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Exponential differencing BGK method for multiscale flow simulation: deterministic and stochastic solvers

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Abstract

Aerospace applications often involve gas flows that are particularly difficult to reproduce or measure experimentally, and include different regimes where usual numerical simulation methods can become inaccurate or computationally expensive. Therefore, a multiscale method to simulate gas flows, based on an exponential differencing of the BGK operator, is presented here. It is second-order accurate and preserves asymptotic limits towards both continuum and free-molecular limits. Furthermore, its mathematical structure allowed for an implementation as both a discrete velocity and a particle-based method sharing the aforementioned properties. The accuracy and performance of this scheme is validated on several test cases.

1. Introduction

When a gas flow is rarefied up to a point where the continuum assumption no longer holds, the Navier-Stokes (NS) equations fail to describe it accurately. The common numerical tool used to simulate such flows with a high Knudsen number is the Discrete Simulation Monte-Carlo (DSMC)[1] method. This method, widely developed in recent years, becomes however computationally costly in transition regimes, and conducting coupled NS-DSMC simulations is particularly challenging due to the inherent differences between the two approaches. A multiscale method would thus greatly improve the efficiency and accuracy of simulations in cases where the Knudsen number varies by several orders of magnitude, such as atmospheric re-entry flows or nozzle expansions.

The Bhatnagar-Gross-Krook (BGK) model[2] offers this possibility, since it is an approximation of the Boltzmann equation that remains valid for non-equilibrium flows while allowing for numerical solvers with less strict resolution requirements as DSMC. This model can be developed into gas kinetic schemes by fully discretizing it in phase space and using a wide range of partial differential equation solvers, leading to a variety of discrete velocity methods (DVM).[3,4] Although significant progress has been made on DVM, with many solvers offering different stability and convergence properties, the accurate discretization of the velocity space remains problematic for three-dimensional cases when the distribution function is far away from equilibrium (e.g., shocks, high Mach number flows). Another type of BGK methods, based on stochastic simulation particles similarly as DSMC, has therefore recently come to the fore as an efficient way to handle such flows.[5] However, the operator splitting approach it implies usually limits such stochastic particle BGK methods to explicit schemes with first order accuracy, thus requiring fine spatiotemporal resolutions.

The multiscale method presented here, based on an exponential differencing of the BGK operator (EDBGK), achieves second order accuracy and asymptotic preserving behavior towards both continuum and free-molecular limits. Moreover, it was constructed so as to allow its implementation as both a deterministic discrete velocity method and a stochastic particle solver,[6] in the open-source code PICLas. This dual approach would then make possible a coupling in either velocity or physical space, using each method where it performs best. This article begins by summarizing the theory of the kinetic description of rarefied gas flows and the construction of the EDBGK scheme. Then, several cases are simulated to validate the method and demonstrate its possibilities to reproduce accurately different types of gas flows interesting for aerospace applications, while comparing the efficiency of the deterministic and stochastic approach.

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2. Theory

2.1 Bhatnagar-Gross-Krook model

The kinetic theory describes gases using a distribution function $f(\mathbf{x}, \mathbf{v}, t)$ which is the probability density of gas particles having a velocity $\mathbf{v}$ at the position $\mathbf{x}$ and time t. The evolution of this function is given by the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}. \tag{1}$$

The collision term $\left.\frac{\partial f}{\partial t}\right|_{\text{coll}}$ is originally a complex integral over the velocity space, but can be approximated by the BGK operator.[2] The equation then becomes

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = \nu(f^t - f), \tag{2}$$

where ν is a relaxation frequency, chosen in order to match the viscosity $\mu = \frac{\rho RT}{\nu}$, with R the specific gas constant and T the temperature. The target distribution f^t towards which f relaxes can be chosen as the Maxwellian distribution that corresponds to the thermal equilibrium of the gas:

$$f^M = \rho\left(\frac{1}{2\pi RT}\right)^{3/2} \exp\left[-\frac{\mathbf{c}\cdot\mathbf{c}}{2RT}\right], \tag{3}$$

with the density ρ and the thermal velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$, where $\mathbf{u}$ is the flow velocity. However, this choice gives rise to a fixed Prandtl number $Pr = 1$, so corrected distribution functions have to be introduced. The most common options are the Shakhov[7] and the ellipsoidal statistical (ESBGK)[8] models, using respectively the corrected distributions f^S and f^{ES}:

