International Journal for Multiscale Computational Engineering, 2(2)189–202(2004)

Discussion of Hybrid Atomistic-Continuum Methods for Multiscale Hydrodynamics

Hettithanthrige S. Wijesinghe & Nicolas G. Hadjiconstantinou*

Mechanical Engineering Department,
Massachusetts Institute of Technology, Cambridge, MA 02139

ABSTRACT

We discuss hybrid atomistic-continuum methods for multiscale hydrodynamic applications. Both dense-fluid and dilute-gas formulations are considered. The choice of coupling method and its relation to the fluid physics as well as the need for timescale decoupling is highlighted. In particular, by relating the molecular integration timestep to the CFL timestep, we show that compressibility is important in determining the choice of a coupling method. Appropriate coupling techniques for various flow regimes are discussed and proposed. We also discuss recently developed incompressible and compressible hybrid methods for dilute gases. The incompressible framework is based on the Schwarz alternating method, which provides timescale decoupling; the compressible method is a multispecies, fully adaptive mesh and algorithm refinement approach that introduces the direct-simulation Monte Carlo at the finest level of mesh refinement.

*Address all correspondence to ngh@mit.edu

0731-8898/04/$20.00

1. INTRODUCTION

By limiting the molecular treatment to regions where it is needed, a hybrid method allows the simulation of complex thermo-fluid phenomena, which require modeling at the microscale without the prohibitive cost of a fully molecular calculation. In what follows we provide an overview of this rapidly expanding field and discuss recent developments. We also describe archetypal hybrid methods for incompressible and compressible flows; the hybrid method for incompressible gas flow is based on the Schwarz alternating coupling method; and the hybrid method for compressible flow is based on the recently developed [34] flux-coupling, multispecies adaptive mesh and algorithm refinement scheme that extends adaptive mesh refinement by introducing the molecular description at the finest level of refinement.

Over the years a fair number of hybrid simulation frameworks have been proposed leading to some confusion over the relative merits and applicability of each approach. Original hybrid methods focused on dilute gases [10, 20, 28, 29], which are arguably easier to deal with within a hybrid framework than dense fluids, mainly because boundary condition imposition is significantly easier in gases. The first hybrid methods for dense fluids appeared a few years later [11, 16, 17, 26]. These initial attempts have led to a better understanding of the challenges associated with hybrid methods.

To a large extent, the two major issues in developing a hybrid method is the choice of a coupling method and the imposition of boundary conditions on the molecular simulation. Generally speaking, these two can be viewed as decoupled, in the sense that the coupling technique can be developed on the basis of matching two compatible and equivalent over some region of space hydrodynamic descriptions and can thus be borrowed from the already existing and extensive continuum-based numerical methods literature. The choice of coupling technique is further discussed in Section 2.1–2.3. Boundary condition imposition can again be considered in a decoupled sense and can be posed as a general problem of imposing "macroscopic" boundary conditions on a molecular simulation. In our opinion, this is a very challenging problem that has not been, in general, resolved to date completely satisfactorily. Boundary condition imposition on the molecular subdomain is discussed in Section 2.4. Boundary condition imposition on the continuum subdomain is generally well understood, as is the process of extracting macroscopic fields from molecular simulations (typically achieved through averaging).

In Section 3, we give a brief description of the direct simulation Monte Carlo (DSMC), the dilute-gas simulation method used in this work. In Section 4, we demonstrate a hybrid scheme suitable for low-speed, incompressible gaseous flows based on the Schwarz alternating method. The current paper introduces Chapman-Enskog boundary condition imposition in incompressible hybrid formulations. Subsequently, in Section 5 we discuss a recently developed multispecies compressible formulation [34] for gases that introduces the molecular simulation at the finest level of refinement within a fully adaptive mesh refinement framework. We finish with some concluding remarks.

2. DEVELOPING A HYBRID METHOD

2.1. The Choice of Coupling Method

Coupling a continuum to a molecular description is meaningful in a region where both can be presumed valid. In choosing a coupling method, it is therefore convenient to draw upon the wealth of experience and large cadre of coupling methods nearly 50 years of continuum computational fluid dynamics have brought us. Coupling methods for compressible and incompressible formulations generally differ, since the two correspond to two different physical and mathematical hydrodynamic limits. The compressible formulation lends itself naturally

to time-explicit flux-based coupling while incompressible formulations are typically coupled using either state (Dirichlet) properties or gradient (Neumann) variables.

Given that the two formulations have different limits of applicability and/or physical regimes in which each is significantly more efficient than the other, care must be exercised when selecting the ingredients of the hybrid method. In other words, the choice of a coupling method and continuum subdomain formulation needs to be based on the degree to which compressibility effects are important in the problem of interest and not on a preset notion that a particular coupling method is more appropriate than all others. The latter approach was recently pursued in a variety of studies, which enforce the use of a compressible, time-explicit, flux-matching coupling scheme to steady and essentially incompressible physical problems. This approach is not recommended. On the contrary, for an efficient simulation method, similar to the case of continuum solution methods, it is important to allow the flow *physics* to dictate the appropriate formulation, while the numerical implementation is chosen to cater to the particular requirements of the latter. Below, we expand on some of the considerations that influence the choice of coupling method under the assumption that the hybrid method is applied to problems of *practical interest* and, therefore, the continuum subdomain is appropriately large. Our discussion extends to timescale considerations that are more complex, but equally important to limitations resulting from length scale considerations, such as the size of the molecular region(s).

