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Non-equilibrium flows in aerodynamic and microsystems: a new field of study in fluid dynamics

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Abstract
Fluid flows that do not have local equilibrium are characteristic of some of the new frontiers in engineering and technology, for example, high-speed high-altitude aerodynamics and the development of micrometre-sized fluid pumps, turbines and other devices. However, this area of fluid dynamics is poorly understood from both the experimental and simulation perspectives, which hampers the progress of these technologies. This paper reviews some of the recent developments in experimental techniques and modelling methods for non-equilibrium gas flows, examining their advantages and drawbacks. We also present new results from our computational investigations into both hypersonic and microsystem flows using two distinct numer- ical methodologies: the direct simulation Monte Carlo method and extended hydro- dynamics. While the direct simulation approach produces excellent results and is used widely, extended hydrodynamics is not as well developed but is a promising candidate for future more complex simulations. Finally, we discuss some of the other situations where these simulation methods could be usefully applied, and look to the future of numerical tools for non-equilibrium flows.

Keywords: non-equilibrium flows; microfluidics; hypersonics; transition-continuum; direct simulation Monte Carlo; extended hydrodynamics

Introduction
To design the next generation of space re-entry vehicles and intercontinental passen- ger aeroplanes, engineers will need a good understanding of high-speed high-altitude aerodynamics (East 1999). At the other end of the scale, in order to make the best use of the new capabilities that micrometre-sized devices can offer, an appreciation of how to manipulate fluids in small spaces is essential (Gad-el-Hak 1999). Unfor- tunately, these emerging technologies have exposed a weak point in our ability to predict how fluids flow in unusual and extreme circumstances. Some surprising and curious effects occur in these types of flows that do not happen under more conven- tional circumstances. This paper describes the tools that engineers and mathemati- cians are just starting to develop to deal with these new situations. Our particular concern here will be gas flows, but we will also make some comments on how liquid and other flows may be dealt with in the future.

The classical mathematical expressions for momentum and heat transfer in fluids are the Navier–Stokes equations. These work very well for modelling fluids flowing in everyday situations, e.g. around cars, in water turbines and in the human body. However, these equations have been derived by assuming a strong separation exists between effects occurring on a microscopic scale and those on a macroscopic scale— essentially that the fluid can be regarded as a continuum. In practice, this requires heat and momentum to be equilibrated almost instantaneously throughout the fluid. For a monatomic gas, the molecules need some three or four collisions in order to equilibrate their energy with surrounding molecules. As, at normal temperatures and pressures, these molecules only travel on average a few tens of nanometres before they collide with another molecule, for most practical situations the continuum description is acceptable. However, at high altitude and in highly confined flows, the situation is not always so clear-cut.

The important parameter that indicates whether a gas can maintain conditions of thermodynamic equilibrium is the Knudsen number, Kn. This is the ratio of the average distance the gas molecules travel between collisions (called the 'mean free path', λ) to a characteristic length-scale, L, of the fluid system:

$$Kn = \frac{\lambda}{L}. \qquad (1.1)$$

(Sometimes the product of *Kn* and the Mach number of the flow is used as a classifica- tion parameter as well.) For gas flows in micrometre-sized devices, the characteristic length of the system is the width of the channel through which the gas is travelling, or a measure of the typical gradients in the flow. For aerospace vehicles, the char- acteristic length could be the radius of curvature of the bow or wing of the vehicle. In either case, if *Kn* is less than about 10^{-3}, the gas can be assumed to undergo a large number of collisions over the typical length-scale, and the conventional Navier– Stokes equations are an appropriate model (and the Euler equations can be used for flows away from solid boundaries when *Kn* is even lower). Difficulties appear when *Kn* rises, either due to the low density of the gas (which makes the mean free path larger) or in regions of high local gradients. Specifically, the relative flow velocity at any surface, which is normally assumed to be zero due to friction, takes on a finite value. Analogously, the temperature of the gas near the surface also differs from the surface temperature itself. This velocity 'slip' and temperature 'jump' mean that the boundary conditions normally required by the Navier–Stokes equations have to be changed. The situation becomes even more problematic as *Kn* rises to the range 0.1–1. This is the so-called 'transition-continuum regime'. For flows in this regime, the continuum assumption has essentially broken down, and the Navier–Stokes equations themselves become inappropriate. A schematic of these regimes and their methods of analysis is given in figure 1. Because of the development of new technologies and pro- cesses, a major focus of research in fluid dynamics is now the transition-continuum regime and, in particular, the construction of new modelling methodologies for those

