A New Heterogeneous Multiscale Technique for Microscale Gas Flows

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Abstract We present a new hybrid method for dilute gas flows that heterogeneously couples a continuum-fluid description to the direct simulation Monte Carlo (DSMC) method. A continuum-fluid model is applied across the entire domain, while DSMC is applied in spatially-distributed micro regions. Using a field-wise coupling approach, DSMC sub-domains of any size can be placed at any location. The sub-domain arrangement can therefore be adjusted for each problem to capture non-equilibrium behaviour both close to bounding walls and in the bulk. We demonstrate our method on a test case of high-speed micro Couette flow. With large differences in wall velocity, significant viscous heating is present, and so our coupling considers the transfer of both momentum and heat. Our hybrid results are validated against a pure DSMC simulation, and the results show that the method can deal with missing boundary and constitutive information.

Keywords: Heterogeneous Multiscale Method, Molecular/Continuum, Hybrid, DSMC, Micro Gas Flow.

1. Introduction

The conventional hydrodynamic model is excellent for the majority of fluid flows, but in some cases, the presence of localised regions of thermodynamic non-equilibrium can result in inaccuracy. Molecular simulation tools can provide an accurate alternative, but are usually much too computationally expensive for resolving typical engineering spatial and temporal scales. Multiscale methodologies have therefore been developed over the past decade. Often referred to as 'hybrids', these multiscale methods integrate continuum and molecular descriptions within the same solver, effectively combining the computational efficiency of continuum methods with the detail and accuracy of molecular techniques.

In the literature, two hybrid frameworks have emerged for fluids: a) the domain-decomposition technique, and b) the Heterogeneous Multiscale Method (HMM). For liquids, molecular dynamics (MD) is the appropriate molecular tool. This is, however, inefficient for dilute gases. The direct simulation Monte Carlo (DSMC) method developed by Bird (1998) can instead provide a coarse-grained molecular description.

Domain-decomposition is currently the most popular hybrid framework for liquids (O'Connell et al., 1995; Hadjiconstantinou and Patera, 1997; Flekkøy et al., 2000) and dilute gases (Hash and Hassan, 1996; Aktas and Aluru, 2002; Sun et al., 2004; Wijesinghe et al., 2004; Schwartzentruber et al., 2007). With the simulation domain partitioned, a molecular solver is typically applied in micro regions close to bounding interfaces while a conventional continuum solver is implemented in the remainder. These solvers are then coupled through an overlap region. A problem with this approach is that computational efficiency can be increased above that of a full molecular simulation only when non-equilibrium is confined to 'near-wall' regions.

The less-common HMM framework overcomes this limitation by adopting a micro-resolution approach: a continuum model is applied across the entire flowfield, and the molecular solver is applied in spatially-distributed micro regions (near bounding surfaces, and in the bulk). These micro regions provide missing data that is required for closure of the local continuum model, either in the form of unknown boundary conditions, or unknown constitutive information. Existing HMM studies are based mainly on liquid

flows, with MD as the molecular solver (see Ren and E, 2005; Yasuda and Yamamoto, 2008; Borg et al., 2013a).

Despite the advantages of HMM over domain-decomposition, there has been little development of HMM hybrids that incorporate DSMC. The Coupled Multiscale Multiphysics Method (CM^3) of Kessler et al. (2010) retains fully-coupled length scales, as the continuum description and DSMC are applied over the same flow domain. Recently, Patronis et al. (2013) adapted the Internal-flow Multiscale Method (IMM) to simulate dilute gas flows in high-aspect ratio channels with DSMC as the molecular solver.

In this paper we propose a new form of the HMM technique that is designed to deal with inaccuracy in traditional boundary conditions and/or constitutive relations. We adopt DSMC as the molecular description, which is linked to the continuum fluid solver using a field-wise coupling (HMM-FWC) approach (see Borg et al., 2013b). Rather than supplying a correction to a node on the continuum mesh, each micro region corrects a continuum sub-region, the spatial dimensions of which are identical to those of the micro region itself. This means that the position and size of our micro regions can be optimised for each problem, making HMM-FWC suitable for problems with varying degrees of spatial scale separation.

The form of the method we present in this paper is general and is suitable for modeling both momentum and heat transfer in gases at the microscale. To validate our method, we consider a one-dimensional test case of high-speed Couette flow.

2. Simulation Methodology

In our method, the continuum description is applied across the full macro domain and is corrected using dispersed DSMC sub-domains. In turn, these sub-domains are constrained by the local continuum description. We present a new strategy to achieve this two-way coupling.

