



## Research Highlight

## To overcome memory barrier of kinetic solvers for non-equilibrium flow study

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For the non-equilibrium flow study, there are very few analytical solutions. Most studies are based on the simulation techniques. At the current stage, there are mainly two types of numerical methods for the study of non-equilibrium gas dynamics. The dominant numerical method for rarefied gas flow, especially for the high speed one, is the Direct Simulation Monte Carlo (DSMC) method [1]. The essential DSMC technique is the direct modeling in its algorithm development, which mimics the physical process in the construction of the Boltzmann equation. More specifically, the DSMC simulates the gas dynamics in small scales, such as time step  $\Delta t$  and cell size  $\Delta x$  being less than the particle collision time  $\tau$  and mean free path  $\ell$ . Only under such a condition, the decoupling of the particle transport and collision in DSMC will not introduce much numerical error and the physical solution can be faithfully obtained in the rarefied flow regime. Even though the DSMC is a single scale method for capturing flow physics in the kinetic level  $(\tau, \ell)$ , for rarefied high speed flow, the DSMC is very efficient and is the only reliable method which has been routinely used in aerospace industry.

Another method for rarefied flow is the direct Boltzmann solver [2], which basically follows the numerical partial differential equation methodology, to solve the Boltzmann equation numerically. Instead of following individual pseudo-particles, here the velocity distribution function is the only dependent variable which is a function of space, time, and particle velocity. As a result, the Boltzmann solver needs to follow the evolution of a gas distribution function in a computational space with seven dimensions. If 100 grid points are used in each direction, for a three dimensional unsteady flow calculation theoretically there requires  $10^{14}$  grid points, which is a unreasonable big number even for super computers. As a result, the direct Boltzmann solver is only limited to the study of simple flows in one or two-dimensional physical space.

However, the history may be changed due to the techniques developed in the current paper “A unified implicit scheme for kinetic model equations. Part I. memory reduction technique” [3]. In this paper, the authors developed a technique which does not require to update the gas distribution function. Instead, the only updated variables are the macroscopic ones, which take the same memory as conventional Navier–Stokes solvers. Therefore, even for the non-equilibrium flow, the computations can be conducted in a three dimension space  $(x, y, z)$ . Certainly, the success and the

outstanding achievement of the current method depend strictly on the following conditions. First, the memory-free method is only for steady state solution, where the time variable is not involved. Second, the full Boltzmann collision term has to be replaced by a relaxation model, such as the BGK [4], ES-BGK [5], or Shakhov-type [6] for a monatomic gas. Under these conditions, in a three dimensional physical space the approximate Boltzmann equation becomes an equation which connects two variables, the distribution function  $f$  and the equilibrium state  $g$ , such as the BGK model in 1-D case,

$$u \frac{d}{dx} f = (g - f) / \tau, \quad (1)$$

where  $f$  is the distribution function,  $g$  is the equilibrium state,  $\tau$  is the particle collision time, and  $u$  is the particle velocity. Since the equilibrium state  $g$  depends only on the local macroscopic flow variables, the above equation implicitly and uniquely connects  $f$  with the macroscopic flow variables. It had been first realized by Liepmann et al. [7] for the shock structure calculation. In their approach, an integral solution for  $f$  is obtained,

$$f = \int_{-\infty}^x \frac{g(x')}{\tau u} \exp\left(-\int_{x'}^x \frac{dx''}{\tau u}\right) dx', \quad (2)$$

where  $x'$  and  $x''$  are dummy variables and the negative and positive signs on the lower limit apply for positive and negative  $u$  (upwind), respectively. The above equation was solved numerically by Liepmann et al. [7] using an iterative scheme that required an initial guess for  $g$ , or macroscopic flow distributions. Essentially, the current paper is to extend the above method to design a discrete ordinate method (DOM) for rarefied flow computations in multiple dimensions.

Numerically, even though the current implicit scheme has similar efficiency or computational cost as the implicit unified gas kinetic scheme (UGKS) in the rarefied flow regime [8], the memory reduction in the current approach is a big step to make the 3D rarefied flow simulation possible with a lab cluster. The numerical tests in this paper [3] fully validate the current approach for the flow simulation when the cell size is less than the particle mean free path.

For the adoption of the first order upwind scheme, such as Eq. (12) in Ref. [3], the pseudo time step for the inner iteration is  $\tau$ , which can be effective in the rarefied regime when  $\ell \gg \Delta x$ , as the pseudo time step  $\tau$  is much larger than the explicit time step.