2.2. Timescale Decoupling

It is well known [31] that the timestep for explicit integration of the compressible Navier-Stokes formulation τ_c, scales with the physical timestep of the problem $\tau_{\Delta x} (= \Delta x/U$, where Δx is the numerical grid spacing and U is the characteristic velocity), according to

$$\tau_c \leq \frac{M}{1+M}\tau_{\Delta x}, \tag{1}$$

where M is the Mach number. As the Mach number becomes small, we are faced with the well-known stiffness problem whereby a) the numerical efficiency degrades due to disparity of the timescales in the system of equations and b) the accuracy of the compressible solution degrades due to mismatch of magnitudes between fluxes in the original equations and corresponding terms in the numerically added artificial viscosity [36]. For this reason, when the Mach number is small, the incompressible formulation is used that allows integration at the physical timestep $\tau_{\Delta x}$. In the hybrid case, matters are complicated by the introduction of the molecular integration timestep, τ_m, which is at most of the order of τ_c (in some cases in gases when $\Delta x \leq \lambda$, where λ is the molecular mean free path) and in most cases significantly smaller. One consequence of Eq. (1) is that as the global domain of interest grows, the total integration time grows, and transient calculations in which the molecular subdomain is explicitly integrated in time become more computationally expensive and eventually infeasible. The severity of this problem increases with decreasing Mach number and makes unsteady incompressible problems very computationally expensive. New integrative frameworks, which coarse grain the time integration of the molecular subdomain, are therefore required.

Fortunately, for coupling low-speed steady problems implicit (iterative) coupling methods exist that provide solutions without the need for explicit integration of the molecular domain to the global problem steady state. The particular method used here is known as the Schwarz method and is discussed further in Section 4. This method decouples the global evolution timescale from the molecular evolution timescale (and timestep) by achieving

convergence to the global problem steady-state through an iteration between steady state solutions of the continuum and molecular subdomains. Because the molecular subdomain is small, explicit integration to its steady state is feasible. Although the steady assumption may appear restrictive, it is interesting to note that the vast majority of both compressible and incompressible test problems solved to date by hybrid methods have been steady.

A variety of other iterative methods may be suitable as they provide for timescale decoupling. The choice of the Schwarz coupling method, which uses state variables instead of fluxes to achieve matching, was motivated by the fact (as explained below) that state variables suffer from smaller statistical noise and are thus easier to prescribe on a continuum formulation.

The above observations do not preclude the use of the compressible formulation in the continuum subdomain for low-speed flows. In fact, preconditioning techniques, which allow the use of the compressible formulation at very low Mach numbers, have been developed [31]. Such a formulation can, in principle, be used to solve the continuum subproblem while this is being coupled to the molecular subproblem via an implicit (e.g., Schwarz) iteration. What should be avoided is a compressible, time-explicit, flux-based coupling procedure for solving essentially incompressible steady-state problems.

The issues discussed above have not been very apparent to date because in typical test problems published so far the continuum and atomistic subdomains are of the same size (and, of course, small). In this case the large cost of the molecular subdomain masks the cost of the continuum subdomain and also typical evolution timescales (or times to steady state) are small. It should not be forgotten, however, that hybrid methods make sense when the continuum subdomain is significantly larger than the molecular subdomain.

2.3. Statistical Noise Considerations

The use of a compressible formulation with flux coupling in the $M \to 0$ limit leads to two additional disadvantages. The first, continuum subdomain stiffness (see Eq. 1), may be remedied by implicit timestepping methods [38] or preconditioning approaches [31]. The second, more serious disadvantage, is linked to adverse signal to noise ratios (compared to non-flux-based schemes) in connection with the averaging required for imposition of boundary conditions from the molecular subdomain to the continuum subdomain. More specifically, in the case of an ideal gas (where compressible formulations are typical) it has been shown in [19] that, for the same number of samples, flux (shear stress, heat flux) averaging exhibits relative noise E_f, which scales with E_{sv}, the relative noise in the corresponding state variable (velocity, temperature) according to,

$$E_f \sim \frac{E_{sv}}{Kn}. \tag{2}$$

Here $Kn = \lambda/L$ is the Knudsen number based on the characteristic length scale of the transport gradients L, and λ is the mean-free path, which is expected to be much smaller than L, because, by assumption, a continuum subdomain is present. It thus appears that flux coupling will be significantly disadvantaged in this case, because the number of samples required to make $E_f \approx E_{sv}$ scales as $1/Kn^2$ times the number of samples required by state-variable averaging.

On the other hand, Schwarz-type iterative methods based on the incompressible physics of the flow require a fair number of iterations for convergence [$O(10)$]. These iterations require the re-evaluation of the molecular solution. This is an additional computational cost that is not shared by time-explicit approaches. At this time, the best choice for *incompressible unsteady problems* appears to be an explicit incompressible approach, such as the one used by O'Connell and Thompson [26]. We should recall, however, that unless time coarse-graining

techniques are developed, large, low-speed, unsteady problems are currently too expensive to be feasible by any approach (see discussion in Section 2.2).

2.4. Boundary Condition Imposition

Consider the molecular region Ω on the boundary of which, $\partial\Omega$, we wish to impose a set of hydrodynamic (macroscopic) boundary conditions. Typical implementations require the use of particle reservoirs $\mathcal{R}$ (see Fig. 1) in which particle dynamics may be altered in such a way that the desired boundary conditions appear on $\partial\Omega$; the hope is that the influence of the perturbed dynamics in the reservoir regions decays sufficiently fast and does not propagate into the region of interest, that is, the relaxation distance both for the velocity distribution function and the fluid structure is small compared to the characteristic size of Ω.

In a dilute gas, the nonequilibrium distribution function in the continuum limit has been characterized [8] and is known as the Chapman-Enskog distribution. Use of this distribution to impose boundary conditions on molecular simulations of dilute gases results in a robust, accurate, and theoretically elegant approach. Typical implementations [14] require particle generation and initialization within $\mathcal{R}$. Particles that move into Ω within the simulation timestep are added to the simulation whereas particles remaining in $\mathcal{R}$ are discarded. More details on implementation are provided in Section 4.

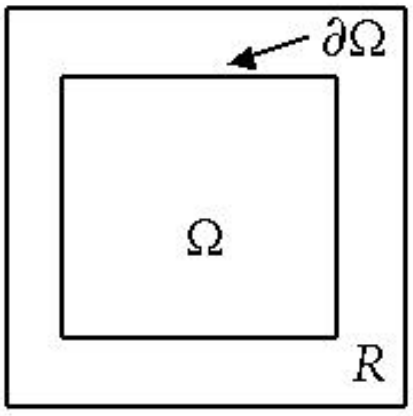

FIGURE 1. Continuum to atomistic boundary condition imposition using reservoirs.

