsymbol{u}t,\boldsymbol{u},t,\xi)\right].$$

(resolved to unresolved turbulent modeling)

$$\simeq (1-\mathrm{e}^{-t/\tau_t}) P^{\mathrm{pdf}}_{\mathrm{tur}} + \mathrm{e}^{-t/\tau_t} f^{\mathrm{ns}}_{\mathrm{laminar}},$$

where τ_t is the turbulent relaxation time. P^{pdf} is the "equilibrium" state approached by the turbulent flow, such as the probability density function (PDF) of the large eddy simulation (LES). The above equation presents a transition process from the laminar to turbulent description. The real solution used for the flux evaluation depends on the flow structure and cell size resolution. The turbulent relaxation time needs to be constructed through the modeling of the time scale for the energy dissipation.

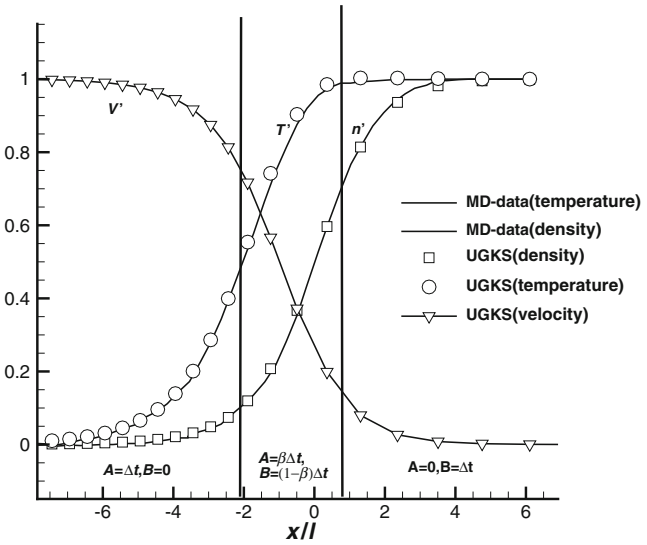

Fig. 4 Normalized number density, temperature and velocity distributions from UGKS (*symbols*) and molecular dynamics (MD) solutions (*lines*) [30]

5 A few applications for non-equilibrium flows

The UGKS has been used in a gigantic amount of engineering applications [11]. Here we only present two cases to demonstrate the usefulness of the UGKS.

5.1 Shock structure simulation

The shock structure is one of the most important test case for the non-equilibrium flow. In this calculation, a nonuniform mesh in physical domain is used, such as a fine mesh in the upstream and a relative coarse mesh in the downstream [29]. In addition, a local time step is used in order to get the stationary solution more efficiently. The UGKS with the inclusion of the full Boltzmann collision term will be tested. The parameters to determine the switching between full Boltzmann and Shakhov models in the current UGKS depends on the relative values of the local time step and particle local collision time.

The shock wave of argon gas with Lennard–Jones potential at $M = 5$ is calculated by UGKS and is compared with a molecular dynamics simulation of Ref. [30]. Figures 4 and 5 show the shock wave structure and the distribution functions inside the shock layer.

5.2 Lid-driven cavity flow

In the cavity flow case [31], the gaseous medium consists of monatomic molecules of argon with mass, $m = 6.63 \times 10^{-26}$ kg. The variable hard sphere (VHS) model is used, with a reference particle diameter of $d = 4.17 \times 10^{-10}$ m. In the current study, the wall temperature is kept at the same reference temperature of $T_w = T_0 = 273$ K, and the up wall velocity is kept fixed at $U_w = 50$ m/s. Maxwell's diffusion model with full accommodation is used for the boundary condition. In the following test cases, a nonuniform mesh is used in order to capture the boundary layer effect. The grid point follows, in the x-direction

$$x = (10-15s+6s^2)s^3 - 0.5, \quad s = (0,1,\ldots,N)/2N. \quad (9)$$

A similar formula is used in the y-direction.