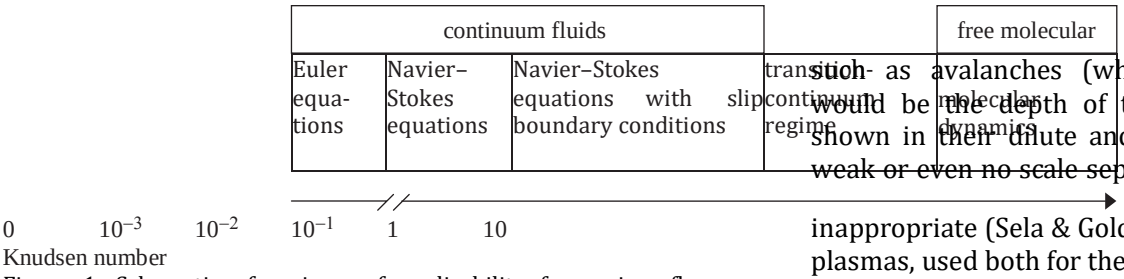

Figure 1. Schematic of regimes of applicability for various flow models over the range of Knudsen numbers.

gas flows that are too dense for computational molecular dynamics but so rarefied that standard continuum-equilibrium mathematical models cannot capture the flow physics.

The applicability of such models will be substantial. For example, it is important in high-altitude high-speed aerodynamics to be able to predict phenomena such as the rate and distribution of heating on the nose cone of a shuttle re-entering the atmosphere, or create the optimum design of aerodynamic surfaces for hypersonic airliners. If the aerodynamic control surfaces of such a vehicle have a characteristic length of, say, 0.1 m, the vehicle would encounter air at sea level with $\lambda \sim 10^{-7}$ m, which gives a *Kn* well into the continuum regime. However, at altitudes of 100 km (in which re-entry vehicles need to manoeuvre), $\lambda \sim 10^{-1}$ m, which would indicate that the flow is well into the transition-continuum regime. So the flight envelope of a vehicle such as a space shuttle encompasses the full range of *Kn*, and a comprehensive aerodynamic design methodology needs to recognize and be able to handle this.

In the technology of micro-electro-mechanical systems (MEMS), a major advance would be a fluid dynamical model which can predict the slip on the inner surfaces of flow devices (Craig *et al* . 2001), or handle the breakdown of the second law of thermodynamics in these tiny systems (Wang *et al* . 2002; Blau 2002). This branch of fluid dynamics is called 'microfluidics', and it is particularly important because of the multiplicity of applications for which MEMS have been proposed, including computer hard disk reading heads which are less than a micrometre above the spinning disk (Ng & Liu 2002), microducts for gas chromatographs and filters for environmental and biological monitoring, microactuators for flow control (Ho & Tai 1998), microturbinesand pumps, etc.

Other flow systems which have a coarse, particulate structure can also be ascribed a Knudsen number. When this is high enough, any continuum model of the sys- tem is likely to be inaccurate. For example, granular shear flows such as avalanches (where the reference length-scale would be the depth of the avalanche itself) have been shown in their dilute and semi-dense state to have very weak or even no scale separation, so a continuum model is inappropriate (Sela & Goldhirsch 1998). High- temperature plasmas, used both for the confinement of gases for nuclear fusion and for advanced spacecraft propulsion systems (Garrigues *et al* . 2002), are typically in the transition-continuum regime (although long-range Coulomb interactions add a further complication).

Transition-continuum flows

Experimental techniques

Recent experimental work on fluid flows in micrometre-sized systems illustrates some of the key problems in non-local-equilibrium flows. For example, the fact that the relative velocity of the gas at a solid boundary is not zero is well known (Maxwell 1879), but this has also been confirmed experimentally for liquid flows (Craig *et al* . 2001). It is even more intriguing to trace the consequences of the second law of thermodynamics at these small space and time-scales (Wang *et al* . 2002). New results are being uncovered all the time, but the development and validation of computational models for such flows is hampered by the difficulty of making *in situ* experimental measurements within microscale devices under, in the case of gas flows, rarefied and compressible conditions. Important physical quantities, such as tangential-momentum accommodation coefficients, thermal-accommodation coeffi- cients, electric wall-potential effects and wall-roughness effects, are all either inferred from external bulk flow measurements or derived implicitly or explicitly from analyt- ical or numerical schemes. Estimates of these coefficients and effects can vary by as much as 50% for common materials under controlled conditions. Unlike other areas of fluid dynamics, there is a dearth of experimental data and, even more importantly, a lack of established and reliable techniques for acquiring them.

To obtain detailed, spatially resolved and accurate experimental measurements of, for example, gas velocity within MEMS devices, the measurement technique must have certain characteristics. Firstly, it must be non-intrusive. Because the devices of interest are typically 1–500 μm in size, any probe would severely block and therefore alter the velocity distribution within the device. Secondly, for measurements to be meaningful they should reflect the actual mean velocity of the gas molecules. Non-continuum effects are evident mostly in the near-wall regions of the flow, but particle tracers and even large molecules do not react to the wall in the same way that gas molecules react. Therefore, the particle-based non-intrusive velocity-measurement techniques used for standard fluid dynamics, such as particle image velocimetry and laser Doppler velocimetry, are not options. Additionally, standard molecular tracking velocimetry is not an option, since the molecules used for this technique are generally very complex, and will not react within the near-wall region in the same way as, say, a diatomic gas molecule. Finally, the experimental technique must not severely alter the state of the gas molecules being probed. Because the individual molecules' velocities are much greater than the bulk velocity of the fluid, and the direction of the particles is random, radically altering the state of the molecules within the measurement volume potentially affects successive measurements.