2.1 Correcting the Continuum Description

For steady-state fluid flows, the governing equations for the conservation of mass, momentum, and energy can be written,

$$\nabla \cdot \rho \mathbf{u} = 0, \tag{1}$$

$$\rho \mathbf{u} \cdot (\nabla \mathbf{u}) = -\nabla \cdot p\mathbf{I} + \nabla \cdot \boldsymbol{\sigma} + \mathbf{F}, \tag{2}$$

$$\nabla \cdot (\rho \mathrm{E} \mathbf{u}) = -\nabla \cdot (p\mathbf{I} \cdot \mathbf{u}) + \nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}, \tag{3}$$

where, ρ is the mass density, $\mathbf{u}$ is velocity, p is the pressure, $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{F}$ is a body force, E is the total energy, and $\mathbf{q}$ is the heat-flux vector. Typically, these expressions are closed using the traditional Navier-Stokes-Fourier (NSF) constitutive relations for $\boldsymbol{\sigma}$ and $\mathbf{q}$. These relations are, however, known to fail in certain conditions, e.g. in conditions of thermodynamic non-equilibrium, or in flows of complex fluids. We can therefore obtain 'corrections' to these constitutive relations from our cluster of DSMC sub-domains. We obtain a 'stress correction' field $\boldsymbol{\Omega}$, i.e.

$$\boldsymbol{\sigma} = \mu(\nabla \mathbf{u}) + \mu(\nabla \mathbf{u})^{\mathrm{T}} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} + \boldsymbol{\Omega}, \tag{4}$$

and a 'heat-flux correction' field $\boldsymbol{\Phi}$, i.e.

$$\mathbf{q} = -\kappa \nabla T + \boldsymbol{\Phi}. \tag{5}$$

Note that these correction fields automatically incorporate any error in the assumed dynamic viscosity μ and thermal conductivity κ. The momentum equation then reads,

$$\rho \mathbf{u} \cdot (\nabla \mathbf{u}) = -\nabla \cdot p\mathbf{I} + \nabla \cdot \mu(\nabla \mathbf{u}) + \nabla \cdot \mu(\nabla \mathbf{u})^{\mathrm{T}} - \frac{2}{3}\nabla \cdot \left[\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right] + \nabla \cdot \boldsymbol{\Omega} + \mathbf{F}, \tag{6}$$

while the energy equation becomes,

$$\nabla \cdot (\rho \mathrm{E} \mathbf{u}) = -\nabla \cdot (p\mathbf{I} \cdot \mathbf{u}) + \nabla \cdot \left[\mu(\nabla \mathbf{u}) \cdot \mathbf{u}\right] + \nabla \cdot \left[\mu(\nabla \mathbf{u})^{\mathrm{T}} \cdot \mathbf{u}\right] - \frac{2}{3}\nabla \cdot \left[\mu(\nabla \cdot \mathbf{u})\mathbf{I} \cdot \mathbf{u}\right] + \nabla \cdot (\boldsymbol{\Omega} \cdot \mathbf{u}) + \nabla \cdot (\kappa \nabla \mathrm{T}) - \nabla \cdot \boldsymbol{\Phi}. \tag{7}$$

The general strategy of our heterogeneous hybrid approach can be summarized as follows. Based on the local continuum description, constraints are applied to each micro sub-domain. Performing DSMC, the velocity and temperature, along with the stress and the heat-flux, are measured across each sub-domain. The stress and heat-flux correction fields across each sub-domain are then computed using Eqs. 4 and 5. By

interpolating between all micro sub-domains, the correction fields across the entire flowfield are approximated. With boundary conditions obtained from near-wall micro simulations, solving Eqs. 1, 6, and 7 results in new 'corrected' velocity, temperature, and pressure fields across the domain. With successive iterations, the hybrid simulation stops once these property fields converge.

2.2 Constraining the DSMC Sub-domains

The open-source C++ toolbox OpenFOAM incorporates a DSMC solver, dsmcFoam, which we use to perform all the micro and full-scale DSMC simulations in this paper.

It is important that the gas state in the DSMC sub-domains (from which we extract the correction fields) is properly representative of the local conditions in the macro domain. However, the particle distribution required at the boundaries of each sub-domain cannot be extracted directly from the continuum flowfield. We circumvent this problem by establishing an artificial 'relaxation' region around each sub-domain that enables the particle distribution to naturally evolve to its correct form at the sub-domain boundaries. Sampling of property fields is then performed only in the core of the sub-domain, i.e. the 'sampling zone'. A schematic of a 3D bulk sub-domain is shown in Fig. 1.