Unfortunately, for dense fluids where not only the particle velocities but also the fluid structure is important and needs to be imposed, no theoretical results for their distributions exist. A related issue is that of domain termination; due to particle interactions, Ω, or in the presence of a reservoir, $\mathcal{R}$ needs to be terminated in a way that does not have a big effect on the fluid state inside of Ω.

As a result, researchers have experimented with possible methods to impose boundary conditions. It is now known that similarly to a dilute gas, use of a Maxwell-Boltzmann distribution for the velocities leads to slip [16]. Li *et al*. [22] used a Chapman-Enskog distribution to impose boundary conditions to generate a dense-fluid shear flow. In this approach, particles crossing $\partial\Omega$ acquire velocities that are drawn from a Chapman-Enskog distribution parametrized by the local values of the required velocity and stress boundary condition. Although this approach was only tested for a Couette flow, it appears to give reasonable results (within molecular fluctuations). Because in Couette flow no flow normal to $\partial\Omega$ exists, $\partial\Omega$ can be used as symmetry boundary separating two back-to-back shear flows; this sidesteps the issue of domain termination.

In a different approach, Flekkoy *et al*. [11] use external forces to impose boundary conditions. More specifically, in the reservoir region they apply an external field of such magnitude that the total force on the fluid particles in the reservoir region is the one required by momentum conservation. They then terminate their reservoir region by using an ad hoc weighing factor for the distribution of this force on particles within $\mathcal{R}$ that prevents particles from leaving the reservoir region from its

outer edge. In particular, they chose a weighing factor that diverges as particles approach this boundary such that particles do not escape the reservoir region while particles introduced there move towards Ω. Particles introduced into the reservoir are given velocities drawn from a Maxwell-Boltzmann distribution, while a Langevin thermostat keeps the temperature constant. The method appears to be successful although the nonunique (ad hoc) choice of force fields and Maxwell-Boltzmann distribution makes it not very theoretically pleasing. It is also not clear what the effect of these forces are on the local fluid state (it is well known that even in a dilute gas [25] gravity-driven flow exhibits significant deviations from Navier-Stokes behavior), but this effect is probably negligible since force fields are only acting in the reservoir region. Delgado-Buscalioni and Coveney [9] refined the above approach by using an Usher algorithm to insert particles in the energy landscape such that they have the desired specific energy, which is beneficial to imposing a desired energy current while eliminating the risk of particle overlap at some computational cost. This approach, however, uses a Maxwell–Boltzmann distribution, for the initial velocities of the inserted particles. Temperature gradients are imposed by a small number of thermostats placed in the direction of the gradient. Although no proof exists that the disturbance to the particle dynamics is small, it appears that this technique is successful at imposing boundary conditions with moderate error. Boundary conditions on MD simulations can also be imposed through the method of constraint dynamics [26]. Although the approach in [26] did not allow hydrodynamic fluxes across the matching interface, this feature can be integrated into this approach with a suitable domain termination.

A method for terminating molecular dynamics simulations with small effect on particle dynamics has been suggested and used in [16]. This simply involves making the reservoir region fully periodic. In this manner, the boundary conditions on $\partial\Omega$ also impose a boundary value problem on $\mathcal{R}$, where the inflow to Ω is the outflow from $\mathcal{R}$. As $\mathcal{R}$ becomes bigger, the gradients in $\mathcal{R}$ become smaller; thus, the flow field in $\mathcal{R}$ will have a small effect on the solution in Ω. The disadvantage of this method is the number of particles that are needed to fill $\mathcal{R}$ that is fairly large, especially in high dimensions.

We believe that significant contributions can still be made by developing methods to impose boundary conditions in hydrodynamically consistent and, most importantly, rigorous approaches.

3. THE DIRECT SIMULATION MONTE CARLO

The DSMC method was proposed by Bird [7] in the 1960s and has been used extensively to model rarefied gas flows. A comprehensive discussion of DSMC can be found in the review article by Alexander *et al*. [2]. The DSMC algorithm is based on the assumption that a small number of representative "computational particles" can accurately capture the hydrodynamics of a dilute gas as given by the Boltzmann equation. Air under standard conditions narrowly meets the dilute gas criterion. Empirical results [7] show that a small number (≈ 20) of computational particles per cubic molecular mean-free path is sufficient to capture the relevant physics. This is approximately two orders of magnitude smaller than the actual number of gas atoms/molecules contained in the same volume. This is one source of the DSMC's significant computational advantage over a fully molecular simulation.

The DSMC solves the Boltzmann equation using a splitting approach: the time evolution of the system is approximated by a sequence of discrete timesteps Δt in which particles undergo successively collisionless advection and collisions. Collisions are performed between randomly chosen particle pairs within small cells of linear size Δx. The flow solution is determined by averaging the individual parti-

cle properties over space and time. This approach has been shown to produce correct solutions of the Boltzmann equation in the limit Δx, $\Delta t \to 0$ [30]. The splitting approach eliminates the computational cost associated with integrating the equations of motion of all particles, but most importantly allows the timestep to be significantly larger (see also below) than a typical timestep in a hard sphere molecular dynamics simulation. This is another reason why the DSMC is significantly more computationally efficient than "brute force" molecular dynamics.

Recent studies [15, 18] have shown that for steady flows or flows that are evolving at timescales that are long compared to the molecular relaxation times, a finite timestep leads to a truncation error that manifests itself in the form of timestep-dependent transport coefficients; this error has been shown to be of the order of 5% when the timestep is of the order of a mean-free time and goes to zero as Δt^2. Quadratic dependence of transport coefficients on the collision cell size Δx was shown in [3].