Several new diagnostic techniques are demonstrating promise under these con- straints, including fluorescent Doppler anemometry (FDA), emission detection of Doppler-shifted absorption (EDDA) and Raman excitation plus laser-induced elec- tronic fluorescence (RELIEF). FDA and EDDA are optically based techniques that directly measure the velocity of a gas species by examining the Doppler-shift effect on either the gas absorption characteristics (EDDA) or its fluorescence-emission effects (FDA) (Hiller *et al* . 1983; Paul *et al* . 1989). EDDA has been successfully employed in both supersonic and subsonic macro-flows, using NO and I_2 fluorescence, respec- tively. The advantages of this approach are that the experimental set-up is relatively simple and that a two-dimensional velocity field can be imaged. The disadvantage is that the spectral linewidth of the exciting laser beam must be very small, of the order of 100–500 MHz, to provide enough sensitivity in the velocity measurements for subsonic flow conditions. FDA determines the flow-field velocity by heterodyn- ing the Doppler-shifted fluorescence signal gathered from collection optics located upstream (blueshifted) and downstream (redshifted) of the measurement location. This experimental set-up is appreciably more complex and sensitive to alignment than the first option, but is advantageous because of its increased measurement sensitivity and loosened constraints on the spectral linewidth of the laser illumination. RELIEF, the third technique, is in essence a molecular tagging technique that uses oxygen as the measuring medium (Miles *et al* . 1989, 2000). Oxygen molecules are excited along the path of two coincident laser beams tuned to the oxygen Q-branch to a long-lived (*ca*. 30 ms lifetime) metastable state by a stimulated Raman process. Fluorescent emission is stimulated after a predetermined time delay by an analys- ing argon-fluoride laser beam. The velocity is determined by the displacement of the fluorescence signal from the initial excitation location. Like EDDA, the optical set-up and data analysis of the RELIEF technique are substantially more straightforward than for the FDA technique. The potential drawbacks to RELIEF are that the quan- tum efficiency of the process is very low, and the resolution of the measurements is limited by both the focus of the Raman-excitation beams and diffusion of the gas particles.

The difficulties in measuring the transition-continuum regime and other slip flows

accurately mean that the amount of reliable experimental data available is very small. However, this has not halted the development of numerical techniques for the simulation of such flows. Indeed, the most widespread technique—the direct simulation Monte Carlo method (DSMC, see below)—is used with confidence to check the results of measurements. We shall now examine some of the modelling techniques.

Modelling

From an engineering perspective, there are two practical and competing approaches to simulating gas flows in the transition-continuum regime: the DSMC (e.g. Bird 1994), and extensions of the continuum equations so they are appropriate for rarefied flows (e.g. Chapman & Cowling 1970; Agarwal *et al* . 2001). In the physics community, molecular dynamics simulations and lattice-based schemes with simplified collision dynamics are popular (Mareschal 1997). The former method simulates the motion of individual gas molecules, so for applications of any size or for transient flows it requires prohibitively large computational resources. The latter approach offers better possibilities for the future but, although work is progressing in this area, it is proving difficult to extend the lattice methodology reliably to hypersonic flow situations, which limits its usefulness (Chen & Doolen 1998).

The fundamental kinetic equation, which describes gas flows in all regimes, is the Boltzmann equation. Both the DSMC and extended hydrodynamics are, in essence, different ways of solving the Boltzmann equation for the transition-continuum regime. In its most basic form, the Boltzmann equation describes the evolution of a system of monatomic gas molecules, assuming molecular chaos and that only binary inter-molecular collisions occur (i.e. the gas needs to be dilute, although there are modifications which can allow for the multiple collisions typical of dense gases). This

Boltzmann equation can be represented as

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = C(f), \quad (2.1)$$

where $f(\boldsymbol{r}, \boldsymbol{v}, t)$ is a function describing the number density of gas molecules with position $\boldsymbol{r}$ and velocity $\boldsymbol{v}$ at a certain time t. The left-hand side of equation (2.1) represents the drift motion of the molecules, without collisions, under the influence of a body force $\boldsymbol{F}$ (gravity, say). The right-hand side of equation (2.1) is the collision function, $C(f)$, which represents the scattering of molecules due to intermolecular collisions. It is this term that causes the problems with solving the kinetic equation as it stands. Because the collision integral includes the velocity–space coordinates as independent variables, this increases the dimensions to be solved for. This not only means that analytical solutions for gas flows in complex geometries are intractable, but even a computational approach represents a formidable problem when trying to solve the Boltzmann equation in three dimensions. However, there have been two recent proposals for getting around this problem: simulating the movement and collisions of gas molecules directly, and using an approximation based on Kn to solve the Boltzmann equation. We shall describe each of these approaches in turn.