The first few tests are in the rarefied and transitional regime, where the UGKS solutions are compared with DSMC ones. Figures 6, 7, 8 show the results from UGKS and DSMC solutions of Ref. [31] at Knudsen numbers 10, 1, and 0.075. The computational domain for $Kn = 10$ and $Kn = 1$ cases is composed of 50×50 nonuniform mesh in the physical space and $72 \times 72 \times 24$ points in the velocity space. Because of the decreasing Knudsen number, the mesh size over the particle mean free path can be much enlarged. The computational domain for $Kn = 0.075$ case is composed of 23×23 nonuniform mesh in physical space and $32 \times 32 \times 12$ points in the velocity space. Because of the use of non-uniform of mesh and the local time step, Fig. 8 also includes the switching interface between the use of the full Boltzmann collision term and the Shakhov model.

In order to validate the AP property of the current scheme in the continuum limit, the case at Knudsen number 1.42×10^{-4} or $Re = 1000$ is tested. The computational domain for $Re = 1000$ is composed of 61×61 nonuniform mesh in physical space and 32×32 points in the velocity space. In both cases, the freedom of molecules is restricted in a 2D

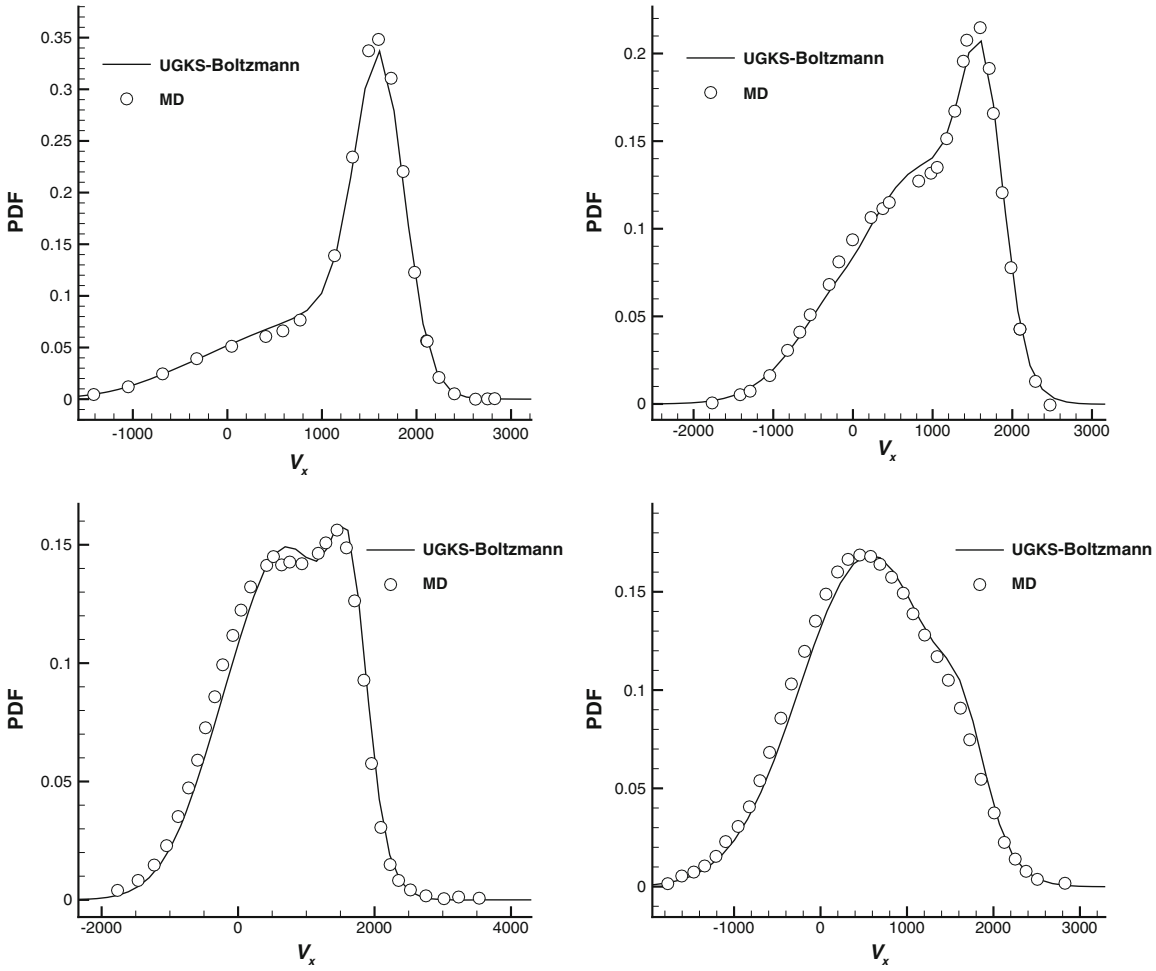

Fig. 5 The distribution function $\iint f \frac{\mathrm{d}v\mathrm{d}w}{n}$ at locations of density $n' = 0.151, 0.350, 0.511$, and 0.759. UGKS solutions (*lines*) and MD solution (*symbols*) [30]

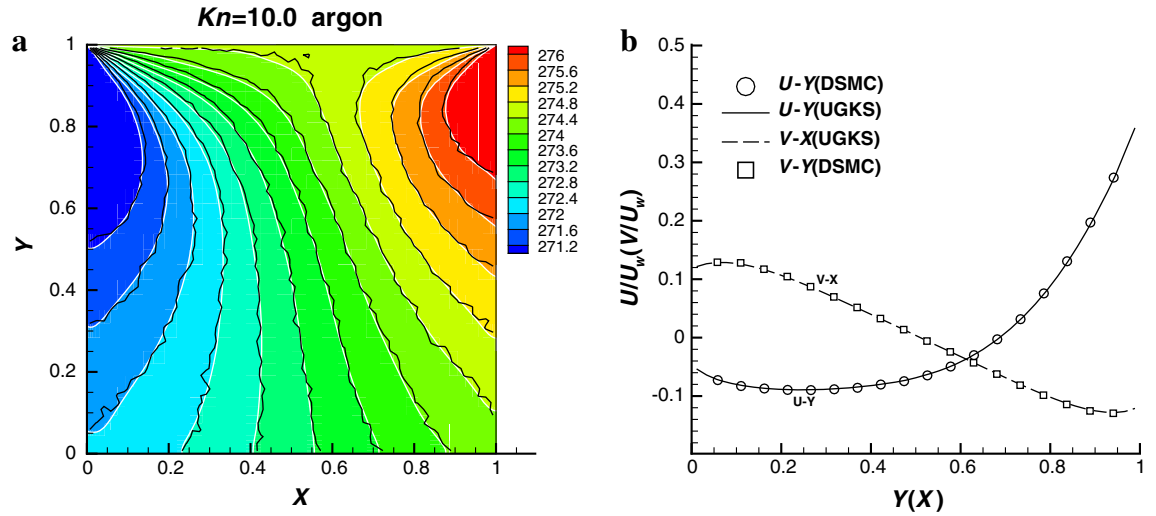

Fig. 6 Cavity flow at $Kn = 10$. **a** Temperature contours, *black lines* DSMC, *white lines* and *background* UGKS. **b** $\boldsymbol{U}$-velocity along the central *vertical line* and $\boldsymbol{V}$-velocity along the central *horizontal line*, *circles* DSMC, *line* UGKS