$$f^S = f^M\left[1 + (1 - Pr)\frac{\mathbf{c}\cdot\mathbf{q}}{5\rho(RT)^2}\left(\frac{\mathbf{c}^2}{RT} - 5\right)\right], \tag{4}$$

$$f^{ES} = \frac{\rho}{\sqrt{\det \mathcal{A}}}\left(\frac{1}{2\pi RT}\right)^{3/2} \exp\left[-\frac{\mathbf{c}^T\mathcal{A}^{-1}\mathbf{c}}{2RT}\right] \qquad \text{with} \qquad \mathcal{A} = \mathcal{I} - \frac{1 - Pr}{Pr}\left(\frac{3\mathcal{P}}{\text{Tr}\,[\mathcal{P}]} - \mathcal{I}\right). \tag{5}$$

These correction are based on the inclusion of the deviation from equilibrium due to high order moments of the distribution function, either the heat flux vector $\mathbf{q} = \frac{1}{2}\int \mathbf{c}(\mathbf{c}\cdot\mathbf{c})f d\mathbf{v}$ or the pressure tensor $\mathcal{P} = \int \mathbf{c}\mathbf{c}^T f d\mathbf{v}$. Even though these two model can give slightly different results,[5] both will be used in the rest of this paper for the sake of simpler implementation: the Shakhov model for the deterministic solver and the ESBGK model for the stochastic one.

It should however be noted that the BGK model, regardless of the target distribution, is only a good approximation of the Boltzmann equation when non-equilibrium effects remain limited, notably in the so-called transition regime. For more rarefied cases, when the Knudsen number increases before reaching the free-molecular limit, BGK-based simulations become less accurate than actually solving the Boltzmann equation or using the well-known DSMC method. Nevertheless, the Knudsen range covered by BGK methods is large enough to make them very beneficial thanks to their low resolution requirements compared with DSMC, as the spatio-temporal discretization can be larger than the mean free path and mean collision time.

The various numerical methods that solve the BGK equation can mainly be classified as either discrete velocity methods[3,9–11] where the equation is fully discretized deterministically, using a grid in physical space as well as in velocity space, or stochastic particle-based solvers,[5,12,13] in which the velocity space discretization is done with simulation particles whose velocity is sampled stochastically from the distribution function. These different approaches lead to different regimes of best performance for each method. Indeed, the deterministic nature of DVMs ensures good accuracy regardless of the temporal evolution of the flow, while particle-based solver are often used with time averaging in order to decrease the level of statistical noise in the results, a procedure that is only possible for steady flows. Besides, as the Knudsen number decreases, the distribution function, getting closer to equilibrium, becomes easier to discretize deterministically using appropriate quadratures. However, for hypersonic flows, the stochastic approach is more efficient in reproducing the highly non-equilibrium distribution that would require many quadrature points, and the statistical noise becomes negligible compared to the high velocity and temperature. Furthermore, the number of velocity discretization points required by DVMs naturally increases with the flow dimension, as 3 dimensions of space result in an effective equation to solve in a phase space with 6 dimensions.

To summarize, DVMs perform best on one or two dimensional near-continuum cases with low flow velocity while stochastic BGK methods become more efficient on more rarefied high-Mach number 3D problems. Setting apart the dimension, a hybrid method would therefore be very advantageous. Such a solver has been developed with the

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unified gas-kinetic wave-particle (UGKWP) solver,[14] but its stochastic part is based on a classical particle-based BGK solver that only achieves first-order accuracy. The method presented here is therefore constructed with the goal of reaching second-order accuracy while making possible both a deterministic and a stochastic-particle implementation.

2.2 Exponential differencing of the BGK equation

A good candidate to be extended from a DVM to a second-order particle-based solver would be the discrete unified gas-kinetic scheme[11,15] (DUGKS) because the second-order accuracy is achieved while keeping the overall method explicit. However, the operations realized on the distribution function can include negative factors when the time step increases and can therefore not be seen as probabilities, with which particles would be sampled from a distribution in the stochastic approach. The main idea behind the exponential differencing BGK (EDBGK) method is thus to obtain a second-order accurate solver in a similar way as DUGKS while retaining positivity in every operation made on the distribution functions, as detailed in Pfeiffer et al.[6]