The DSMC method

In the late 1950s, Alder & Wainwright (1957) introduced a new numerical method that traced the paths of individual molecules. This molecular dynamics was com- pletely deterministic, in the sense that the motion and the collisions of each molecule were computed using the laws of classical mechanics. In 1963, Bird proposed calcu- lating the molecular collisions using stochastic rather than deterministic procedures (Bird 1963). This improved the computational efficiency greatly, so that today this method—the direct simulation Monte Carlo method—is almost universally used in the area of rarefied gas dynamics or where mean-free-path phenomena are of interest. In the DSMC methodology a gas flow is represented by the motion of a number of 'computational molecules', each of which represents a large number of real molecules. A computational molecule travels at constant velocity until it experiences a collision with another computational molecule. Collisions are binary and change the veloci- ties and the internal energies but not the positions of the colliding pair. It should be noted that computational molecules have three-dimensional velocity vectors for collision purposes, regardless of the dimensionality of the geometry. The result of this approach is a statistical, physical simulation of the dynamics and interactions
of thousands of gas molecules.

There are several choices of collision models that can be used, including the hard sphere (HS), variable hard sphere (VHS), and variable soft sphere (VSS) models. The HS model is capable of matching the viscosity of a gas at only one temperature, the VHS model matches the temperature-dependent viscosity of a gas, and the VSS model matches the temperature-dependent viscosity and self-diffusion coefficient of a gas. During a move, computational molecules travel at constant velocity for the entire time-step or until a boundary is encountered. In the latter situation, the appropriate boundary condition is applied. Typical boundary conditions are 'inflow' (computa- tional molecules enter the domain with a prescribed Maxwellian

supersonic applications), 'diffuse wall' (computational molecules are reflected usu- ally with a prescribed Maxwellian distribution) and 'specular wall' (computational molecules are reflected with mirror symmetry).

A computational mesh is used in the DSMC method for identifying possible col- lision partners and to accumulate statistical information. Moments of the molecular velocity distribution function are accumulated over one or more time-steps within each mesh cell to yield gas quantities such as the number density, velocity and tem- perature. Forces on molecules, such as gravity or electrostatic forces for ions, can be incorporated. To preclude non-physical behaviour, time-steps and mesh cells are constrained to be less than about one-third of a collision time and one-third of a mean free path, respectively.

The relationship between the DSMC and the Boltzmann equation, and the lack of a rigorous mathematical foundation for the method, was a cause of much discus- sion as the DSMC became widely used. Bird argued that DSMC procedures were mimicking the physical reasoning behind the Boltzmann equation and in 1970 he proved that the Boltzmann equation could be derived through DSMC procedures (Bird 1970). The lack of a complete theoretical foundation was settled in 1992 when Wagner presented a description of the DSMC as a Markov process converging to the Boltzmann equation in the limit of an infinite number of molecule simulators (Wag- ner 1992). It is now generally accepted that the DSMC is not a mere simulation of gas flows but a definite solution method for the kinetic equation, in the sense that stochastic processes derived from the Boltzmann equation can be simulated by the DSMC method.

The DSMC has been used successfully in many applications of hypersonics (Bird 1994) and, more recently, microfluidics. As it is an atomistic method, the DSMC is ideally suited to deal with complicated physics and chemistry in the gas flow field. However, the application of the DSMC to subsonic flows becomes computationally expensive due to the statistical scatter inherent in any DSMC simulation. Assuming Gaussian statistics for a measured quantity (for example, velocity) the standard deviation decreases by the square root of the number of independent samples. Bearing in mind that not all DSMC steps produce statistically independent samples (as a rule of thumb, every third move produces an independent sample), to reduce the velocity scatter to 0.1 m s^{-1} one needs roughly five million samples. To further reduce the scatter by one order of magnitude to 0.01 m s^{-1} one needs 100 times more samples. Therefore, resolving subsonic velocities of the order of 1–0.1 m s^{-1} becomes costly in computer time even for relatively simple applications (Gallis *et al* . 2001). Complex applications of the DSMC are only possible in a massively parallel computational environment employing thousands of processors, so its use as a design tool is still out of the reach of most researchers or industry (Gallis *et al*. 2002).

As an alternative to pure DSMC for gas flow fields with mixed densities (for example, the entire flow around a hypersonic vehicle), hybrid schemes are being pro- posed which combine both the DSMC and Navier–Stokes solvers. The aim is to try to reduce the computational load of the DSMC by using traditional computational fluid dynamics in regions where this is physically acceptable (Garcia *et al* . 1999; Hadjiconstantinou 1999). Depending on the application, speed-ups of two orders of magnitude can be obtained. The main problem that these methods have to address is the communication of information from one region to another (or from one numer- ical scheme to the other). However, hybrid codes lose their appeal in the area of microfluidics, where the subsonic speeds still require a very large number of statisti- cal samples in the DSMC regions of the simulation. This makes the computational requirements of the hybrid scheme still practically intractable. Alternative schemes have recently been proposed (Fan & Shen 2001; Sun & Boyd 2002; Kaplan & Oran 2002) that try to reduce the statistical noise either during the calculation or at the end as a post-processing step. While this computational problem is opening up a whole new area of research into efficient and physically realistic methods, even in the best-case scenarios, the computational efficiency of particle schemes still lags behind that of traditional fluid dynamics. However, a different method which applies solu- tion techniques similar to the standard continuum fluid equations but applicable to higher *Kn* flows is showing promise. We now turn to examine this approach.