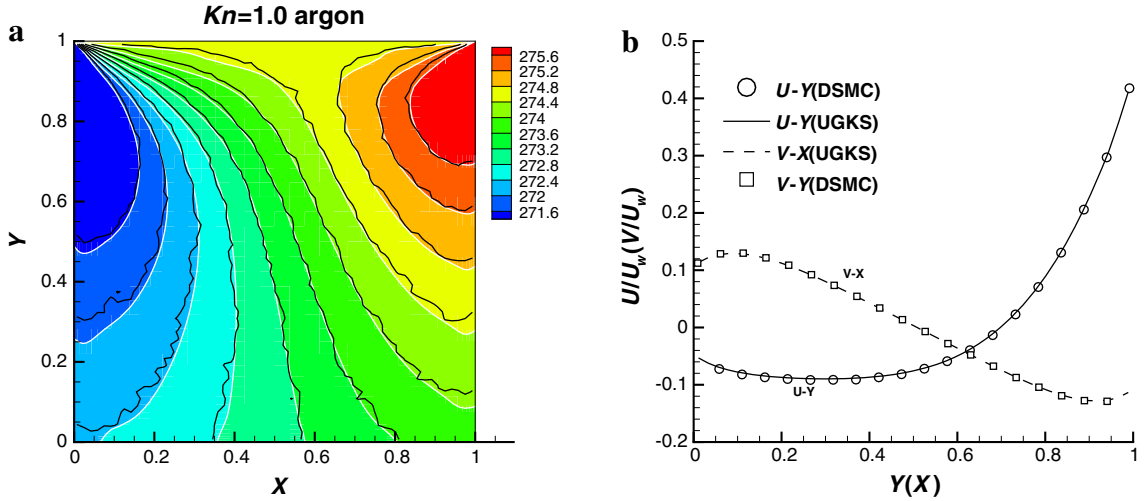

Fig. 7 Cavity flow at $Kn = 1$. **a** Temperature contours, *black lines* DSMC, *white lines* and *background* UGKS. **b** U-velocity along the central *vertical line* and V-velocity along the central *horizontal line*, *circles* DSMC, *line* UGKS

