# Switching Criteria for Hybrid Rarefied Gas Flow Solvers

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**Abstract.** A set of local Knudsen numbers are defined, which are demonstrated to be more appropriate than conventional ones for the purposes of identifying gas flow non-equilibrium. The problematic area of choosing an appropriate switching criteria is addressed by adopting a local Knudsen number definition based on higher-order constitutive relations; the R13 equations are chosen. A procedure is then described that allows the estimation of the R13 local Knudsen number within a Navier-Stokes solver, and the efficacy of this as a switching criterion is tested within an illustrative hybrid BGK/Navier-Stokes procedure. For the test case investigated, the results from the hybrid procedure compare very well with the full BGK solution, and are obtained at a fraction (depending on the global Kn) of the computational cost.

**Keywords:** local Knudsen number; switching criteria; breakdown parameter; hybrid code.

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## INTRODUCTION

The Knudsen number is a dimensionless parameter that represents the degree of rarefaction in a gas flow; more specifically, the extent to which the gas flow departs from local thermodynamic equilibrium. It is commonly accepted that the Knudsen number can be used to characterise different rarefied regimes and therefore indicate which modelling methods are appropriate to use, e.g. continuum-fluid, molecular dynamics, etc. The Knudsen number, in global form, depends on a somewhat arbitrary choice of the macroscopic length scale. In a 2D channel flow, for example, it is not clear whether this length should be half the channel, or the full channel height – the choice would affect the Knudsen number by a factor of two. Because of this ambiguity a local Knudsen number is often adopted which replaces the macroscopic length scale with a formulation based on the spatial gradients of hydrodynamic variables, e.g.:

$$Kn_{\mathrm{L}} = \frac{\lambda}{\phi}\left|\frac{\mathrm{d}\phi}{\mathrm{d}x}\right| , \tag{1}$$

where $\lambda$ is the molecular mean free path, and $\phi$ is some significant flow quantity, typically density, temperature or pressure. Since this number is intended to represent the degree of departure from equilibrium at a particular point in a flow field, it has been used as a switching criterion (sometimes known as a breakdown parameter [1]) for use in hybrid continuum-molecular solvers; i.e., an indicator as to where within the same domain continuum models, rather than costly molecular methods, can be accurately applied. However, since there are a variety of ways in which to define the local Knudsen number, and each can give significantly different values, the choice of what to use as a switching criterion has proven a problem in itself [2]. This is especially apparent when considering micro flows. For example, a low-speed micro gas flow will have a uniformly negligible local Knudsen number, based on definition given in equation 1), since the gradients of the flow variables are negligibly small. However, evidently, non-equilibrium effects are far from negligible in these cases. At the opposite extreme, for hypersonic flows, it has also been suggested [3] that eq (1) should be multiplied by local Mach number for a more appropriate breakdown parameter – a definition such as this is clearly not compatible with low-speed gas flows, either. These issues prompt the question: is there a local Knudsen number definition, and hence switching criterion, that is appropriate for both hypersonic *and* micro gas flows?

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## LOCAL KNUDSEN NUMBER

A local Knudsen number should reflect the degree of departure from equilibrium at a given point in the flow field. More precisely, if it is to be used to establish when the Navier-Stokes equations can or cannot be employed, it should indicate the degree of departure from *near* local equilibrium (the thermodynamic state that must exist for the Navier-Stokes equations to be valid). Furthermore, it is not departure from near equilibrium in an absolute sense that we are interested — magnitude does not affect the rarefied characteristics of low-speed flows — it is departure *relative* to near equilibrium, i.e. relative to the Navier-Stokes non-equilibrium. With these considerations in mind, an expression for a local Knudsen number that expresses the fractional departure from Navier-Stokes non-equilibirum at a point in a gas flow is given:

$$Kn_{\mathrm{L}} = \frac{\left|\int \phi(f - f_{NS})\mathbf{dc}\right|}{\left|\int \phi(f_{NS} - f_e)\mathbf{dc}\right|}, \tag{2}$$

where $\mathbf{c}$ are the set of molecular velocities, $f$ the distribution function, $f_e$ the equilibrium distribution, $f_{NS}$ the distribution corresponding to the Navier-Stokes assumption, and the moment variable $\phi$ is chosen to generate expressions for $Kn_{\mathrm{L}}$ in terms of different hydrodynamic variables. Disregarding trivial moments, hydrodynamic local Knudsen number definitions can be generated from equation (2) as follows:

$$Kn_{\sigma_{ij}} = \frac{\left|\sigma_{ij} - \sigma_{NS,ij}\right|}{\left|\sigma_{NS,ij}\right|}, \tag{3}$$

and

$$Kn_{q_i} = \frac{\left|q_i - q_{NS,i}\right|}{\left|q_{NS,i}\right|}, \tag{4}$$

where $\sigma_{ij}$ is the stress tensor, $q_i$ is the heat-flux vector, and the subscript $NS$ denotes values obtained using Navier-Stokes constitutive relations. Note, *nine* unique Knudsen numbers are defined for use in a three-dimensional non-isothermal flow field. An *overall* Knusden number could be taken as the maximum of these values, i.e.:

$$Kn_L = \max\left(Kn_{\sigma_{ij}}, Kn_{q_i}\right), \tag{5}$$

## SWITCHING CRITERIA

The local Knudsen number, in the form (5), will not always be an appropriate guide for switching between molecular and continuum modeling approaches. A truly useful switching criterion, for a particular point in flow, must also take into account the *range* of non-equilibrium in the simulation being considered (i.e., the range in stress or heat flux). For example, in the same simulation there might be regions of high local Knudsen number at relatively low stress, and other regions with much greater stress, but negligible local Knudsen number. In this case, you would not want a simulation to switch to a molecular model to calculate stress in the regions of high local Knudsen number because values for the stress, although highly non-equilibrial, would be negligible in magnitude compared to other regions of the flowfield. For this reason, for a switching criterion, we propose the following modification to the local Knudsen numbers given in (3) and (4):

$$Kn_{\sigma_{ij}} = \frac{\left|\sigma_{ij} - \sigma_{NS,ij}\right|}{\left|\sigma_{NS,ij}\right|_{\max}}, \tag{6}$$

and

$$Kn_{q_i} = \frac{\left| q_i - q_{NS,i} \right|}{\left| q_{NS,i} \right|_{\max}}, \tag{7}$$

where the subscript max denotes a global(/spatial) maximum.

To test the performance of these local Knudsen number definitions as switching criteria, switching directions in both directions must be considered: molecular to continuum and continuum to molecular. In some respects determining appropriate switching from a molecular to a continuum solution is academic, since the more accurate solution (the molecular one) has already been obtained. However, this may not be so clear cut in time-dependent simulations.

## Molecular-to-Continuum Switching

To test the ability of the local Knudsen number to inform molecular-continuum switching, we consider low-speed Poiseuille flow with a global Kn=0.1 (=$\lambda/H$); where $H$ is the channel width and the mean free path is defined as:

$$\lambda = \mu \sqrt{\frac{\pi}{2\rho p}}, \tag{8}$$

where $\mu$ is the viscosity, $\rho$ is the density, and $p$ is the pressure. In figure 1, A Navier-Stokes solution (with second-order slip boundary conditions [4]) is plotted alongside a solution to the BGK Boltzmann equation obtained using a Discrete Velocity Method (similar to that used by Valougeorgis [5,6]); in both simulations, 500 grid points are used. The new local Knudsen number, from equation (6), is also plotted (calculated from the BGK data); for this case given as follows:

$$Kn_L = \frac{\left| \tau + \mu \dfrac{du}{dx} \right|}{\left| \mu \dfrac{du}{dx} \right|_{\max}}, \tag{9}$$

where $\tau$ is the shear stress, and $x$ is in a direction perpendicular to the flow velocity $u$. The local Knudsen number is identifying non-equilibrium in the Knudsen layers clearly and distinctly from the near-equilibrium bulk flow, where switching to a continuum solution could occur without significant error. Conventional local Knudsen number definitions, based on equation (1), could not provide this information since their values are negligibly small throughout the channel.