4. THE SCHWARZ METHOD FOR INCOMPRESSIBLE FORMULATIONS

Although in some cases compressibility may be important, a large number of applications are typically characterized by flows where use of the incompressible formulation results in a significantly more efficient approach [31]. As explained in the introduction section, our definition of incompressible formulation is based on the *flow physics* and not on the numerical method used. Although we have used here a finite element discretization based on the incompressible formulation, we believe that a preconditioned compressible formulation could also be used to solve the continuum subdomain problem provided that it is matched to the molecular solution through a coupling method which takes into account the flow physics as outlined in Section 2.

Here, matching is achieved through an iterative procedure based on the Schwarz alternating method for the treatment of steady-state problems. The Schwarz method was originally proposed for molecular dynamics-continuum methods in [16] and extended in [17], but it is equally applicable to DSMC-continuum hybrid methods [1, 33]. This approach was chosen because of its ability to couple different descriptions through Dirichlet boundary conditions (easier to impose on dense-system molecular simulations compared to flux conditions because fluxes are nonlocal in dense systems), and its ability to reach the solution steady state in an implicit manner by using only *steady* solutions from each subdomain. The importance of the latter characteristic cannot be overemphasized; the implicit convergence in time through exchange of steady solutions guarantees timescale decoupling that is necessary for the solution of macroscopic problems: while the integration of molecular trajectories at the molecular timestep for total times corresponding to macroscopic evolution times is, and will for a long time be, infeasible, integration of the molecular region to *its* steady state is feasible.

Within the Schwarz coupling framework, an overlap region facilitates information exchange between the continuum and atomistic subdomains in the form of Dirichlet boundary conditions. A steady-state continuum solution is first obtained using boundary conditions taken from the atomistic subdomain solution. For the first iteration, this latter solution can be a guess. A steady-state atomistic solution is then found using boundary conditions taken from the continuum subdomain. This exchange of boundary conditions corresponds to a single Schwarz iteration. Successive Schwarz iterations are repeated until convergence, i.e., until the solutions in the two subdomains are identical in the overlap region.

The Schwarz method was recently applied [1] to the simulation of flow-through micromachined filters. These filters have passages that are sufficiently small that require a molecular description for the simulation of the flow

through them. Depending on the geometry and number of filter stages, the authors have reported computational savings ranging from 2 to 100. The approach in [1] used a Maxwellian velocity distribution and a "control mechanism" to impose the flow field on the molecular simulation. This approach, although successful in quasi-one-dimensional flows, is not very general; additionally, it is well known that using a Maxwellian distribution to impose hydrodynamic boundary conditions, in general, if uncorrected will lead to slip (discrepancy between the imposed and observed boundary conditions). As discussed in Section 2.4 general boundary condition imposition on dilute-gas molecular simulations can be performed using the Chapman-Enskog velocity distribution [8, 14]. This approach eliminates the need for a feedback correction since supplying the correct local distribution function eliminates slip. A Chapman-Enskog procedure for the Schwarz method is described below.

Extensions of the Schwarz method to time-dependent problems is currently under investigation [32], although, as discussed in Section 2.3, when the Mach number is low, the disparity between the molecular and hydrodynamic timescales makes this a very stiff problem.

Before proceeding with an example, a subtle numerical issue associated with the incompressible formulation should be discussed. Let Γ_1 be the portion of the continuum subdomain that receives boundary data from the molecular subdomain. Due to inherent statistical fluctuations in this data, the boundary condition on the complete continuum subdomain boundary ($\phi \supseteq \Gamma_1$) may not conserve mass exactly. Although this phenomenon is an artifact of the finite sampling of the atomistic solution (if a sufficiently large —"infinite"— number of samples are taken, the mean field obtained from the atomistic simulation should be appropriately incompressible), it is sufficient to cause a numerical instability in the continuum calculation. The most common remedy is to apply a correction to $\mathbf{v}_{\Gamma_1}$, the atomistic boundary data to be imposed on Γ_1, namely

$$(\mathbf{v}_{\Gamma_1}.\mathbf{n})_{corrected} = \mathbf{v}_{\Gamma_1}.\mathbf{n} - \frac{\int_\phi \mathbf{v}_\phi.\mathbf{n} dS}{\int_{\Gamma_1} dS}, \qquad (3)$$

where $\mathbf{n}$ is the unit outward normal vector to the boundary and dS is an element of the boundary. This correction essentially removes the discrepancy in mass flux equally across all normal velocity components of $\mathbf{v}_{\Gamma_1}$. Tests with various problems [16, 17, 33] indicate that it is successful at removing the numerical instability.

4.1. Driven Cavity Test Problem

In this section we discuss the Schwarz alternating method in the context of the solution of the driven cavity problem. We pay particular attention to the imposition of boundary conditions on the DSMC domain using a Chapman-Enskog distribution, which is arguably the most rigorous and general approach. For illustration and verification purposes we solve the steady driven cavity problem (see Fig. 2), in which the continuum subdomain is described by the Navier-Stokes equations solved by finite-element discretization. The hybrid solution is expected to recover the fully continuum solution because the atomistic subdomain is far from solid boundaries and from regions of large velocity gradients. This test, therefore, provides a consistency check for the scheme.

Standard Dirichlet velocity boundary conditions for a driven cavity problem were applied on the system boundaries; the horizontal velocity component on the left, right, and lower walls were held at zero while the upper-wall horizontal velocity was set to 50 m/s. The vertical velocity component on all boundaries was set to zero. Despite the relatively high velocity, the flow is essentially incompressible and isothermal. The pressure is scaled by setting the middle node on the lower boundary at atmospheric pressure (1.013×10^5 Pa).