The EDBGK method is based on an integration of the BGK equation using exponential time differencing[16] in order to handle the stiff linear term νf:

$$f(t^{n+1}) = f(t^n)e^{-\nu\Delta t} + e^{-\nu\Delta t}\int_0^{\Delta t} e^{\nu s}\left(\nu f^t(t^n+s) - \mathbf{v}\frac{\partial f}{\partial \mathbf{x}}(t^n+s)\right) ds. \tag{6}$$

Then, a linear approximation is used on the non-linear stiff term νf^t to integrate it while keeping the second-order accuracy:

$$f^t(t^n+s) = f^t(t^n) + \frac{s}{\Delta t}(f^t(t^n+\Delta t) - f^t(t^n)). \tag{7}$$

From this point, introducing "re-scaled" distribution functions and reordering terms leads to

$$\widetilde{f}_{n+1} = \hat{f}_n - \mathcal{F}_n, \tag{8}$$

where

$$\hat{f}_n = \frac{1}{\gamma}\left(f(t^n)e^{-\nu\Delta t} + (1-e^{-\nu\Delta t})Af^t(t^n)\right) \quad \text{and} \quad \widetilde{f}_n = \frac{1}{\gamma}\left(f(t^n) - (1-e^{-\nu\Delta t})Bf^t(t^n)\right) \tag{9}$$

with

$$\gamma = \frac{1-e^{-\nu\Delta t}}{\nu\Delta t}, \quad A = \frac{1}{\nu\Delta t} - \frac{e^{-\nu\Delta t}}{1-e^{-\nu\Delta t}} \quad \text{and} \quad B = \frac{1}{1-e^{-\nu\Delta t}} - \frac{1}{\nu\Delta t}. \tag{10}$$

For the next time step, $\hat{f}_{n+1}$ can easily be obtained from $\widetilde{f}_{n+1}$ via

$$\hat{f} = e^{-\nu\Delta t}\widetilde{f} + (1-e^{-\nu\Delta t})f^t. \tag{11}$$

The flux term $\mathcal{F}_n = e^{-\nu\Delta t}\int_0^{\Delta t} e^{\nu s}\mathbf{v}\frac{\partial f}{\partial \mathbf{x}}(t^n+s)\,ds$ can then be handled in different ways. In a similar manner as in DUGKS, it can be integrated with a midpoint rule using a finite volume scheme with second-order reconstruction. This approach, combined with a discretization of the velocity space using either Gauss-Hermite (in near-equilibrium cases) or Newton-Cotes quadratures, results in a second-order DVM, presented in Garmirian and Pfeiffer.[17] Otherwise, using a Lagrangian frame of reference by following the trajectory of simulation particles simply removes this term in the initial equation. By sampling the particle velocities from $\widetilde{f}$ and making them relax by re-sampling them from f^t with a probability $P = 1 - e^{-\nu\Delta t} \in [0,1]$ at every time step acording to equation (11), a second-order stochastic solver is constructed.[6] Both of these solvers are implemented in the open-source gas and plasma simulation framework PICLas.[18]

3. Results

The simulation results shown in this section, either from the presented methods or DSMC, are all obtained with PICLas running in parallel on AMD Epyc 7713 processors, each made of 128 cores. For the deterministic EDBGK solver, the Courant-Friedrichs-Lewy (CFL) number is defined using the highest possible velocity on the discretization grid. The boundary interactions are either fully specular or diffusive, assuming a Maxwellian distribution at the wall. In the particle-based methods, all particles hitting the diffusive walls are sampled from this distribution, while in the deterministic case, ghost cells are employed to ensure second-order accuracy at the boundaries.[19] In all cases, a variable hard sphere (VHS) model of argon gas is used, with monatomic molecules of mass $m = 6.63 \times 10^{-26}$, and an initial temperature equal to the temperature of diffusive walls $T_0 = 273$K.

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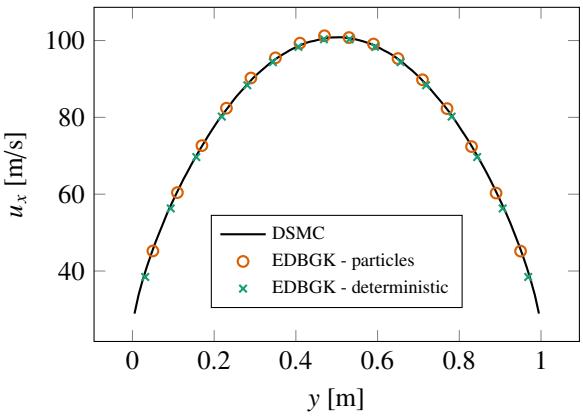

Figure 1: Poiseuille flow at Kn= 0.1: velocity profile comparison.