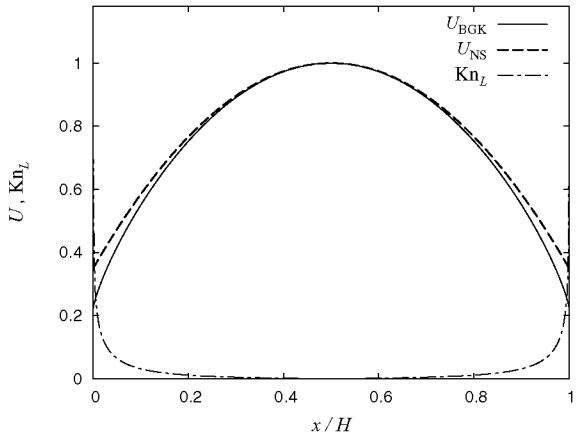


**FIGURE 1.** Normalised velocity profiles for Poiseuille flow (global $Kn$=0.1); BGK solution (——); Navier-Stokes with slip (— —). Local Knudsen number (— · —), equation (6), calculated from BGK data.

## Continuum-to-Molecular Switching

In contrast to molecular-to-continuum switching, equations (6)-(7) are little use as criteria to decide switching from a Navier-Stokes solution to a molecular-based simulation, since $\sigma_{ij}=\sigma_{NS,ij}$ and $q_i=q_{NS,i}$. For example, for Poiseuille flow, the Navier-Stokes constitutive relations are simply $\tau = -\mu\, du/dx$, which substituted into equation (9) reduces to $Kn_L=0$. If, though, high-order constitutive relations can be used to estimate the non-equilibrium values of $\sigma_{ij}$ and $q_i$, a means for continuum-to-molecular switching exists.

There are many competing high-order equation sets in the literature (space precludes a detailed discussion here, instead, see [7,8]). Of the most famous, perhaps, are the Burnett equations, variants of which have shown to accurately reproduce the viscous structure of one-dimensional shock waves. For normal shock waves, the dominant nonlinear term featuring in these high-order constitutive relations for normal stress, is as follows:

$$\sigma_B = \frac{A\mu^2}{p}\left(\frac{dv}{dx}\right)^2, \tag{10}$$

where $v$ is the velocity in the direction of shock structure variation, $x$, and $A$ is a constant for the particular gas. If this term is used to predict the non-equilibrium stress $\sigma_{11}$, the following local Knudsen number can be obtained from (6):

$$Kn_{\sigma_{11}} = \frac{\dfrac{A\mu^2}{p}\left(\dfrac{dv}{dx}\right)^2}{\dfrac{4\mu}{3}\left|\dfrac{dv}{dx}\right|_{\max}} \tag{11}$$

At the point of maximum normal stress, for steady one-dimensional shock waves, eq (11) can be reposed as follows (using continuity):

$$Kn_{\sigma_{11}} = \frac{3A\mu}{4p}\left|\frac{dv}{dx}\right| \propto M\frac{\lambda}{\rho}\left|\frac{d\rho}{dx}\right|, \tag{12}$$

where $M$ is the local Mach number. The form given in (12) is exactly the same as the local 'breakdown parameter' identified by Bird for high-speed expanding flows [9], and closely related to Tsein's parameter [10], also identified by Macrossan [3] as a better indicator for high-speed flows than the local Knudsen number (1) alone.