Figure 3 shows the detailed structure of the approach used for exchanging boundary condi-

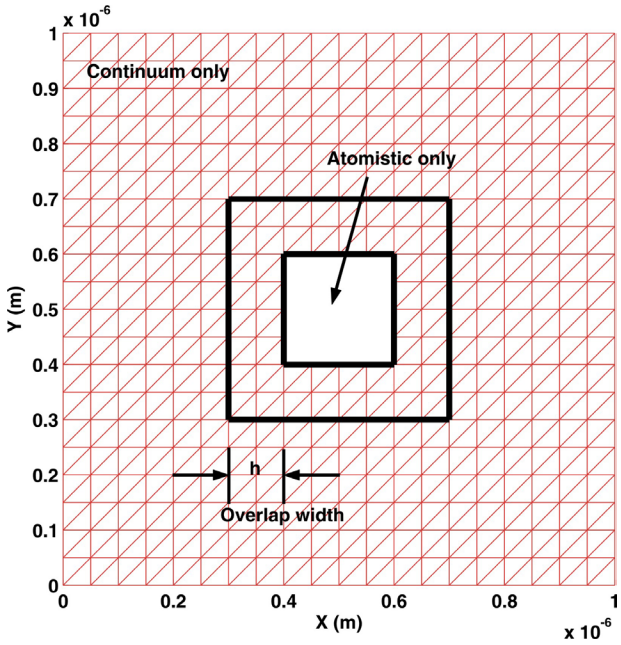

FIGURE 2. Continuum and atomistic subdomains for Schwarz coupling for the two-dimensional driven cavity problem.

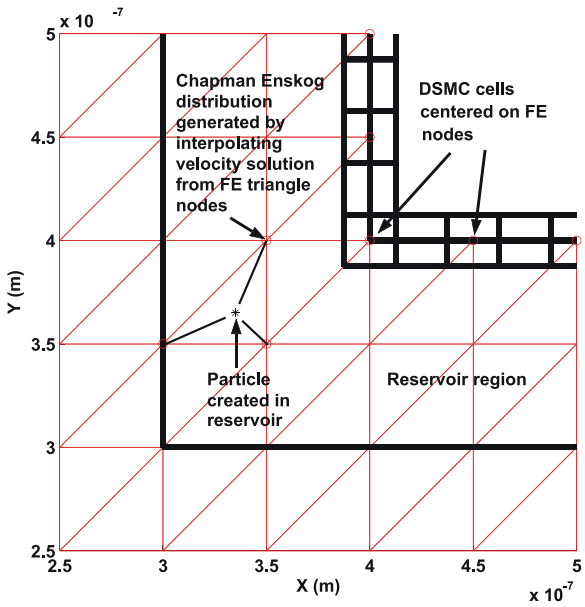

FIGURE 3. Schematic of the boundary condition imposition approach. Only the bottom left corner is shown.

tions between the two subdomains. By centering DSMC cells on the finite element (FE) nodes we can directly impose the molecular solution onto the continuum calculation (after correcting for mass conservation using Eq. 3). The imposition of boundary conditions on the atomistic subdomain is facilitated by the particle reservoir shown in Fig. 3 which, in this implementation acts also as part of the overlap region. Particles are created at locations x, y within the reservoir with velocities $\mathbf{C} = (C_x, C_y, C_z)$ drawn from a Chapman-Enskog velocity distribution $f(\mathbf{C})$ given by [13],

$$f(\mathbf{C}) = f_0(\mathbf{C})\Gamma(\mathbf{C}), \tag{4}$$

where, if $\tilde{\mathbf{C}} = \mathbf{C}/(2kT/m)^{1/2}$ is the normalized thermal velocity,

$$f_0(\tilde{\mathbf{C}}) = \frac{1}{\pi^{3/2}} e^{-\tilde{C}^2} \tag{5}$$

and,

$$\begin{aligned} \Gamma(\tilde{\mathbf{C}})=1 \quad &+ \quad (q_x\tilde{C}_x + q_y\tilde{C}_y + q_z\tilde{C}_z)\left(\frac{2}{5}\tilde{C}^2 - 1\right) \\ &- \quad 2(\tau_{xy}\tilde{C}_x\tilde{C}_y + \tau_{xz}\tilde{C}_x\tilde{C}_z + \tau_{yz}\tilde{C}_y\tilde{C}_z) \\ &- \quad \tau_{xx}(\tilde{C}_x^2 - \tilde{C}_z^2) - \tau_{yy}(\tilde{C}_y^2 - \tilde{C}_z^2) \end{aligned} \tag{6}$$

with,

$$q_i = -\frac{\kappa}{P}\left(\frac{2m}{kT}\right)^{1/2}\frac{\partial T}{\partial x_i}, \tag{7}$$

$$\tau_{ij} = \frac{\mu}{P}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3}\frac{\partial v_k}{\partial x_k}\delta_{ij}\right). \tag{8}$$

Here q_i and τ_{ij} are the dimensionless heat flux and stress tensor, respectively, with μ, κ, P and $\mathbf{v} = (v_1, v_2, v_3)$ being the viscosity, thermal conductivity, pressure, and mean fluid velocity. The Chapman-Enskog distribution of velocities can be generated using an "acceptance-rejection" scheme as detailed by Garcia and Alder [13].

The number and spatial distribution of particles in the reservoir are chosen according to the overlying continuum cell mean density

and density gradients. After particles are created in the reservoir they move for a single DSMC timestep. Particles that enter DSMC cells are incorporated into the standard convection/collision routines of the DSMC algorithm. Particles that remain in the reservoir are discarded. Particles that leave the DSMC domain are also deleted from the computation. The rapid convergence of the Schwarz approach is demonstrated in Fig. 4. The continuum numerical solution is reached to within $\pm 10\%$ at the third Schwarz iteration and to within $\pm 2\%$ at the tenth Schwarz iteration. Our error estimate, which includes the effects of statistical noise [19] and discretization error due to finite timestep and cell size, is approximately 2.5%. Similar convergence of the vertical velocity field is also observed.

The close agreement with the fully continuum results indicates that the Chapman-Enskog procedure is not only theoretically appropriate, but also robust. Despite a Reynolds number of $Re \approx 1$, the Schwarz method (originally only shown to converge for elliptic problems [23]) converges with negligible error. This is in agreement with the findings of Liu [24] who has recently shown that the Schwarz method is expected to converge for $Re \sim O(1)$. Extension of the the Schwarz method to flows with higher $Re \sim O(100)$ has also been possible [12] provided suitable preconditioning is utilized.