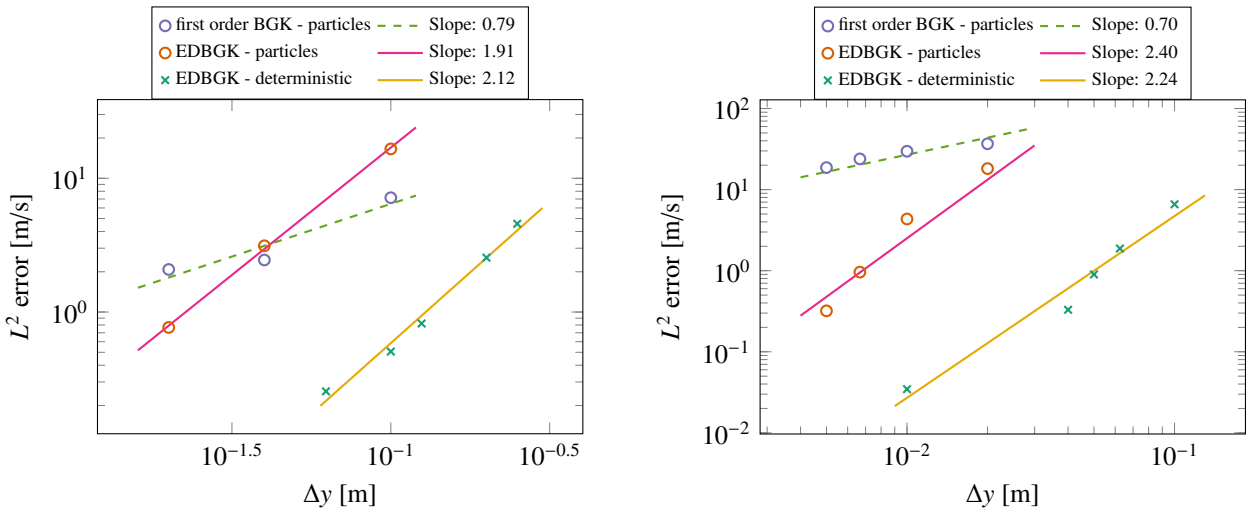

Figure 2: Poiseuille flow: comparison of error convergence. (a) Kn = 0.1; (b) Kn = 0.001.

3.1 Poiseuille flow

First, a force-driven Poiseuille flow is simulated, where a uniform force defined by $\frac{\rho}{m}F_x = 10^{-2}$ Pa/m is applied perpendicularly to the $L_y = 1$m-long domain. In order to retain the second-order accuracy, the force is applied in two steps using a Strang splitting approach as done in Wang et al.[20] This study focuses on the profile of the x velocity component that appears between the two diffusive plates at $y = 0$ m and $y = 1$ m.

On Figure 1, results obtained at Kn = 0.1 with both variants of the EDBGK method are compared to a highly resolved DSMC solution. The different approach to reach second-order accuracy in space, between the linear interpolation used for particles and the reconstruction using the gradients of the distribution function for the DVM, resulted respectively in the need for 50 and 16 mesh cells. A 101×101 uniform velocity grid with boundaries $v_{max} = -v_{min} = 9\sqrt{2RT_0}$ and a CFL number of 0.9 were used for the deterministic results, resulting in a relaxation factor of $\nu\Delta t = 0.04$ and a simulation time on one CPU core of 314 s to reach steady state. The Lagrangian particle-based method having no stability condition to respect, a larger time step could be used with this solver ($\nu\Delta t = 0.15$). However, the simulation had to be continued after reaching steady state to obtain time-averaged results, in order to minimize the amount of noise in the results and reach a similar level of L^2 error with both approaches:

$$\frac{1}{N_{cells}}\left(\sum_{i=1}^{N_{cells}}[u_x(x_i) - u_{x,DSMC}(x_i)]^2\right)^{-1/2} \approx 0.2. \tag{12}$$

A longer CPU time of 516 s was therefore necessary for the stochastic EDBGK on one core, but this is a good example

