A kinetic switching criterion for hybrid modelling of multiscale gas flows

Jianping Meng, Nishanth Dongari, Jason M Reese, Yonghao Zhang
Department of Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, United Kingdom
E-mail: jianping.meng@strath.ac.uk; nishanth.dongari@strath.ac.uk; jason.reese@strath.ac.uk; yonghao.zhang@strath.ac.uk

Abstract. In some important engineering applications, gas flows are often found to be hydrodynamic in one part of device and highly rarefied in the others. To solve this kind of multi-scale flow problems efficiently and accurately, hybrid methods coupling hydrodynamic and kinetic methods are attractive. The successful implementation of hybrid methods relies on the accurate assessment of the level of non-equilibrium (rarefaction) in the local flowfield. Currently available criteria, such as Knudsen and Mach numbers, are based on macroscopic parameters and have been shown to be restrictive. Here, we propose a new kinetic criterion that utilises the fundamental molecular distribution function to assess the local flow field. Through numerical evaluation we show that our criterion provides a reasonable assessment and, in particular, it behaves consistently for both high-speed and low-speed flows, which is not the case for the other criteria based on macroscopic parameters. As our criterion fully utilises the accurate information provided by the molecular distribution function, it is particularly suitable for recently developed multi-scale kinetic methods.

1. Introduction

Physical phenomena may occur over a broad range of spatial and temporal scales in practical engineering problems. In gas flows, for instance, equilibrium and non-equilibrium phenomena may co-exist within the same device [1]. To qualitatively identify the non-equilibrium level of the local flowfield, the Knudsen number $Kn$ can be used, which is the ratio of the mean free path of a gas to the characteristic length scale of the flow process. It is commonly accepted that the conventional hydrodynamic description is only valid for $Kn < 0.001$. When $Kn$ is larger than 0.001, rarefaction effects have to be considered. These rarefied flows can be further classified into the slip ($0.001 \leq Kn < 0.1$), transitional ($0.1 \leq Kn < 10$) and free molecular ($Kn \geq 10$) flow regimes.

Multi-scale methods are designed to model gas flows with a broad range of Knudsen numbers [2]-[13]. Conventional continuum type solvers based on the Navier-Stokes (NS) framework are efficient, but only valid in the hydrodynamic flow regime. Their modelling capabilities may be extended to the slip flow regime by providing appropriate velocity-slip and temperature-jump boundary conditions. By contrast, kinetic solvers, such as the direct simulation Monte Carlo (DSMC) method [14] or direct solvers of the Boltzmann equation [15], can provide accurate solutions. However, they are computationally much more expensive, and may be prohibitively so for realistic 3D simulations of multiscale flows. To take advantages...
of both methods, the central idea of a multi-scale method is to deploy a kinetic solver in rarefied flow regions only, and apply a hydrodynamic solver in the other regions. Hence it is practically possible to provide not only efficient but also sufficiently accurate solutions for multi-scale problems.

An appropriate model switching criterion is a key factor in the success of a multi-scale method. It should be able to accurately assess the local flowfield in order to deploy appropriate solvers. The global Knudsen number may not be appropriate for this purpose [2], due to its arbitrariness in choosing a characteristic length. Various criteria are proposed ([2, 13, 16, 17, 18] and references therein). A commonly-used one is the so-called local Knudsen number, where the length scale is a formulation based on the local spatial gradients of hydrodynamic variables, i.e., \( K_{nl} = \frac{\lambda}{\phi \frac{d\phi}{dx}} \), where \( \phi \) denotes a significant flow quantity, typically density, temperature or pressure. For hypersonic aerodynamic flows, in particular, it has been suggested that \( Ma \cdot Kn_{nl} \), where \( Ma \) is the Mach number, is a more appropriate switching parameter [16]. Although these parameters have been proven to be applicable to a range of problems, they may not be generally optimal. For instance, they may become a negligible quantity in low speed flows even for high Knudsen numbers.

On the other hand, there are several proposed multi-scale methods that are built purely on the kinetic theory [19, 20]. For these kinds of methods a criterion based on macroscopic quantities does not take advantage of the available kinetic information. So recently, we propose using the molecular distribution function, instead of macroscopic flow properties, to assess the level of thermodynamic non-equilibrium in the local flowfield [21]. Here, we will numerically evaluate this approach as a model switching criterion.