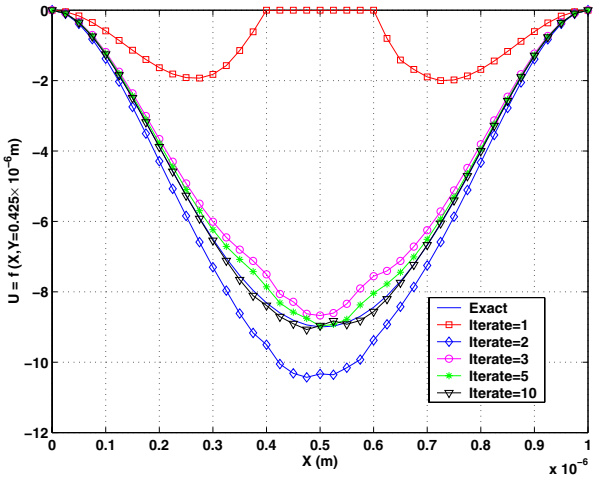

FIGURE 4. Convergence of the horizontal velocity component along the $y = 0.425 \times 10^{-6} m$ plane with successive Schwarz iterations.

5. ADAPTIVE MESH AND ALGORITHM REFINEMENT FOR COMPRESSIBLE FORMULATION

As discussed above, consideration of the compressible equations of motion leads to hybrid methods that differ significantly from their incompressible counterparts. The hyperbolic nature of compressible flows means that steady-state formulations typically do not offer a significant computational advantage, and as a result, explicit time integration is the preferred solution method and flux matching is the preferred coupling method. Given that the characteristic evolution time, τ_h, scales with the system size, the largest problem that can be captured by a hybrid method is limited by the separation of scales between the molecular integration time and τ_h. Local mesh refinement techniques [14, 34] minimize the regions of space that need to be integrated at small CFL timesteps (due to a fine mesh), such as the regions adjoining the molecular subdomain. Implicit timestepping methods [38] can also be used to speed up the time integration of the continuum subdomain. Unfortunately, although both approaches enhance the computational efficiency of the continuum subproblem, they do not alleviate the issues arising from the disparity between the molecular timestep and the total integration time.

As discussed in the introduction, overwhelming computational costs can be incurred when using a time-explicit flux-based coupling approach to capture steady phenomena where compressibility effects are negligible, as is in most cases, in dense fluids. In this case the integration timestep of the continuum subdomain also becomes of the order of the molecular timescale, while the continuum subdomain

is, presumably, much larger than the molecular subdomain and evolves at a much longer timescale. This appears to not have been fully appreciated by various groups that have attempted to develop dense-fluid hybrid methods based on the compressible continuum formulation and flux-based matching procedures to solve steady and essentially incompressible problems.

On the other hand, for compressible gas flow, locally refining the continuum solution cells to the size of DSMC cells leads to a particularly seamless compressible hybrid formulation in which DSMC cells differ from the neighboring continuum cells only by the fact that they are inherently fluctuating (the DSMC timestep required for accurate solutions, see [3, 15, 18], is very similar to the CFL timestep of a compressible formulation). Thus a finite volume formulation can be used to couple the two subdomains quite naturally. In such a method [18, 19] the fluxes of mass, momentum, and energy from DSMC to the continuum subdomain given by particles leaving the DSMC region and traveling toward the continuum subdomain can be used directly for finite volume integration. Imposition of the continuum "interface conditions" onto DSMC requires the use of reservoirs similarly to the procedure outlined in Section 4.1. The flux of mass, momentum, and energy from the continuum to the atomistic domain is provided by the particles that, upon initialization in the reservoir at the continuum solution conditions, travel into the DSMC region. In this paper we review recent developments [34, 35] that embed this methodology into an adaptive mesh refinement framework.

Another characteristic inherent to compressible formulations is the possibility of describing parts of the domain by the Euler equations of motion [34]. In that case, consistent coupling to the molecular formulation can be performed using a Maxwell-Boltzmann distribution [14].

In a recent paper [4], Alexander *et al*. have shown that explicit time-dependent flux-based formulations preserve the fluctuating nature of the molecular description within the molecular regions, but the fluctuation amplitude decays rapidly within the continuum regions; correct fluctuation spectra can be obtained in the entire domain by solving a fluctuating hydrodynamics formulation [21] in the continuum subdomain.

5.1. Fully Adaptive Mesh and Algorithm Refinement for a Dilute Gas

The compressible formulation of Garcia *et al*. [14], referred to as AMAR (Adaptive Mesh and Algorithm Refinement), pioneered the use of mesh refinement as a natural framework for the introduction of the molecular description in a hybrid formulation. In AMAR, the typical continuum mesh refinement capabilities are supplemented by an algorithmic refinement (continuum to atomistic) based on continuum breakdown criteria. This seamless transition is both theoretically and practically very appealing.

In what follows we briefly discuss a recently developed [34, 35] *fully adaptive* AMAR method. In this method, the DSMC provides an atomistic description of the flow while the compressible two-fluid Euler equations serve as the continuum-scale model. The continuum and atomistic representations are coupled by matching fluxes at the continuum-atomistic interfaces and by proper averaging and interpolation of data between scales. This is performed in three steps: a) the continuum solution values are interpolated to create DSMC particles in the reservoir region, here called buffer cells; b) the conserved quantities in each continuum cell overlaying the DSMC region are replaced by averages over particles in the same region; and c) fluxes recorded when particles cross the DSMC interface are used to correct the continuum solution in cells adjacent to the DSMC region. This coupling procedure makes the DSMC region appear as any other level in an AMAR grid hierarchy. Similarly to the over-

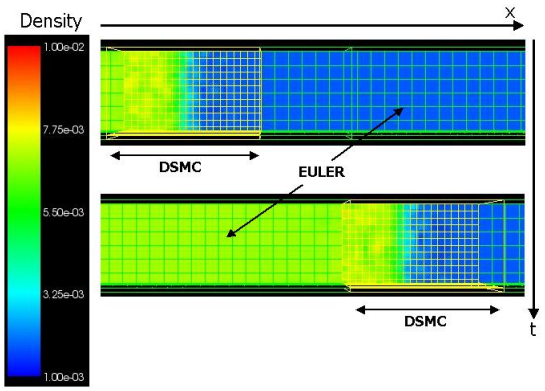

FIGURE 5. Moving Mach 10 shock wave though Argon. The AMAR algorithm tracks the shock by adaptively moving the DSMC region with the shock front.