Extended hydrodynamics

Although the DSMC method is currently the most popular route to simulating transition-continuum flows, its computational cost—especially for applications in three dimensions and for mixed density (continuum/rarefied) flows—limits its appli- cability to simulations of flows in quite simple geometries. However, there is an alter- native: so-called 'extended hydrodynamics' (which is a generic term covering all the methods outlined below, and not to be confused with the 'extended thermodynamics' of Müller & Ruggeri (1993)). This approach is not nearly so well developed as the DSMC method, but offers interesting possibilities for the future. Extended hydro- dynamics

uses equations in the form of the standard fluid equations of mass, momen- tum and energy, but in the momentum and energy equations the stress tensor and the heat flux vector are constructed to be mathematically more applicable to flows with a high *Kn*. This means, in practice, that the expressions for the stress tensor and heat flux contain higher-order, and typically nonlinear, terms in the gradients of the gas properties (velocity, temperature, etc.) than the Navier–Stokes equations. One advantage of these higher-order constitutive relations is that, in principle, solving them should not be much more computationally expensive than solving the stan- dard Navier–Stokes equations, so complex simulations in three dimensions become numerically much more tractable. Another important advantage is that the equations of extended hydrodynamics reduce to the Navier–Stokes equations in areas of low flow gradients (and low *Kn*) or higher densities. Therefore, the same set of equations can be applied across an entire mixed-density flow field.

There are many competing sets of higher-order constitutive relations, mostly derived from the fundamental Boltzmann equation (or some approximation thereof) using differing approaches. The classical approach is the Chapman–Enskog tech- nique, which determines a hierarchy of approximate solutions to the Boltzmann equation. Using a Kn series approximation, the velocity distribution function, f in equation (2.1), can be written in terms of a perturbation of the local equilibrium or Maxwellian distribution function, f_0,

$$f = f_0\{1 + a_1(Kn) + a_2(Kn)^2 + \cdots\}, \quad (2.2)$$

where the coefficients a_n are functions of density, velocity and temperature only. One prerequisite for the Chapman–Enskog expansion technique to work is that the series (2.2) converges, limiting this approach mathematically to gases that are not too far from local equilibrium (i.e for gas flows with *Kn* up to about 0.3). Taking just the first term in the series (2.2) (i.e. for an equilibrium gas) results in a distribution function corresponding to a viscous stress tensor equal to the pressure, and zero heat flux. So this zeroth-order approximation (in *Kn*) yields the governing equation set known as the Euler equations. In the same way, taking the first two terms in the series results in the Navier–Stokes equations, and at second order in *Kn* the complicated set of constitutive relations known as the Burnett equations is obtained. As the Burnett equations are accurate to second order in *Kn*, they are presumed to extend the validity of the continuum model to flows at higher *Kn* than the Navier–Stokes equations.

Since the derivation of these original equations by Burnett (1935), there have been several modifications proposed. Agarwal *et al* . (2001) derived their equations from a slightly different starting point. They used the Bhatnagar–Gross–Krook approxima- tion, a simplified expression for the Boltzmann collision integral in equation (2.1). This gives expressions of the same form as Burnett, although the coefficients in the nonlinear terms are different. Woods (1993) went a stage further when he pointed out that the Burnett equations predict some anomalous effects, including an initial heat flux generated in an isothermal sheared flow. Tracing these difficulties to the fact that the solution technique is dependent on the frame of the observer, he modified the kinetic operator and collision function to make them frame indifferent. His set of second-order constitutive relations is similar to the Burnett equations, but contains fewer terms and modified coefficients. More recently, Chen *et al* . (2001) have pro- posed a reformulation of the Chapman–Enskog expansion which does not use results from lower orders in the formulation of higher-order equations. However, the equa- tions obtained do not yield solutions to supersonic flows beyond about Mach 2.1, so the use of this theory seems limited.