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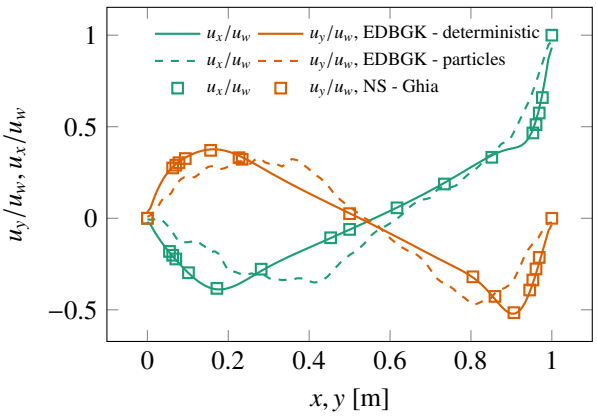
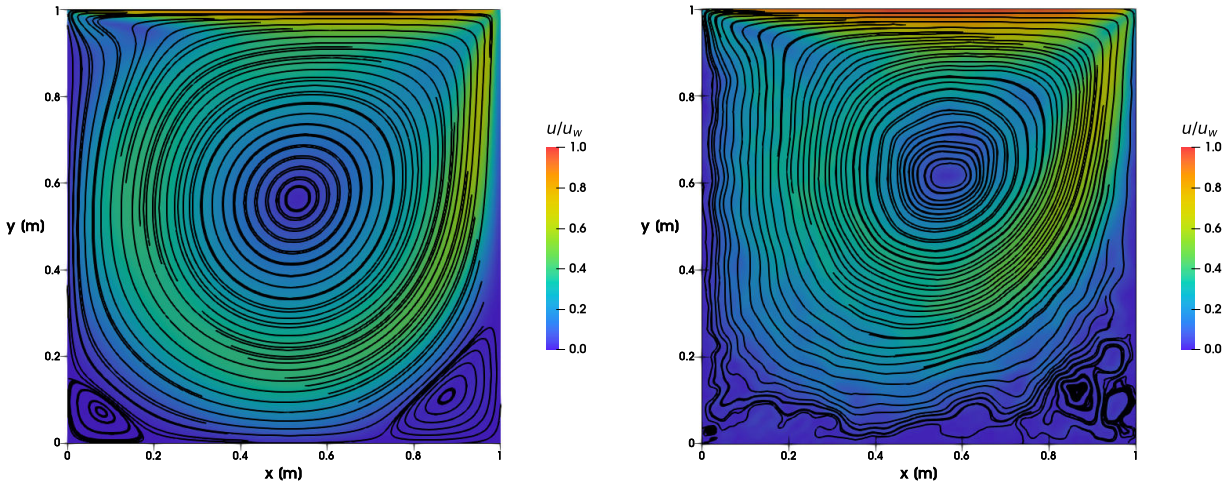


Figure 3: Lid-driven cavity flow at Re = 1000: x-velocity along a central vertical line (green) and y-velocity along a central horizontal line (orange).



(a) (b)

Figure 4: Lid-driven cavity flow at Re = 1000: velocity field lines and magnitude. (a) ED - deterministic; (b) ED - particles.

of a case where the computational cost remains low and similar with both solvers: only 2D velocity grids are necessary for the DVM, the transition regime is exactly where BGK methods are efficient, and the flow is subsonic but the velocity gradients are large enough to limit the relative importance of statistical noise.

For the purpose of validating the space and time convergence order of the method, simulations were carried out using different resolutions while keeping the same ratio between time step and mesh size. As shown on Figure 2, the second-order accuracy of the EDBGK scheme is as clear in the rarefied as in the near-continuum regime. It also demonstrates the advantage over the classical first-order particle-based BGK solver.

3.2 Lid-driven cavity flow

The EDBGK method is then applied to a common validation test case for computational fluid dynamics, the lid-driven cavity flow. A 1m-large square cavity is filled with a gas that is set in motion by the top side moving at the constant speed $u_w = 50$ m/s. The density is set so as to obtain a Reynolds number of Re = 1000, resulting in a Knudsen number of Kn $= 2 \times 10^{-4}$. The mesh used is a 100×100 non-uniform grid, with more resolution near the boundaries where vortices appear.