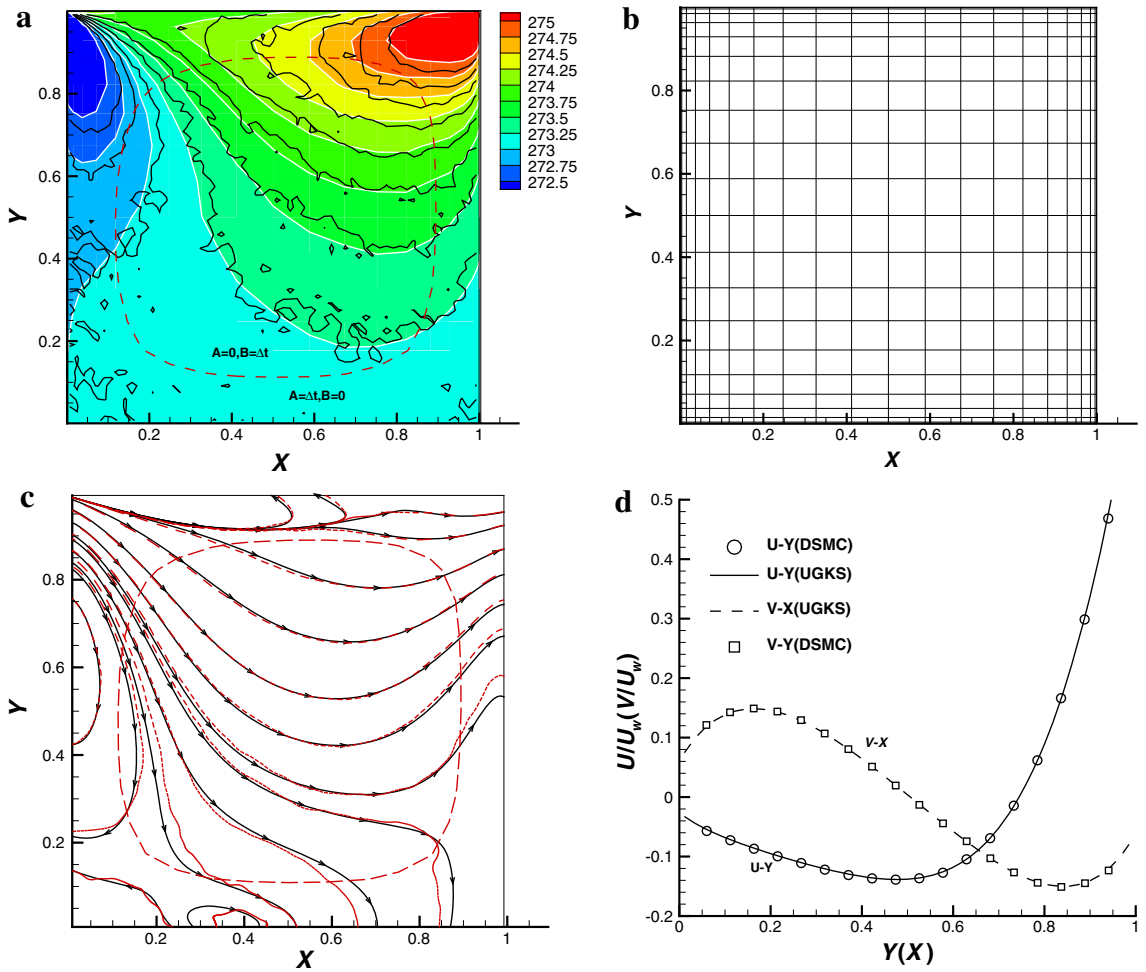

Fig. 8 Cavity flow at $Kn = 0.075$. **a** Temperature contours with domain interface for different collision models, *black lines* DSMC, *white lines* and *background* UGKS. **b** Computational mesh in physical space. **c** Heat flux, *dash lines* DSMC, *solid lines* UGKS. **d** U-velocity along the central *vertical line* and V-velocity along the central *horizontal line*, *circles* DSMC, *line* UGKS

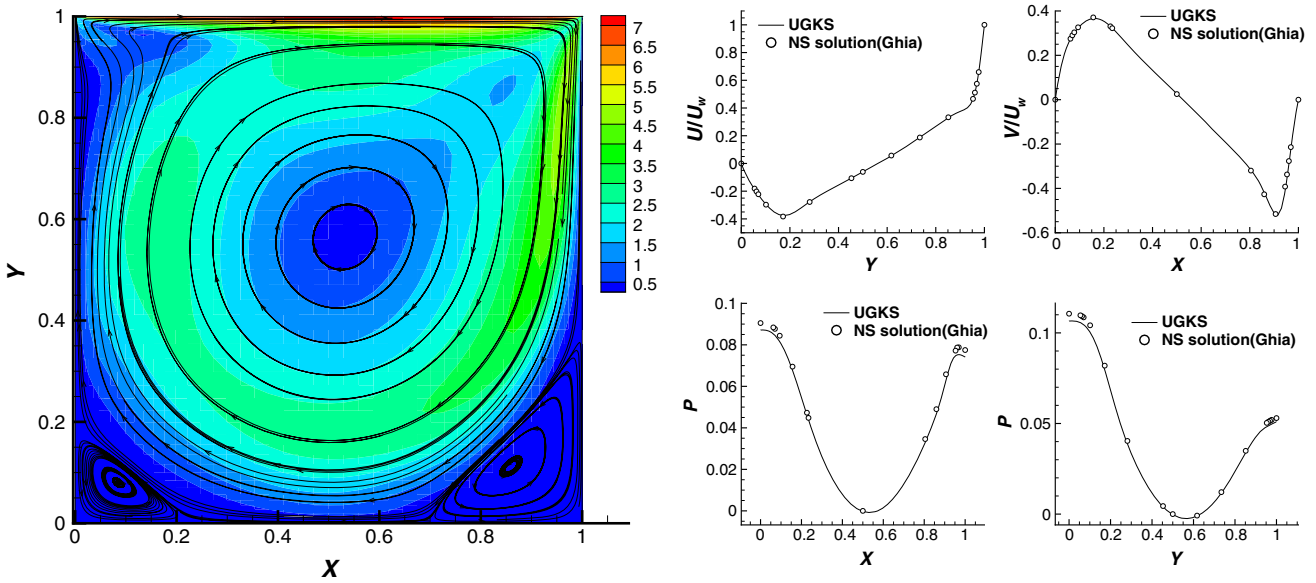

Fig. 9 Cavity flow at $Kn = 1.42 \times 10^{-4}$ and $Re = 1000$. (*left*) Velocity stream lines with temperature background; (*right*) $\boldsymbol{U}$-velocity along the central *vertical line*, $\boldsymbol{V}$-velocity along the central *horizontal line*, pressure along the central *vertical line*, and pressure along the central *horizontal line*, *circles* NS solution, *line* UGKS

space in order to get the flow condition close to the 2D incompressible flow limit. Also, the non-slip boundary condition is imposed in the calculation. Figure 9 shows the UGKS results and reference NS solutions [32]. This clearly demonstrates that the UGKS converges to the NS solutions accurately in the hydrodynamic limit.