A slightly different path was followed by Grad (1949). He expanded the distribution function as a series of Hermite tensor polynomials, with variable parameters, around the Maxwellian equilibrium state. To evaluate the distribution function at second- order, moment equations are needed for 13 dependent variables in the conservation equation set. This process led to Grad's 13 moment equations, which are yet another version of the second-order transport terms. Aside from questions which have recently been raised over inconsistencies in this mathematical approach (Velasco *et al* . 2002), it is in any case possible to retrieve the Burnett equations from Grad's equations (Agarwal *et al* . 2001). So it is unclear whether the Grad equations are an attractive alternative, although they have recently been used to solve stationary heat-transfer problems (Struchtrup 2002). The equations of 'generalized hydrodynamics' proposed by Eu (1992) and developed by Myong (2001) are based on a modification of Grad's approach. The main difference lies in the way the dissipation terms of the evolution equations are dealt with. By introducing a non-equilibrium canonical distribution function in exponential form, and using a cumulant expansion method, the resulting generalized hydrodynamic equations are consistent with the thermodynamic laws at every order of approximation. This is a promising approach as it deals with a major problem of many of the extended hydrodynamic equations, which we shall now outline.

There is active debate around the thermodynamic consistency of the various sets of equations. For example,

ables (and their gradients) take and is not an intrinsic property of the equations. A violation of the second law does not, in this regime, necessarily mean that a non-physical process is occurring (Wang *et al* . 2002). However, it may partly explain why researchers over the last few decades have encountered so many problems with the stability of the equation set. The question then remains whether thermodynamic consistency is a good guide to the computational stability of extended hydrodynamic equations in every application. In any case, there are still substantial practical prob- lems to obtaining numerical solutions for even simple flow situations. Most of the proposed equation sets are mathematically ill-posed in their original formulations, displaying some or all of the following problems:

they are numerically difficult to solve and sensitive to initial conditions;

there are time-dependent instabilities arising in the solution of the equations (which often, as stated above, coincide with the thermodynamic inconsistency of the equations);

although they are required by the higher-order derivatives in the equations, it is uncertain which additional boundary conditions should be imposed.

The first problem is at least partly receding with the commercial availability of flex- ible and efficient fluid dynamics codes and numerical techniques. The second problem is more challenging. In the past, the Burnett equations, for example, have been both stabilized and made thermodynamically consistent by eliminating the terms in the equations that cause the instability (Fiscko & Chapman 1988), or adding selected linear terms of even higher order (Zhong *et al* . 1991), or substituting the convec- tive derivative terms that appear in the Burnett relations with expressions obtained by rearranging the Navier–Stokes equations, or extending the entire equation set to third-order (Agarwal *et al* . 2001). Yet another approach has been proposed by Jin & Slemrod (2001), who used a unique viscoelastic relaxation approximation which, fol- lowing a Chapman–Enskog expansion, eliminates the instability and thermodynamic inconsistency up to Burnett order. Although this approximation could be regarded as 'ad hoc', this approach seems to offer excellent possibilities for a stable and robust equation set.

The final problem to do with boundary conditions is also a major issue. The flow fields calculated using higher-order continuum equations are particularly sensitive to the variables and gradients imposed at the boundaries. It is therefore imperative to prescribe these conditions accurately. However, for rarefied flows, wall boundary conditions are particularly difficult to predict and require the use of semi-empirical models that take into account the slip that occurs between fluid and surface. Also, because of higher-order gradients in the equations, additional boundary conditions are usually required and in many flows it is not always clear how and on what physical basis these should be chosen.

Applications

In this section we present new results that demonstrate the potential that both the DSMC and extended hydrodynamic equations have for addressing some important transition-continuum gas flow problems.

Hypersonics

The space programme was the main thrust behind the development of the DSMC method in the 1970s and early 1980s. Early publications on DSMC are dominated by studies of shock layers and compression flows in front of blunt bodies. These studies were mainly concerned with the effect of chemical non-equilibrium on the surface heating rates. Although this problem is complex, its solution was made possible by one- or two-dimensional axisymmetric simulations that were within the range of computer technology at that time. However, it was not until recently that the simulation technology (including both computer technology and software) allowed DSMC to be applied to complicated flow physics phenomena.

One currently important topic is the use of air-breathing technology for hypersonic vehicles (Holden 2000). The performance of the vehicle can be greatly influenced by the interaction of an internally produced shock wave with a boundary layer. In addi- tion to the high thermal loads that can occur in the shock–boundary layer-interaction region, the adverse pressure gradients can lead to flow separation, significantly reduc- ing the effectiveness of control surfaces. Despite the significance of such flow phenom- ena, the mechanisms by which thermochemical non-equilibrium and real-gas effects influence the extent of the separation zone are not well understood.

The significance of thermochemical non-equilibrium can be assessed by DSMC simulations. Recently, however, Harvey *et al* . (2001) questioned the ability of the DSMC to deal with recirculating flows. Although the application of DSMC has not been demonstrated for such complicated flow fields there is no evidence to sug- gest that the method could not provide useful information about such flows. Roy *et al* . (2003) compared the performance of a traditional computational fluid dynamics solver and DSMC, with the aim of demonstrating the ability of DSMC to deal with such flow fields. This work is part of the international effort to validate DSMC and Navier–Stokes codes (Holden *et*

al . 2002). The geometry we selected was a 25/55 spherically blunted biconic, as proposed in an experimental study by Harvey *et al* . (2001) and Holden *et al* . (2002). This geometry was selected because a recircula- tion region was formed in the region between the two cones. The Knudsen number of the flow field was such that it was clearly placed in the continuum regime. We performed the calculations using the SNL DSMC code ICARUS (Bartel *et al* . 2001) on 2048 processors of ASCI Red, the massively parallel platform at Sandia National Laboratories (USA), for 120 hours. Figure 2 shows in detail the pressure profiles in the recirculation region in the area of the intersection of the two cones. The two predictions are in very good agreement, demonstrating that DSMC can deal with such complicated phenomena.