### 2. Kinetic criterion

The Boltzmann equation describes the dynamical behaviour of dilute gases, and assumes both binary collisions between gas molecules and molecular chaos to enable a single molecular velocity distribution function to describe the gas motion. The conventional macroscopic equations, such as the NS equations, can be considered as approximate solutions of the Boltzmann equation in the hydrodynamic flow regimes, via the Chapman-Enskog approach. In this approach the solution of the Boltzmann equation, is assumed to be of the form

\[
f = f^{(0)} + f^{(1)} + f^{(2)} + \cdots + f^{(\alpha)} + \cdots,
\]

where the distribution functions \( f^{(\alpha)} \) can be asymptotically obtained from the Boltzmann equation. The Maxwell-Boltzmann equilibrium distribution,

\[
f^{eq} = \frac{\rho}{(2\pi RT)^{3/2}} \exp \left[ -\frac{\xi^2}{2RT} \right],
\]

is the zeroth-order solution \( f^{(0)} \), and leads to the Euler equations. Here, \( \rho \) denotes the gas density, \( T \) the temperature, \( R \) the gas constant, and \( \xi \) the peculiar velocity of molecules, which is \( \xi = u - \bar{u} \) where \( \bar{u} \) represents the molecular velocity and \( u \) is the macroscopic fluid velocity. In Eq. (1), \( f^{(1)} \) provides a non-equilibrium correction of order \( Kn \). To recover the Navier-Stokes equations,

\[
f^{(1)} = f^{eq} \left[ \left( \frac{\sigma_{ij} \xi_i \xi_j}{2pRT} \right) + \frac{2q_i \xi_i}{5pRT} \left( \frac{\xi^2}{2RT} - \frac{5}{2} \right) \right],
\]

where \( p \) is the gas pressure, and the shear stress \( \sigma_{ij} \) and the heat flux \( q_i \) are related to the following first-order gradients of velocity and temperature,

\[
\sigma_{ij} = -2\mu \frac{\partial u_i}{\partial x_j}, \quad q_i = -\kappa \frac{\partial T}{\partial x_i},
\]
where \( \mu \) and \( \kappa \) denote the viscosity and thermal conductivity, respectively. We can continue the series to obtain higher-order corrections in terms of the Knudsen number.

As indicated by the Chapman-Enskog procedure, the Euler equations are appropriate for thermodynamically equilibrium flows with \( Kn \to 0 \), while the Navier-Stokes equations are valid for linear departures from equilibrium, where the Knudsen number is close to zero. In high altitude applications, such as spacecraft re-entry into planetary atmospheres, or vacuum applications, such as low-pressure chemical processes, the flows can be highly non-equilibrium. The Navier-Stokes equations fail to provide an adequate description in such cases. However, the Knudsen number alone may not be sufficient to describe the level of non-equilibrium in the flowfield, and therefore to assess whether the Navier-Stokes equations are applicable or not. Both simulation data [16] and theoretical analysis [22] show that the level of non-equilibrium is also strongly influenced by the Mach number.

In our recent work, we have proposed two kinetic parameters for indicating the level of non-equilibrium in the local flowfield [21]. These parameters can be used as model switching criteria as well. Here, we give a brief summary. Considering Eq. (1), the distribution function may be naturally split into two parts: the equilibrium and the non-equilibrium components, i.e.,

\[
    f = f^{eq} + f^{neq}. \tag{5}
\]

The ratio of the non-equilibrium to the equilibrium parts can be used to measure the departure from equilibrium. However, it is not a practical criterion for low-speed flows, and it may be more appropriate to utilise higher order corrections. If the validity of the Navier-Stokes equations is of interest, the non-equilibrium part \( f^{neq} \) may be further divided into two components, i.e.,

\[
    f^{neq} = f^{(1)} + f^{(H)}, \tag{6}
\]

where \( f^{(1)} \) is the Navier-Stokes level correction, which is given by Eq. (3), and \( f^{(H)} \) is the higher-order non-equilibrium correction beyond the Navier-Stokes level. Obviously, only when \( f^{(1)} \gg f^{(H)} \), can the Navier-Stokes equations be a valid approximation of the Boltzmann equation. Moreover, a \( L^2 \) norm of

\[
    C_1 = \sqrt{\frac{\int (f^{(H)})^2 d\xi}{\int (f^{(1)})^2 d\xi}} = \sqrt{\frac{\int (f - f^{eq} - f^{(1)})^2 d\xi}{\int (f^{(1)})^2 d\xi}}, \tag{7}
\]

may then be defined to assess the non-equilibrium level, and is a direct indicator of the relative error introduced by using a Navier-Stokes solution on the flowfield. As discussed above, another parameter

\[
    C_0 = \sqrt{\frac{\int (f^{neq})^2 d\xi}{\int (f^{eq})^2 d\xi}} = \sqrt{\frac{\int (f - f^{eq})^2 d\xi}{\int (f^{eq})^2 d\xi}} = \sqrt{\frac{\sqrt{8\pi^3/4}(RT)^{3/4}}{\rho} \int (f - f^{eq})^2 d\xi}, \tag{8}
\]

may be defined similarly, as a measure of the relative error of \( f \) to the Maxwellian \( f^{eq} \). In the following numerical simulations, we will solve the ellipsoidal statistical BGK (ES-BGK) model [23] to evaluate these two parameters for Couette flows over a broad range of Knudsen and Mach numbers.