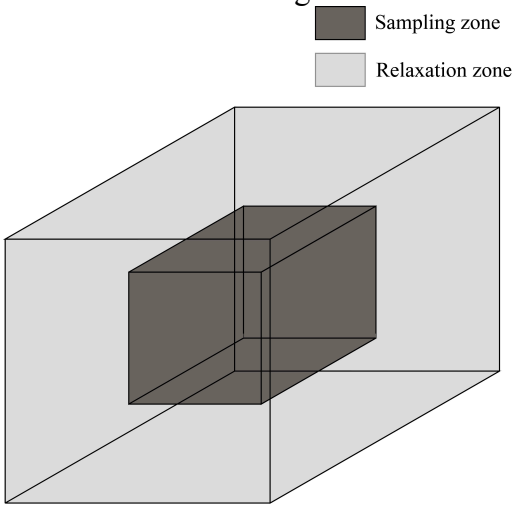

Fig. 1. 3D bulk micro sub-domain.

Note that, to capture regions of non-equilibrium that appear at bounding walls, the sampling zone in a 'near-wall' micro element must be adjacent to the wall itself.

The sole purpose of the 'relaxation zone' is to generate the proper boundary conditions to the sampling zone. We achieve this by using particle controllers (see Borg et al. 2010) to enforce the local continuum state throughout the relaxation zone, while a Maxwellian particle distribution (for simplicity) is imposed at the outer boundaries of the relaxation zone. The relaxation zone must then be large enough that complete relaxation of the particle distribution occurs before reaching the inner sampling zone.

2.3 Iterative algorithm

The general coupling procedure is:

0. Initially, $\boldsymbol{\Omega} = \boldsymbol{\Phi} = 0$. Assuming no velocity slip or temperature jump, solve Eqs. 1, 6, and 7, to obtain an initial estimate for the continuum velocity, temperature, and pressure fields: $\mathbf{u}_{NSF}$, T_{NSF}, and p_{NSF}.

   Compute the initial density field from the ideal gas law, $\rho_{NSF} = p_{NSF}/RT_{NSF}$.

1. Constrain each micro sub-domain by applying boundary conditions:
   a. Enforce the local continuum velocity, temperature, and density fields (computed in the previous step) throughout each relaxation zone using particle controllers.
   b. At the outer boundaries of each relaxation zone, impose a Maxwellian particle distribution at the local continuum velocity and temperature.
2. Perform DSMC in each sub-domain. From each sampling zone, extract the time-averaged property fields. Also, from near-wall sampling zones, extract the velocity and temperature of the gas at the wall surface.
3. Using the extracted velocity and stress fields in Eq. 4, compute the stress correction across each sampling zone. Similarly, compute the heat-flux correction across each sampling zone using the extracted temperature and heat-flux fields in Eq. 5.

4. Carry out appropriate interpolations between the sampling zones to approximate the correction fields, $\mathbf{\Omega}$ and $\mathbf{\Phi}$, across the full domain.

   Similarly, interpolate between near-wall sampling zones to obtain gas velocity and temperature information at all bounding walls.

5. Using this boundary information, and $\mathbf{\Omega}$ and $\mathbf{\Phi}$, solve Eqs. 1, 6, and 7, to obtain new corrected velocity, temperature, and pressure fields: $\mathbf{u}_{new}$, T_{new}, and p_{new}.

   Compute the new corrected density field, $\rho_{new} = p_{new}/RT_{new}$.

6. Replace the initial NSF property fields with the new corrected property fields and repeat from Step 1. Continue until the solution converges.

3. High-speed Couette Flow

We require a simple test case that can easily be validated against a full-scale DSMC simulation. We therefore choose a steady-state case with one-dimensional momentum and heat transfer, i.e. high-speed Couette flow. This consists of a gas confined between two infinite parallel walls that are maintained at the same temperature T_{wall}, and are moving in their own plane at different velocities, u_{lower} and u_{upper}. If these velocities are large (such that the gas has a Mach number $Ma > 0.2$), significant viscous heating occurs in the gas.

3.1 Numerical Implementation

In reality, μ and κ will vary with the hydrodynamic properties of the gas. However, with the exact variations unknown, we assume constant reference values μ_r and κ_r in this work. The correction fields automatically adjust for any resulting error.