Based on the above simulations, we can confidently use the UGKS in the whole flow regime. In the near continuum regime, it will be interesting to use the UGKS to test the validity of the NS solution. Before the development of the UGKS, an accurate gas-kinetic scheme (GKS) for the NS solutions was constructed and validated thoroughly [25]. The comparison between the solutions from the UGKS and GKS is basically a comparison of the governing equations of the UGKS and the NS ones. In the following, we test the cavity case at $Re = 5$, 20, and 40, which are shown in Fig. 10. At the above Reynolds numbers, the velocity profiles between the UGKS and GKS are basically the same. But the heat flux can keep differences between the UGKS and GKS. As shown in these figures, the heat flux from the UGKS is not necessarily perpendicular to the temperature contour level, which is the basic assumption of Fourier's law. We believe that the UGKS provides a reliable physical solution in comparison with NS. The UGKS will become an indispensable tool in the study of non-equilibrium flow in the near continuum flow regime.

6 Conclusion

This paper reviews the direct modeling as a general framework for the CFD algorithm development and the construction of the unified gas kinetic scheme. The principle underlying the direction modeling is that the mesh size and time step will actively participate in (describe) the gas evolution, and the aim of CFD is basically to capture the corresponding gas dynamics in the mesh size scale. The unified scheme is constructed under such a principle and provides a multiple scale gas evolution modeling for flow simulations. The flow dynamics in the UGKS provides a continuous spectrum of flow motion from the rarefied to the continuum one. The cell size used in the UGKS can range from the particle mean free path to the hydrodynamic dissipative layer thickness in different locations for the capturing of both the Boltzmann and NS solutions when needed. This CFD principle is distinguishable from the existing CFD methodology, where a direct discretization of the partial differential equations is usually adopted. In the traditional CFD approach, the cell size and time step are basically separated from the flow dynamics. The numerical mesh size seems to introduce error only. The dependence of the flow dynamics on the mesh resolution can be easily understood once we realize that all existing fluid dynamics equations are derived based on the physical modeling in their specific scales. Here we only change the modeling scale to the mesh size and time step. Certainly, we can use the Boltzmann equation or even molecular dynamics all the time to resolve the flow physics in the smallest scale everywhere, but this is not necessary and is not practical at all in the low transition and continuum flow regime. The aim of science is to figure out the most efficient and consistent way to describe the nature. The CFD should present the flow dynamics in different scales as simple as possible, but not simpler. For a gas flow without