3. Numerical evaluation for Couette flow

Due to the simplicity of the Couette flow its characteristics are well understood. Non-equilibrium effect is usually strongest near the wall boundary, and weaker in the bulk, even there is a large global Knudsen number. Therefore it is a suitable benchmark case to numerically examine our proposed model switching criteria.
The ES-BGK kinetic model \[23\] to obtain \( f \) can be written as

\[
\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} = -\frac{1}{\tau} (f - f^{ES}),
\]

(9)

where \( \tau \) is the mean relaxation time, which is assumed to be independent of molecular velocity. The anisotropic Gaussian distribution function can be written as

\[
f^{ES} = \rho \frac{1}{\sqrt{\det[2\pi \lambda_{ij}]}} \exp \left[ -\frac{1}{2} \lambda^{-1} \varsigma \varsigma \right],
\]

(10)

where \( \lambda_{ij} = RT \delta_{ij} + (b \sigma_{ij})/\rho \), \( \sigma_{ij} \) is the shear stress. The parameters \( b \) and \( \tau \) can be determined using either the Boltzmann integral with a known inter-molecular force law, or through experimental values. The relations between the model parameters and the transport coefficients are

\[
\mu = \frac{(p \tau)}{1 - b} \quad \text{and} \quad \kappa = \frac{p R (D + 2)}{2 \tau} \quad \text{(D is the dimension number)},
\]

so that \( Pr = \frac{1}{1 - b} \). Therefore, the Prandtl number can be adjusted via the free parameter \( b \).

To numerically solve Eq.(11), the discrete velocity method is employed. Since this simple Couette flow is actually only one-dimensional, Eq.(11) can be simplified as,

\[
\frac{\partial f}{\partial t} + \xi_y \frac{\partial f}{\partial y} = -\frac{1}{\tau} (f - f^{ES}),
\]

(11)

where the coordinate \( y \) is perpendicular to the stream-wise direction. To save computational cost, a two-dimensional ideal gas, where particle motion is limited to a two-dimensional physical space is considered here. Therefore the particle velocity space can be discretized with a polar coordinate system using Simpson’s rule. For the physical space, the discretization is accomplished by a second-order total variations diminishing (TVD) scheme, as presented below,

\[
f_{j}^{n+1} |_{c_{y} > 0} = A \left\{ f_{j}^{n} - \nu \triangle \phi_{j-} - \frac{1}{2} (1 - \nu) \nu [J_{1} \triangle f_{j+} - J_{2} \triangle f_{j-}] + \frac{1}{\tau \rho} f_{ES,j}^{n} dt \right\},
\]

\[
f_{j}^{n+1} |_{c_{y} < 0} = A \left\{ f_{j}^{n} - \nu \triangle f_{j+} + \frac{1}{2} (1 + \nu) \nu [J_{3} \triangle f_{j+} - J_{4} \triangle f_{j-}] + \frac{1}{\tau \rho} f_{ES,j}^{n} dt \right\},
\]

with

\[
A = \frac{\tau}{\tau + dt},
\]

\[
\triangle f_{j+} = f_{j+1} - f_{j} \quad \triangle f_{j-} = f_{j} - f_{j-1},
\]

\[
\theta_{1} = \frac{f_{j} - f_{j-1}}{f_{j+1} - f_{j}} \quad \theta_{2} = \frac{f_{j+1} - f_{j}}{f_{j+1} - f_{j-1}},
\]

\[
\theta_{3} = \frac{f_{j+2} - f_{j+1}}{f_{j+1} - f_{j}} \quad \theta_{4} = \frac{f_{j+1} - f_{j}}{f_{j+1} - f_{j-1}},
\]

\[
\triangle \phi_{j+} = f_{j+1} - f_{j} \quad \triangle \phi_{j-} = f_{j} - f_{j-1}.
\]

The minmod function is

\[
J_{i} = \max [0, \min(1, \theta_{i})] \quad i = 1 - 4
\]

and

\[
\nu = \frac{\xi_{y} dt}{dy}
\]
Figure 1. Profiles of $C_0$ and $C_1$ across the Couette flow channel at $Kn = 0.01$ and for various Mach numbers.

Figure 2. Profiles of $C_0$ and $C_1$ across the Couette flow channel at $Kn = 0.05$ and for various Mach numbers.

Figure 3. Profiles of $C_0$ and $C_1$ across the Couette flow channel at $Kn = 0.1$ and for various Mach numbers.
is the Courant–Friedrichs–Lewy (CFL) number. Although the molecular velocity is discretized based on the polar coordinate system, the Cartesian components of the molecular velocity is still used. The transformation between tow systems is accomplished as normal. After the solution is converged, the relevant distribution can be obtained directly via Eqs. (2) and (3).