The approach, then, is partially validated, for high-speed flows at least. What is left to decide is which of the competing higher-order constitutive relations to adopt; if a consistent Knudsen number is to be found, this should be based on their performance in both low-speed *and* high-speed problems. In low-speed isothermal flows their main shortcomings have been related to predicting Knudsen-layer phenomena [7] due in part to the lack of additional boundary conditions required for their solution. For switching, though, no estimation of near-wall phenomena is required, since it is already clear that within one or two mean free paths of the wall a molecular treatment (or perhaps accommodation with slip conditions) is needed. On the other hand, non-equilibrium resulting away from the walls can be predicted with less complication using high-order equations. Lockerby and Reese [8] recently tested a number of different high-order continuum-type equations against a simple low-speed benchmark case with no bounding surfaces. It was concluded that the R13 equations, proposed by Torrilhon and Struchtrup [11] as a development of Grad's original 13 moment technique, provided the best model among the several tested. Importantly, the R13 equations also demonstrate good predictive capabilities in high-speed flows [12]. Based on their apparent versatility, we propose the following local Knudsen number definitions for use away from solid bounding surfaces:

$$Kn_{\sigma_{ij}} = \frac{\left|\sigma_{R13,ij} - \sigma_{NS,ij}\right|}{\left|\sigma_{NS,ij}\right|_{\max}}, \tag{13}$$

and

$$Kn_{q_i} = \frac{\left|q_{R13,i} - q_{NS,i}\right|}{\left|q_{NS,i}\right|_{\max}}. \tag{14}$$

If the R13 equations are being solved fully, then these Knudsen numbers are straightforward to calculate. However, they can also be estimated (more cheaply) within a Navier-Stokes solver:

$$Kn_{\sigma_{ij}} = \frac{\left|\sigma'_{R13,ij} - \sigma_{NS,ij}\right|}{\left|\sigma_{NS,ij}\right|_{\max}}, \tag{15}$$

where $\sigma'_{R13,ij}$ is calculated using R13 constitutive relations, but with values for hydrodynamic variables obtained using a Navier-Stokes solution. The error this introduces is acceptable for switching purposes because it is only the accurate calculation of *low* local *Kn* that is important.

## TEST CASE

To test the ability to inform continuum-to-molecular switching of the local Knudsen number given in equation (13), we here investigate the steady-state channel flow response to the following body force (non-dimensionalised with respect to $RT/H$, where $R$ is the gas constant and $T$ the gas temperature):

$$F_y = a_1 Kn\, \hat{x} \exp\left(-a_2 \hat{x}^2\right), \tag{16}$$

where $y$ is in the flow direction (and perpendicular to $x$), $a_1 = 10^5$, $a_2 = 10^3$, $\hat{x} = x/H$, and $Kn$ is the global Knudsen number (based on channel width, $H$). The variation of normalized body force through the channel is shown in Figure 2a) for global $Kn$=0.05. The forcing function has been chosen because it generates a shear flow, shown in Figure 2b), exhibiting both near-equilibrium and strong non-equilibrium behavior in the bulk flow (away from the walls), and is reminiscent in some respects of the velocity variation through a stationary monopole vortex (velocity non-dimensionalisation is with respect to $\sqrt{2RT}$.)

## R13 Local Knudsen Number

The linearised R13 constitutive expression for shear stress, for this steady low-speed one-dimensional example, is as follows:

$$\tau = -\mu\frac{du}{dx} + \frac{104}{15\pi}\lambda^2\frac{d^2\tau}{dx^2} + \frac{18}{5\pi}\lambda^2\mu\frac{d^3u}{dx^3} - \frac{192}{25\pi^2}\lambda^4\frac{d^4\tau}{dx^4}. \tag{17}$$