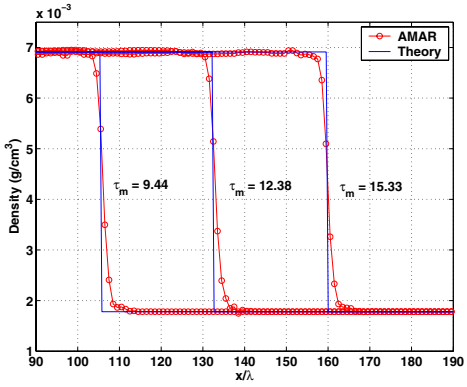

FIGURE 6. Moving Mach 10 shock wave though Argon. The AMAR profile (red dots) is compared with the analytical time evolution of the initial discontinuity (blue lines). τ_m is the mean collision time.

lap region described for the Schwarz method above, the Euler solution information is passed to the particles via buffer cells surrounding the DSMC region. At the beginning of each DSMC integration step, particles are created in the buffer cells using the continuum hydrodynamic values.

The above algorithm allows grid and algorithm refinement based on any combination of flow variables and their gradients. Density gradient-based refinement has been found to be generally robust and reliable [34]. Concentration gradients or concentration values within some interval are also effective refinement criteria especially for multispecies flows involving concentration interfaces. In this particular implementation, refinement is triggered by spatial gradients exceeding user defined tolerances. This approach follows from the continuum breakdown parameter method proposed by Bird [6].

Using the AMAR capabilities provided by the Structured Adaptive Mesh Refinement Application Infrastructure (SAMRAI) developed at the Lawrence Livermore National Laboratory [27], the above adaptive framework has been implemented in a fully 3D, massively parallel form in which multiple molecular (DSMC) patches can be introduced or removed as needed.

Figure 5 shows the adaptive tracking of a shockwave of Mach number 10 used as a validation test for this method. Density gradient-based mesh refinement ensures the DSMC region tracks the shock front accurately. Furthermore, as shown in Fig. 6 the density profile of the shock wave remains smooth and is devoid of oscillations that are known to plague traditional shock capturing schemes [5, 37].

6. DISCUSSION

One of the most important messages of this paper is that boundary-condition imposition on molecular domains is quite independent of the choice of the solution-coupling approach. As an example, consider the Schwarz method, which provides a recipe for making solutions in various subdomains globally consistent subject to exchange of Dirichlet conditions. The imposition of these boundary conditions can be achieved through any method, and no certain method is favored by the coupling approach. Flexibility in adopting *appropriate elements* from previous approaches and the importance of choosing the coupling method ac-

cording to the flow physics are key steps to the development of more sophisticated, next-generation hybrid methods.

Although hybrid methods provide significant savings by limiting molecular solutions only to the regions where they are needed, solution of time-evolving problems, which span a large range of timescales, is still not possible if the molecular domain, however small, needs to be integrated for the total time of interest. New frameworks are, therefore, required that allow timescale decoupling or coarse-grained time evolution of molecular simulations.

Significant computational savings can be obtained by using incompressible formulation when appropriate. Neglect of these simplifications can lead to a problem that is simply intractable when the continuum subdomain is appropriately large. It is interesting to note that, when a hybrid method was used to solve a problem of practical interest [1] while providing computational savings, the Schwarz method was preferred because it provided a steady solution framework with timescale decoupling.

For dilute gases the Chapman-Enskog distribution provides a robust and accurate method for imposing boundary conditions. Further work is required for the development of similar frameworks for dense liquids.

ACKNOWLEDGMENTS

The authors wish to thank R. Hornung, A. L. Garcia, A. T. Patera, and B. J. Alder for helpful comments and discussions. The work outlined in Sec. 5.1 was performed jointly with R. Hornung and A. L. Garcia. This work was supported in part by the Center for Computational Engineering, and the Center for Advanced Scientific Computing, Lawrence Livermore National Laboratory, US Department of Energy, W-7405-ENG-48. The authors also acknowledge the financial support of the Singapore-MIT alliance.

REFERENCES

1. Aktas, O. and Aluru, N. R., A combined continuum/DSMC technique for multiscale analysis of microfluidic filters, *Journal of Computational Physics* **178**:342–372, 2002.
2. Alexander, F. J., and Garcia, A. L., The direct simulation Monte Carlo method, *Computers in Physics* **11**:588–593, 1997.
3. Alexander, F. J., Garcia, A. L., and Alder, B. J., Cell size dependence of transport coefficients in stochastic particle algorithms, *Physics of Fluids* **10**:1540-1542, 1998; erratum, *Physics of Fluids* **12**:731, 2000.
4. Alexander, F., Garcia, A. L. and Tartakovsky D., Algorithm refinement for sochastic partial diffential equations: I. Linear diffusion, *Journal of Computational Physics* **182**(1):47–66, 2002.
5. Arora, M., and Roe, P. L., On postshock oscillations due to shock capturing schemes in unsteady flows, *Journal of Computational Physics* **130**:25–40, 1997.
6. Bird, G. A., Breakdown of translational and rotational equilibrium in gaseous expansions, *AIAA Journal* **8**:1998, 1970.
7. Bird, G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon Press, Oxford, 1994.
8. Chapman, S. and Cowling, T. G., *The Mathematical Theory of Non-Uniform Gases*, Cambridge University Press, Cambridge, 1970.
9. Delgado–Buscalioni, R., and Coveney, P. V., Continuum-particle hybrid coupling for mass, momentum and energy transfers in unsteady fluid flow, *Physical Review E* **67**:046704, 2003.
10. Eggers, J., and Beylich, A., New algorithms for application in the direct simulation Monte Carlo method, *Progress in Astronautics and Aeronautics* **159**:166–173, 1994.
11. Flekkoy, E. G., Wagner, G., and Feder, J., Hybrid model for combined particle and continuum dynamics, *Europhysics Letters* **52**:271–276, 2000.
12. Fortin, M. and Aboulaich, R. Schwarz's decomposition method for incompressible flow problems, *1st Int. Symp. on Domain Decomposition Methods for Partial Differential Equations*, R. Glowinski, G. Golub, G. Meurant, and J. Periaux, Eds., SIAM, Philadelphia, 333–349, 1988.
13. Garcia, A .L., and Alder, B. J., Generation of the Chapman-Enskog distribution, *Journal of Computational Physics* **140**:66–70, 1998.