Microfluidics

In microfluidics in MEMS, gravity and inertia have negligible effects on flows, but the effects of atomic forces and surface morphology dominate the flow field. Due to the small device size, comparable with the gas molecular mean free path even at atmospheric pressures, mean free path effects need to be included in any simulation of the flow within a MEMS device. The force produced on moving microstructures

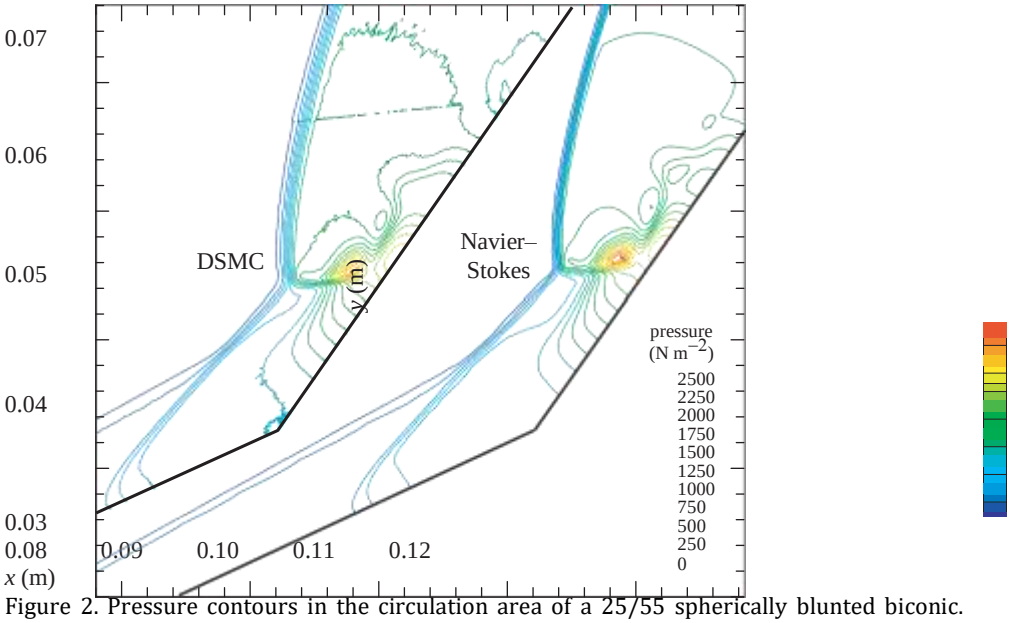

Figure 2. Pressure contours in the circulation area of a 25/55 spherically blunted biconic. Comparison between Navier–Stokes and DSMC predictions.

by the surrounding gas can affect their performance and reliability. As an example, we have simulated the gas flow around the cantilevered microbeams of figure 3. The microbeams shown in this photograph have a width of 20 μm, a thickness of 2 μm and a length of 100 μm (for comparison, a human hair is *ca*. 40 μm thick). They have been manufactured using the SUMMiT V technique at Sandia National Laboratories (USA). The clearance between the microbeam and the bottom surface may vary dueto the motion of the beam.

Although these microbeams are expected to operate at atmospheric conditions, the small size of the domain means that continuum fluid dynamics is questionable and we need to use molecular simulation methods. However, this is a far from triv- ial task since, as outlined above, the simulation of relatively dense subsonic flows with particle simulation codes is very difficult. Figure 4 shows the results of a two- dimensional DSMC simulation of the pressure flow field around the cantilevered microbeams of figure 3 (cross-section of the beams). These simulations were per- formed in 24 hours on 3000 processors of ASCI Red at Sandia. The background pressure was atmospheric and the velocity of the microbeam was 1 m s^{-1}. As the beam moves upwards, it pushes the air above it up as well, creating an area of lower pressure underneath it. It is interesting to note that the Knudsen number of the flow field (based on the clearance between the beam and the lower surface) places the flow field in the transition-

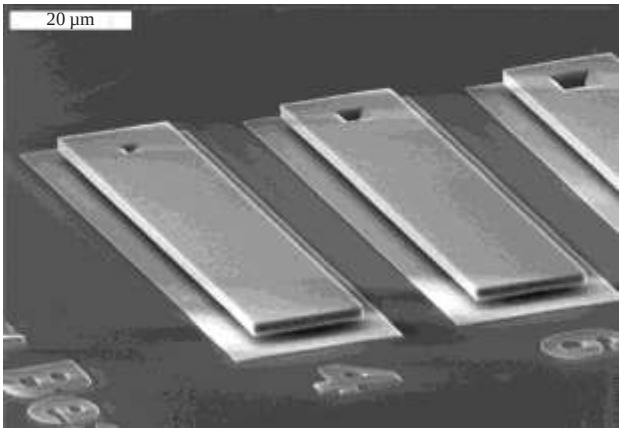

Figure 3. Cantilevered microbeams fabricated at Sandia using SUMMiT V technology.