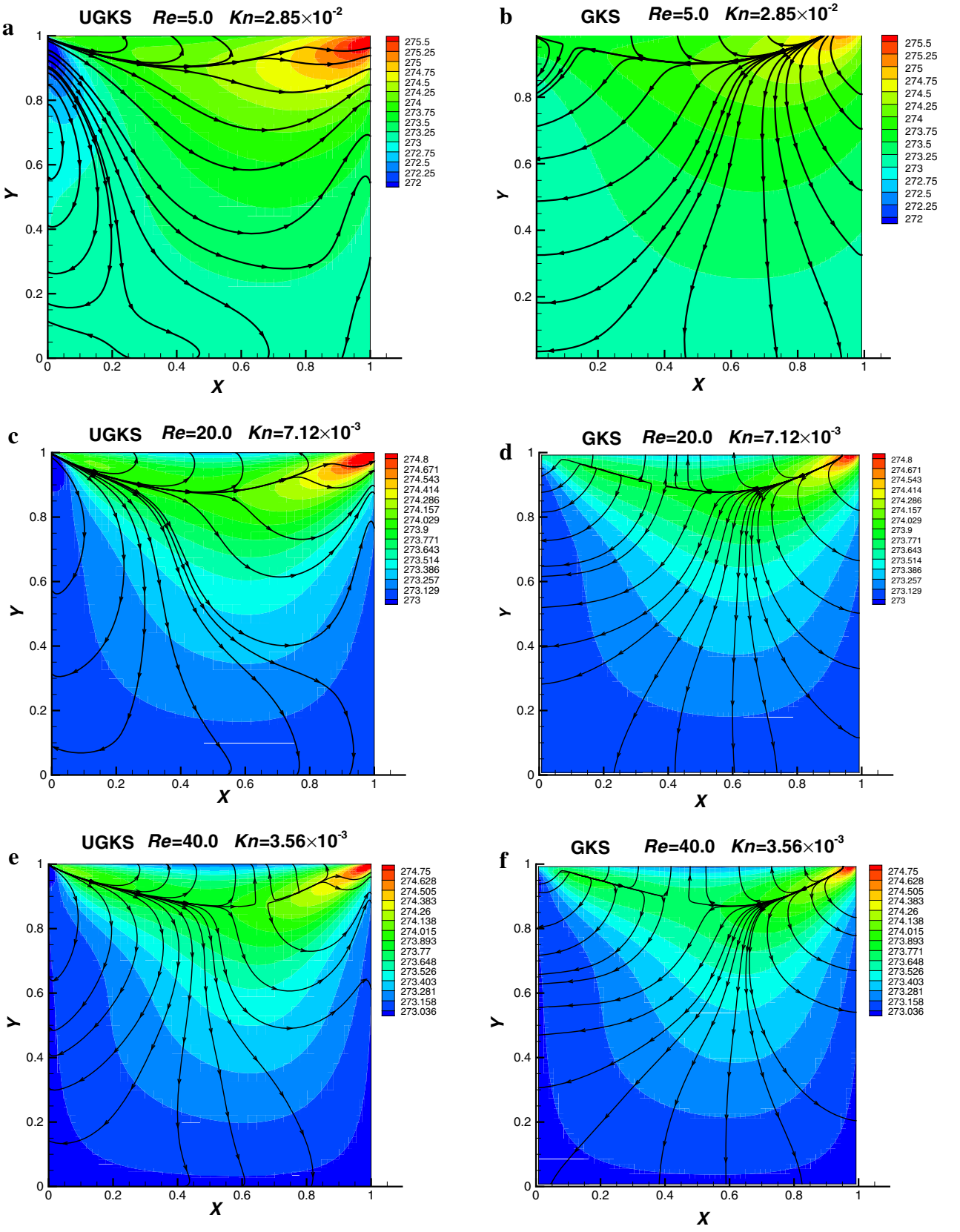

Fig. 10 Cavity simulation using the UGKS and GKS at $Re = 5, 20,$ and 40 with the plots of temperature contour and heat flux. *Left column* UGKS; *right column* GKS

discernible scale separation, it will become hard if not impossible to construct a multiscale method from a few governing equations with distinguishable modeling scales. The multiple scale turbulent problem will not be solved if targeting on the "averaging" of the NS equations only (static approach) without developing a dynamic multiscale modeling principle.

The key in the unified scheme is the modeling of a time- and scale-dependent evolution solution for the interface flux and inner cell collision in the update of both macroscopic flow variables and microscopic gas distribution function. This time evolution solution covers different flow regimes, from kinetic to hydrodynamic. The solution used locally for the numerical flow evolution depends on the ratio of the time step to the local particle collision time. The current study clearly indicates that the UGKS is a valuable and indispensable tool for flow study, especially for the flow simulation with the co-existence of both continuum and rarefied regimes. The direct modeling principle can be naturally used to simulate many multiscale transport dynamics, such as radiation, neutron, and phonon transport. More detailed construction of the kinetic schemes and their applications can be found in a recent monograph [11].

The traditional CFD principle, i.e., the so-called numerical partial differential equations with emphasis on the truncation error analysis and modified equations, has to be re-examined carefully. The final destiny of the direct modeling is to provide a continuous spectrum governing equations with a variation of scales. Besides the traditional partial differential equations for flow description, the discrete dynamic scheme provides another kind of governing equations which may give a more faithful description of gas dynamics.

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