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Under this condition, the high-order extension can be properly conducted since the integration solution (2) can be equivalently evaluated over a few cells. However, as the cell size approaches to the particle mean free path, the main contribution from the integral solution may come from a single numerical cell, because due to collision the particle number decays faster along a particle path. As a result, the current method will become sensitive to the reconstruction of macroscopic variables within each cell. In other words, the reconstructed distribution function is reliable in the rarefied regime because the domain of dependence of  $f(x, u)$  is on the order of  $u\tau$  which is relatively large, and the macroscopic variables are smoothly distributed for the reconstruction of equilibrium state in these cells. However, at a relative small Knudsen number, the exponential term  $\exp(-\int_{x_0}^x \frac{1}{u\tau(x')} dx')$  decays very fast and the domain of dependence shrinks to a small region around  $x$ . Therefore, as Knudsen number decreases, the reconstructed distribution function is highly dependent on the local reconstruction of macroscopic variables. The significant reduction of efficiency at  $Kn = 0.075$  in Table 1 (see Ref. [3]) may be due to the difficulty for the current scheme as the cell size gets closer to the particle mean free path  $\Delta x \rightarrow \ell$ . In an unresolved region or near the shock discontinuity, the situation will become even worse, and an artificial dissipation by enlarging collision time  $\tau$  has to be adopted. On the contrary, due to the multiple scale nature of implicit UGKS [8], as discussed later, its efficiency in near continuum regime gets even higher than that in the rarefied regime.

For high order extension, the inner iteration is used which is expressed as Eq. (21) in Ref. [3]. The essential part is the design of the right hand side residual term which determines the steady state. The steady solution of second inner loop satisfies Eq. (30). Although a high order reconstruction can be used in the construction of the spatial derivative, the numerical PDE approximation for  $\partial f/\partial x$  makes the current scheme be still a single scale method. The current approach is a direct single scale DOM method, which requires small cell size and time step in comparison with the particle mean free path and collision time. In Eq. (30) of [3], the explicit equilibrium distribution  $g^n$  is used. In order to get a convergent solution, an additional second inner loop is needed, which may increase the computational cost. It is possible to add a prediction step to calculate the equilibrium state, such as the methods used in GKS and UGKS [8–10] for the update of macroscopic flow variables, and then use  $g^{n+1}$  in Eq. (30) to increase the convergence rate.

Now let's analyze the physical properties of the current approach and its possible extension to become a multiple scale method. In order to get accurate physical solution in the continuum regime, many asymptotic preserving (AP) schemes have been proposed. However, most AP schemes still need to use a cell size less than the particle mean free path in the continuum regime in order to get accurate Navier–Stokes (NS) solutions, such as high Reynolds number boundary layer. These AP schemes are not real multiple scale methods. If a scheme could not get accurate NS solution in the continuum regime, such as the high Reynolds number boundary layer solution with a cell size being much larger than the particle mean free path, its solution in the near continuum regime would be questionable. The real efficient way to extend the current DOM to the whole flow regime, including the continuum regime for the NS solutions, is to use the methodology in UGKS [9,10] and DUGKS [11,12]. In order to make the above statement clear, let's point out the main difference between traditional DOM and the UGKS. The DOM is based on the conventional numerical PDE approach. For example, in a finite volume DOM, the discretization of  $\partial f/\partial x$  is approximated by

$$\frac{\partial f}{\partial x} \simeq \frac{f_{i+1/2} - f_{i-1/2}}{x_{i+1/2} - x_{i-1/2}}, \quad (3)$$

where  $f_{i+1/2}$  is the distribution function at the cell interface. In DOM, the function  $f_{i+1/2}$  is a simply reconstructed function at a cell interface from the cell averaged values of  $f$  in neighboring cells. The reconstruction can be based on central difference or upwind approach. Its accuracy solely depends on the reconstruction's order of accuracy, and the distribution function  $f$  alone is involved in the determination of  $f_{i+1/2}$ . For any DOM method, like other numerical PDE approach, the solution of DOM will converge to the exact solution of the PDE as cell size and time step approaching to zero. The cell size and time step don't contribute to the description of the physics of the flow, except introducing numerical errors. However, for the UGKS, the time evolution dynamics appears in the determination of  $f_{i+1/2}$ . The solution at the cell interface depends not only the physical reality, such as  $\tau$  and  $\ell$ , but also on the cell size  $\Delta x$  and time step  $\Delta t$ . In other words, the cell size and time step determine the dynamics of flux function across a cell interface. For example, a time averaged distribution function  $\bar{f}_{i+1/2}$  in UGKS at a cell interface can be expressed as

$$\bar{f}_{i+1/2} = \frac{1}{\Delta t} \left[ \int_0^{\Delta t} \left( \frac{1}{\tau} \int_0^t g(u, x - u(t-s), s) e^{-\frac{t-s}{\tau}} ds + e^{-\frac{t}{\tau}} f_0(u, x - ut) \right) dt \right]. \quad (4)$$

For DUGKS,  $\bar{f}_{i+1/2}$  becomes

$$\bar{f}_{i+1/2} = \frac{2\Delta t}{\Delta t + 4\tau} g\left(x - \frac{\Delta t}{2}u\right) + \frac{4\tau - \Delta t}{\Delta t + 4\tau} f_0\left(x - \frac{\Delta t}{2}u\right). \quad (5)$$