This case was simulated with the DVM version of EDBGK using a 5×5 Gauss-Hermite velocity grid, this quadrature being able to capture the shape of the near-equilibrium distribution with a small number of points. A maximum CFL number of 0.9 in the smallest cells was obtained with a time step $\Delta t = 1 \times 10^{-5}$. Although the

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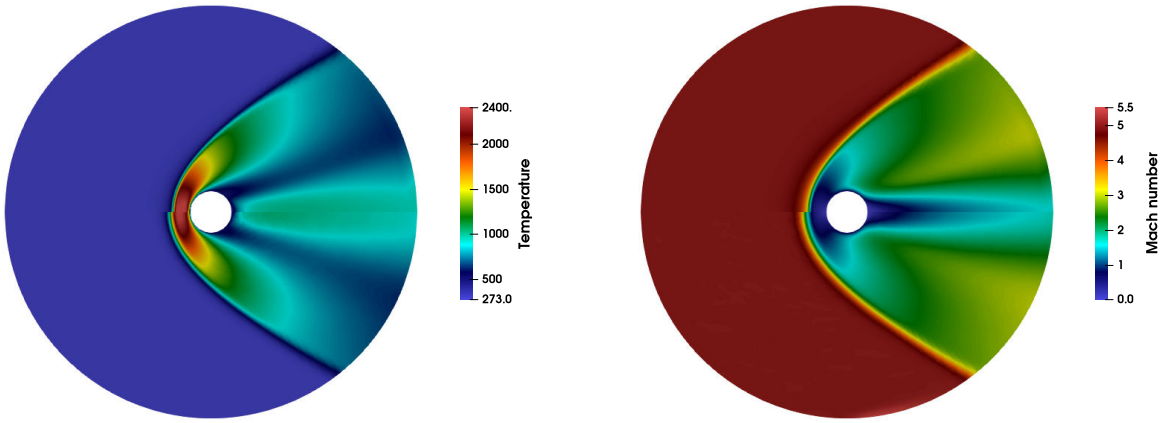

Figure 5: Temperature and Mach number for the flow around a cylinder. Top half of the figures is simulated with the deterministic EDBGK solver, while the bottom half is the DSMC reference.

resulting relaxation factor reached around 11, the coupled integration of the advection and relaxation processes in EDBGK allowed for accurate results that matched very well the Navier-Stokes reference from Ghia and Ghia,[21] as shown on Figure 3. Steady state was considered as reached when the relative change in velocity $\sum_{i=1}^{N_{cells}}(\mathbf{u}(\mathbf{x}_i, t_2) - \mathbf{u}(\mathbf{x}_i, t_1))/\sum_{i=1}^{N_{cells}}\mathbf{u}(\mathbf{x}_i, t_1)$ with $t_2 - t_1 = 0.1$ s fell below 1×10^{-4}. This simulation lasted 539 s on 64 CPU cores.

Using the stochastic particle-based version with the same spatio-temporal resolution, and averaging the results on 20 000 time steps after reaching steady state resulted in noisy results, especially in the low-speed vortex regions, which are visible on Figure 4. However, these results already required 4371 s on the same configuration, showing the superiority of DVM on low-speed continuum cases. Besides, the overall velocity field is slightly shifted compared to deterministic results. Once again, this might be due to the different ways of ensuring second-order accuracy in space, and smaller mesh cells might be needed for the stochastic solver.

3.3 Flow around a cylinder

Although a rarefied flow with a high Mach number implies strong non-equilibrium effects, even the deterministic EDBGK solver can be used on such cases, as long as the velocity discretization can encompass all significant thermal velocities with fine enough resolution. A flow around a circular cylinder is simulated at Kn= 0.1 with an inflow Mach number of Ma= 5. The Venkatakrishnan limiter[22] was used to avoid nonphysical oscillations due to the shock in front of the cylinder. The velocity grid used is the same as the one used by Zhu et al[23] with DUGKS: a 89×89 Newton-Cotes quadrature with $v_{max} = -v_{min} = 15\sqrt{2RT_0}$. The results, obtained on a 100×100 non-uniform half-circle mesh, are compared to DSMC simulations on Figure 5.

4. Conclusion

The second-order asymptotic preserving EDBGK method can simulate a wide range of gas flows in different regimes, and the possibility to use it with the two different common approach to solve the BGK equation make it a particularly versatile toolbox. As future work, coupling the deterministic and the stochastic variants in phase space would provide a highly multiscale method capable of exploiting the advantages of both approaches to reduce the overall computational cost. This would be possible thanks to the shared scheme for time integration.

Besides, the EDBGK solvers could be improved by implementing all mentioned target distributions for both approaches, by extending them to include molecules and mixtures, by making use of moment conservation schemes[3] for the DVM or by improving the spatial interpolation for the stochastic particle-based method.

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