The implicit expression for stress requires iterative solution, with an accordant computational penalty. As an economical alternative, the shear stress can be approximated from within a Navier-Stokes solution by calculating higher-derivatives of stress using Navier-Stokes constitutive relations, i.e. $\tau = -\mu\, du/dx$:

$$\tau'_{R13} = -\mu\frac{du}{dx} - \frac{10}{3\pi}\lambda^2\mu\frac{d^3u}{dx^3} + \frac{192}{25\pi^2}\lambda^4\mu\frac{d^5u}{dx^5}. \tag{18}$$

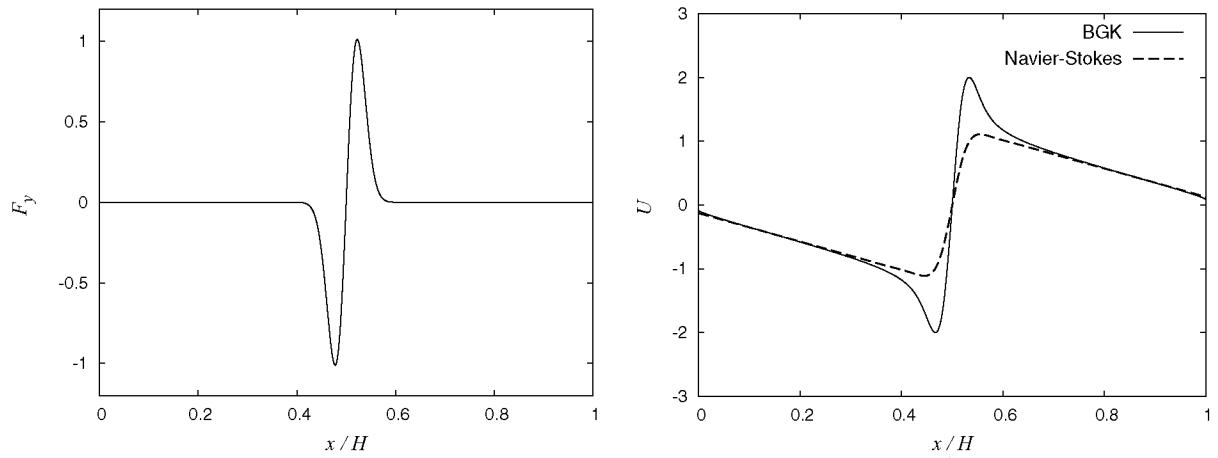


**FIGURE 2.** a) Normalised body forcing through channel (global $Kn$=0.05); and b), resulting non-dimensional velocity response; BGK solution (——); Navier-Stokes with slip (– –).

This approximate non-equilibrium stress, $\tau'_{R13}$, is used to find the local Knudsen number defined in Equation (15), as follows:

$$Kn_L = \frac{\left| -\frac{10}{3\pi}\lambda^2 \frac{d^3u}{dx^3} + \frac{192}{25\pi^2}\lambda^4 \frac{d^5u}{dx^5} \right|}{\left| \frac{du}{dx} \right|_{\max}} . \tag{19}$$

To test the performance of equation (19) as a switching parameter, we have constructed a simple hybrid solution procedure. Firstly, the Navier-Stokes equations are solved (shown by the dotted line in figures 3a,b) for global Kn=0.025, 0.1, respectively.) The local Knudsen number is then calculated as given above, and based on a local Knudsen number threshold of 0.01, some central portion of the domain is handled by the BGK solver (at the same spatial resolution) with the Navier-Stokes velocity gradient, $du/dx_{NS}$, given at the switching points. In the BGK solver, the velocity gradient (and near-equilibrium) is enforced at the switching-point boundaries using:

$$f(v_x) = f(-v_x) - 2v_x v_y \frac{\mu}{PRT} \frac{du}{dx}\bigg|_{NS} \qquad \text{for } v_x > 0 \ , \tag{20}$$

where $f(v_x)$ and $f(-v_x)$ are the distributions of molecules entering and exiting the domain, respectively, and $v_x$ and $v_y$ are components of molecular velocity. The velocity profile, $u$, calculated by the BGK solver is then uniformly scaled (by a few percent) so that the velocities at the switching-point boundaries match the velocities of the Navier-Stokes solution at the same points. The solutions are then combined.