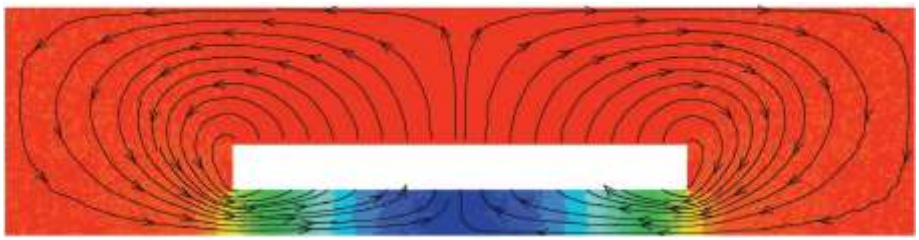

Figure 4. DSMC simulation of cross-section of figure 3 microbeam, 2 μm clearance. The contour lines represent the pressure profile of the flow field. The beam is moving upwards with a velocityof 1 m s^{-1}.

Extended hydrodynamics

As has been stated, extended hydrodynamics is much less well developed than the DSMC method. However, by showing our new results for two benchmark problems, we indicate the potential it has for future applications in aerosciences and microscale engineering. Work on developing stable numerical methodologies for the two- and three-dimensional equations of extended hydrodynamics is ongoing.

Hypersonics

The structure (i.e. the spatial variation of density and temperature) and the stand- off distance of the shock wave at the leading edge of either the bow or wings of high-speed, high-altitude vehicles have implications for the aerodynamic design of next-generation aircraft and transports. The failure of the Navier–Stokes equations to model hypersonic rarefied gas flows is well known. For this reason, we have imple- mented a finite-difference scheme to examine whether extended hydrodynamics (in this case the Burnett (1935) and the Woods (1993) equations) can better predict the essential features of this flow situation. Stability in this case was achieved by enforc- ing the physical constraint that the temperature should not fall below or rise above the upstream and downstream values respectively. Also, discontinuities that arise in the second-order gradients are treated so that they do not produce singularities in the third-order gradients. The equations of extended hydrodynamics were implemented

Future directions

The experimental and numerical investigation of transition-continuum gas flows is still at an early stage. However, the industrial and technological importance of this class of flows is not in question. Future developments in high-speed air vehicles and micro-devices will depend on both reliable experimental and test data, and accurate numerical simulations. We outline here some of the directions and applications that an increased understanding of non-locally equilibrial flows will open up.

Granular gases (inelastically colliding macroscopic solid particles, such as coal, sand or cereals) satisfy a hydrodynamic description on sufficiently large scales. The governing equations for granular gases, usually derived from the Boltzmann equation (modified to account for inelasticity), resemble the Navier–Stokes equations, the

and a good example of transition-continuum regime flows. This is, therefore, an area that is well worth investigating by some of the methods outlined in this paper. Some recent results of applying DSMC to simulate the motion of macroscopic particles suspended in a rarefied medium typical of that in microelectronics applications are given in Gallis *et al*. (2001, 2002).

The study of the transition from laminar to turbulent flow using the Boltzmann equation has also been an active but challenging topic of research (Stefanov & Cer- cignani 1993; Bird 1987). The research so far has been limited by computational resources: a transition to turbulence cannot be uncovered unless three-dimensional simulations are performed. However, as outlined above, a calculation of that size challenges the most modern computational platforms.

Finally, for liquid flows in micrometre-sized geometries, the problems of parti- cle schemes are greatly increased. Using molecular dynamics, only a fraction of a microsecond of liquid flow can be simulated with present computational resources. Although a form of extended hydrodynamics may, in principle, be constructible for liquids, we can speculate about the possibility of building a numerical description of microfluidics that lies between the molecular and the continuum approach, with each numerical component of the simulation perhaps representing some hundreds or thousands of liquid molecules, the aim being to reduce computational effort by con- structing the largest interactive molecular ensemble system that can still capture the essential physics of the flow at the microscale. For example, cellular automata (CAs) can produce complex emergent behaviour that goes well beyond the simplicity of the interaction rules between adjacent automata. CA descriptions of liquids have been shown to reproduce Navier–Stokes behaviour at the macro-scale, so it is certainly possible that, with the correct rule set, a CA model of a liquid may predict unusual physical behaviour at the microscale. We do not yet know whether a rule set can be constructed that captures the physics of the bounded liquid micro-flow, or whether this rule set will produce emergent phenomena that explain micro-flow behaviour, but if a successful CA model can be devised it would open up a whole new area of microfluidic investigation.

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