14. Garcia, A. L., Bell, J. B., Crutchfield, W. Y., and Alder, B. J. Adaptive mesh and algorithm refinement using direct simulation Monte Carlo. *Journal of Computational Physics* **54**:134–155, 1999.
15. Garcia, A. L., and Wagner, W. Time step truncation error in direct simulation Monte Carlo. *Physics of Fluids* **12**:2621–2633, 2000.
16. Hadjiconstantinou, N. G., and Patera A. T. Heterogeneous atomistic-continuum representations for dense fluid systems. *International Journal of Modern Physics C*, **8**:967–976, 1997.
17. Hadjiconstantinou, N. G., Hybrid atomistic-continuum formulations and the moving contact-line problem. *Journal of Computational Physics* **154**:245–265 1999.
18. Hadjiconstantinou, N. G. Analysis of discretization in the direct simulation Monte Carlo. *Physics of Fluids* **12**:2634–2638, 2000.
19. Hadjiconstantinou, N. G., Garcia, A. L., Bazant, M. Z. and He, G., Statistical error in particle simulations of hydrodynamic phenomena. *Journal of Computational Physics* **187**:274–297, 2003.
20. Hash, D., and Hassan, H. A hybrid DSMC/Navier-Stokes solver. AIAA Paper 95-0410, 1995.
21. Landau, L. D., and Lifshitz, E. M. *Statistical Mechanics Part 2*, Pergamon Press, Oxford, 1980.
22. Li, J., Liao, D., and Yip S. Nearly exact solution for coupled continuum/MD fluid simulation. *Journal of Comput-Aided Materials Design* **6**:95–102, 1999.
23. Lions, P. L., On the Schwarz alternating method. I. *1st Int. Symp. on domain decomposition methods for partial differential equations*, R. Glowinski, G. Golub, G. Meurant, and J. Periaux, Eds., SIAM, Philadelphia, 1–42, 1988.
24. Liu, S. H. On Schwarz alternating methods for the incompressible Navier-Stokes equations. *Siam Journal of Scientific Computing* **22**:1974–1986, 2001.
25. Mansour, M. M., Baras, F. and Garcia, A. L. On the validity of hydrodynamics in plane Poiseuille flows. *Physica A* **240**:255–267, 1997.
26. O'Connell, S. T., and Thompson, P.A. Molecular dynamics-continuum hybrid computations: A tool for studying complex fluid flows. *Physical Review E*, **52**:R5792–R5795, 1995.
27. Structured Adaptive Mesh Refinement Application Infrastructure (SAMRAI), http://www. llnl.gov/CASC/
28. Wadsworth, D. C., and Erwin, D. A. One-dimensional hybrid continuum/particle simulation approach for rarefied hypersonic flows. AIAA Paper 90-1690, 1990.
29. Wadsworth, D. C. and Erwin, D. A., Two-dimensional hybrid continuum/particle simulation approach for rarefied hypersonic flows. AIAA Paper 92-2975, 1992.
30. Wagner, W. A convergence proof for Bird's direct simulation Monte Carlo method for the Boltzmann equation. *Journal of Statistical Physics* **66**:1011–1040, 1992.
31. Wesseling, P. *Principles of Computational Fluid Dynamics*, Springer, (2001).
32. Wijesinghe, H. S. Hybrid atomistic-continuum formulations for gaseous flows. PhD thesis, Dep. of Aeronautics and Astronautics, Massachusetts Institute of Technology, 2003.
33. Wijesinghe, H. S., and Hadjiconstantinou, N. G. A hybrid continuum-atomistic scheme for viscous incmpressible flow. *Proc. of 23th Int. Symp. on* Rarefied Gas Dynamics, Whistler, British Columbia, 907–914, 2002.
34. Wijesinghe, H. S., Hornung, R., Garcia, A. L. and Hadjiconstantinou, N. G., "3–dimensional hybrid continuum-atomistic simulations for multiscale hydrodynamics. *Proc. of the 2003 Int. Mechanical Engineering Congress and Exposition, Vol. 2*, Paper No. NANOT-41251.
35. Wijesinghe, H. S., Hornung, R., Garcia, A. L., and Hadjiconstantinou, N. G. Three–dimensional hybrid continuum-atomistic simulations for multiscale hydrodynamics. *Journal of Fluids Engineering (to appear).*
36. Wong, J. S., Darmofal, D. L. and Peraire, J. The solution of the compressible euler equations at low mach numbers using a stabilized finite element algorithm. *Computer Methods in Applied Mechanics and Engineering* **190**:5719–5737, 2001.
37. Woodward, P. R., and Colella, P. The numerical simulation of two-dimensional fluid flow with strong shocks. *Journal of Computational Physics* **54**:115–173, 1984.
38. Yuan, X., and Daiguji, H. A specially combined lower-upper factored implicit scheme for three dimensional compressible Navier-Stokes equations. *Computers and Fluids* **30**:339-363, 2001.