Both formulations are basically equivalent at the second order of accuracy [13], and the solutions are time step or cell size dependent. Whatever the scheme is, i.e., explicit or implicit, the main criterion to distinguish the UGKS and DOM is its underlying “equivalent” distribution function at the cell interface, which is used to evolve its numerical solution inside each cell. The residuals in Eqs. (30) and (32) of Ref. [3] are consistent with the DOM approach only. In order to extend it to simulate flows in all regimes, the above UGKS and DUGKS methodology for the interface distribution function evaluation can be used. For example, the Eq. (1) can be integrated over a cell  $[x_{i-1/2}, x_{i+1/2}]$  and a time step  $\Delta t$ , and the interface fluxes can be modeled as that in Eqs. (4) and (5). For the steady state calculation, the  $\bar{f}_{i+1/2}$  can be simplified as a weighted function between  $g$  and  $f_0$ , such as

$$\bar{f}_{i+1/2} = \mathcal{L}\left(\frac{\Delta x}{u\tau}\right)g + \left(1 - \mathcal{L}\left(\frac{\Delta x}{u\tau}\right)\right)f_0 = f_0 + \mathcal{L}\left(\frac{\Delta x}{u\tau}\right)(g - f_0), \quad (6)$$

where  $\mathcal{L}(\cdot)$  is a certain weighting function which identifies the equilibrium state  $g$  (local equilibrium one) when  $\Delta x \gg \ell \simeq u\tau$ , and the free transport part  $f_0$  (upwind solution from initial  $f$ ) when  $\Delta x \ll \ell \simeq u\tau$ . The UGKS in Eq. (4), especially DUGKS in Eq. (5), are the schemes with special choices of  $\mathcal{L}(\cdot)$ , such as setting  $|u|\Delta t \simeq \Delta x$  to get DUGKS interface distribution function. In unified formulations, the cell size  $\Delta x$  will involve in the physical solution at a cell interface. For the first order scheme, the current DOM method uses Eq. (15) in Ref. [3] to update  $f$ , which has a similar formulation as that in the above Eq. (6), where the collision has been considered inside each cell alone. However, as analyzed in Ref. [14], Eq. (6) has to be implemented in both cell interface and inner cell for a multiscale method. When the current scheme adopts Eq. (6) for the flux evaluation, a memory free UGKS and DUGKS methods can be developed. At the same time, in order to speed up the convergence rate, the update of macroscopic variables as used in UGKS [8,10] can be implemented here as well.

In order to clearly distinguish different kinds of kinetic solvers, here we give a definition of unified preserving (UP). The UP is referred to a scheme with the inclusion of particle transport and collision in the evaluation of the interface distribution function,

and the interface distribution function has the form of Eqs. (4), (5), or (6), where the cell size  $\Delta x$  and time step  $\Delta t$  involve in the gas evolution. The UP is fundamentally different from any previous AP. The AP emphasizes a direct numerical discretization, but UP provides a physical evolution process in the cell size and time step scales. As a requirement, the UP scheme should be able to connect smoothly the solutions from the kinetic Boltzmann equation to the hydrodynamic Navier-Stokes equations. At the same time, if the Navier-Stokes solution has a much larger dissipative thickness than the particle mean free path, the UP scheme should be able to capture the Navier-Stokes solution once the structure can be well resolved by the numerical cell size, such as a few grid points in the Navier-Stokes boundary layer. The UGKS and DUGKS are examples which have the UP properties.

In summary, for the steady state solution the paper [3] developed a memory reduction kinetic solver. The success of the method is due to fact that the kinetic BGK equation gives one to one correspondence between  $f$  and  $g$  in the steady case, and the equilibrium state is uniquely determined by the macroscopic flow variables. Therefore, there is a direct connection between macroscopic flow variables and the construction of the gas distribution function. This is a significant step for kinetic equation solver and for the simulation of rarefied flow. In order to develop a scheme which is applicable to both rarefied and continuum regimes, the methodology of UGKS and DUGKS, or any other equivalent form with the inclusion of both transport and collision in the construction of the interface distribution function (flux function) can be directly implemented here as well. Therefore, it is straightforward to develop a memory free UGKS and DUGKS implicit methods for the steady state solutions. These schemes which could connect the Boltzmann solution in the kinetic scale to the Navier-Stokes solution in the hydrodynamic scale are called unified preserving schemes, or UP-schemes. At end, the conditions for the success of the memory reduction technique is also associated with constraints which limit the appli-

cations of the current technique. The further extension of the memory reduction technique to diatomic gas with non-equilibrium rotational and vibration modes, to the kinetic system with external forcing terms, to the full Boltzmann collision term, and to the plasma simulation with electric-magnetic field coupling, will be interesting and important for the study of multiple scale transport processes.

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