Figure 3a,b) show solutions from this illustrative hybrid method compared to pure Navier-Stokes and BGK solutions, for global Kn=0.025 and 0.1. The simulation at Kn=0.025 is of comparable accuracy to the complete BGK solution, but has been obtained with a BGK domain size that is five times smaller. The relative portions of the deconstructed domain are 20/80% (BGK/Navier-Stokes) for Kn=0.025; 34/66% for Kn=0.05; and 57/43% for Kn=0.1.

Note, had the R13 equations been solved fully, a lesser BGK domain would have been required (a higher local $Kn$ threshold would be permissible), offsetting, partially at least, the additional computational expense of their solution.

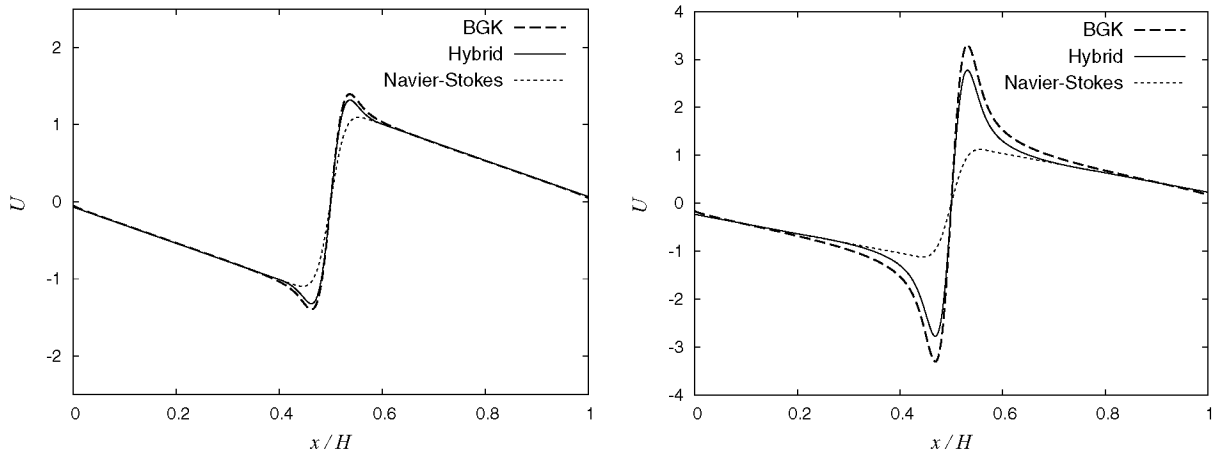


**FIGURE 3.** Non-dimensional velocity response to body forcing within channel, global *Kn* a)=0.025 and b)=0.1; Hybrid BGK/Navier-Stokes solution (——); BGK solution (– –); and Navier-Stokes with slip (·····). The BGK portion of the hybrid solution occurs between *x*=0.4 and 0.6 for global *Kn*=0.025; and x=0.214 and 0.786, for global *Kn*=0.1.

## SUMMARY

A set of local Knudsen numbers have been defined and have been demonstrated to be more appropriate than conventional ones for the purposes of identifying micro gas flow non-equilibrium. The problematic area of choosing an appropriate switching criteria has been addressed by adopting a local Knudsen number definition based on higher-order constitutive relations; here the R13 equations are chosen. A procedure has been described that allows the estimation of the R13 local Knudsen number within a Navier-Stokes solver, and the efficacy of this as a switching criterion has been tested within an illustrative hybrid BGK/Navier-Stokes procedure. For the test case investigated, the results from the hybrid procedure compare very well with the full BGK solution, and are obtained at a fraction (depending on the global Kn) of the computational cost.

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