In the simulations, five global Knudsen numbers ($Kn = [0.01, 0.05, 0.1, 0.5, 0.9]$) and six upper wall speeds ($U_w = [0.03, 0.3, 1.0, 2.0, 3.0, 4.0]\sqrt{RT_0}$) are considered. The variables $p_0$, $T_0$ and $\mu_0$ denote the reference pressure, temperature and viscosity coefficient, respectively, while $L$ is the characteristic length. The non-dimensional number $Kn$ and $Ma$ is then defined as $(\mu_0\sqrt{RT_0})/(p_0L)$ and $U_w/\sqrt{RT_0}$ respectively. While the upper wall is moving with $U_w$, the bottom one is set to be at rest.

The profiles of $C_0$ and $C_1$ are presented in Figs. 4 and 5. Clearly $C_0$ is strongly related not only to the global Knudsen but also to the Mach number with an almost linear correlation. This correlation makes $C_0$ inappropriate for low-speed flows. For instance $C_0$ in the bulk is less than 0.01 for both two cases ($Kn = 0.9, Ma = 0.03$) and ($Kn = 0.05 Ma = 0.3$). Although $C_0$ in the first case is even smaller than in the second one, it is generally accepted that the NS equations

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**Figure 4.** Profiles of $C_0$ and $C_1$ across the Couette flow channel at $Kn = 0.5$ and for various Mach numbers.

**Figure 5.** Profiles of $C_0$ and $C_1$ across the Couette flow channel at $Kn = 0.9$ and for various Mach numbers.
can be applicable in the bulk for the second case and but inappropriate for the first one. However, $C_1$ gives much more consistent indications for both low-speed and high-speed flows. For instance, $C_1$ in the bulk is larger than 0.25 at $Kn = 0.9$ for both $Ma = 0.3$ and $Ma = 0.03$, which clearly indicates inappropriateness of the NS model. At lower Knudsen numbers $C_1$ also reflects the dependency of non-equilibrium on non-linearity, i.e., the Mach number.

The difference in the two parameters lies in the way they assess the departure from equilibrium. According to Eqs. (7) and (8), $C_1$ is assessing the non-equilibrium level with respect to the NS equation, while $C_0$ is measuring the departure from Maxwellian equilibrium. Although the Chapman-Enskog expansion, Eq. (1), indicates that both parameters should reflect the order of the non-equilibrium level, simulations data here show that $C_0$ is greatly influenced by the non-linearity, while $C_1$ can correctly single out the non-equilibrium effect (which is of particular importance for low-speed flows). This observation supports the argument in [2], where the macroscopic quantities are used to assess the level of non-equilibrium in a ‘relative’ sense.

An interesting phenomenon is the variation of $C_1$ for strongly non-linear cases with Knudsen numbers larger than 0.5. Its value in the bulk can be larger than that near the walls. This non-intuitive observation may be explained as follows. As the mean particle speed $\bar{\xi}$ is proportional to $\sqrt{T}$, the mean speed in the bulk may become much larger than the near-wall region due to significant temperature rise caused by viscous heating. On the other hand, when the global Knudsen number is sufficiently large, the wall-molecule rather than molecule-molecule interactions dominate the gas behaviour. Therefore, the molecules in the bulk may actually have a great chance to collide with walls due to their much larger speed. In other words the wall-molecule interactions can be stronger for molecules in the bulk. As the NS solution tends to underestimate this kind of interactions, its error can become more significant in these circumstances.

4. Concluding remarks

We have numerically evaluated the ‘kinetic criterion’ $C_1$ for a multi-scale gas flow method, which can assess the level of non-equilibrium with respect to the NS solution by using the molecular distribution function rather than macroscopic quantities. This criterion is found to give consistent indications for flows over a broad range of Knudsen and Mach numbers. In particular, we have found it is an appropriate criterion for both high-speed and low-speed flows.

As the criterion takes advantage of the accurate molecular level information provided by the distribution function, it may be very useful for some recently developed kinetic multi-scale methods (e.g., those proposed in [19] and [20]), where the distribution function can be explicitly obtained. In these kinds of solvers, to satisfy the accuracy requirement of the difference levels of non-equilibrium, one may only to adjust the discrete velocity number (e.g., [20]), while the governing equation can keep the same. For switching from the higher non-equilibrium level to a hydrodynamic (continuum-fluid) level, it is quite easy as all the information is in hand. For switching from a near-continuum level to higher non-equilibrium level, one can run two level of simulations (e.g., nine-velocity and sixteen-velocity simulations for the lattice Boltzmann method) at the same time, then all the required information can be obtained. We note here, though two simulations are running, the costs are still expected to be less in comparison to those for high non-equilibrium level. Nevertheless, the practical performance of the criterion will be the subject of further work.

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