When following the hybrid procedure of section 2.3, simplifications can be made due to the one-dimensional nature of this problem. Mass conservation (Eq. 1) is automatically satisfied. The conservation of momentum (Eq. 6) takes the form of two separate expressions for the x- and y-directions,

$$\mu_r\left[\frac{d^2u}{dy^2}\right]+\frac{d\Omega_{xy}}{dy}=0, \tag{8}$$

$$\frac{dp}{dy}-\frac{d\Omega_{yy}}{dy}=0, \tag{9}$$

while the conservation of energy (Eq. 7) is reduced to,

$$\kappa_r\left[\frac{d^2T}{dy^2}\right]-\frac{d\Phi_y}{dy}+\mu_r\left[\frac{du}{dy}\right]^2+\frac{du}{dy}\Omega_{xy}=0. \tag{10}$$

From Eq. 4, the shear and normal stress corrections are given by,

$$\Omega_{xy}=\sigma_{xy}-\mu_r\left[\frac{du}{dy}\right], \tag{11}$$

$$\Omega_{yy}=\sigma_{yy}, \tag{12}$$

and, from Eq. 5, the heat-flux correction is given by,

$$\Phi_y=q_y+\kappa_r\left[\frac{dT}{dy}\right]. \tag{13}$$

Discretizing in one-dimensional space, the macroscopic mesh consists of N macro nodes, including a node at each wall. The governing equations 8, 9, and 10, along with the correction fields given by Eqs. 11, 12, and 13, can therefore be approximated using finite difference representations.

An example computational domain for this case is shown in Fig. 2, with a micro sub-domain at each wall, and one in the bulk. This sub-domain arrangement is an example only – the appropriate arrangement depends on the case itself. For this 1D problem, each near-wall sub-domain comprises a single sampling zone and a single relaxation zone, while each bulk sub-domain consists of a single sampling zone with a relaxation zone on either side, as indicated in Fig. 2. To measure and control the variation of the property fields, each sampling zone is divided into a number of 1D measurement bins, while each relaxation zone is divided into a number of 1D control bins. To keep the transfer of data between the solvers as simple as possible, the bin arrangement is set such that the centre of each bin coincides exactly with a macro node. This is, however, merely for convenience and is not essential.

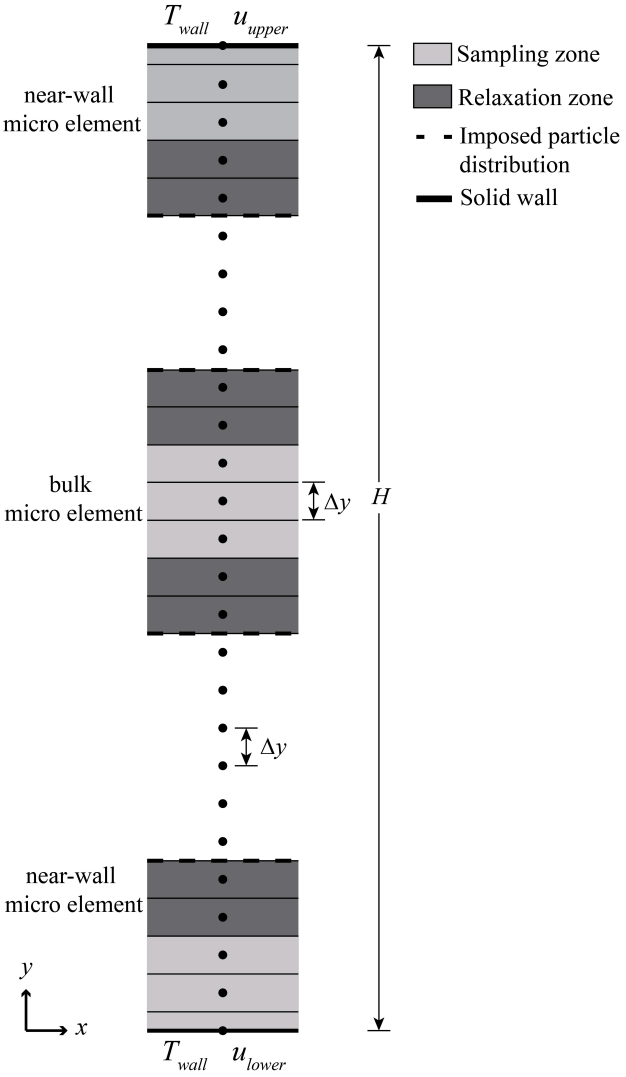

Fig. 2. A schematic of the computational set-up for a planar Couette flow problem.

The application of the general hybrid algorithm to this 1D system is as follows:

0. Assuming no correction ($\Omega_{xy} = \Omega_{yy} = \Phi_y = 0$) and traditional no slip/jump boundary conditions, solving Eqs. 8, 9, and 10 produces the initial NSF property fields, u_{NSF}, T_{NSF}, p_{NSF}, and $\rho_{NSF} = p_{NSF}/RT_{NSF}$.

1. Each sub-domain is then constrained:
   a. The local continuum velocity, temperature, and density fields are enforced across the relaxation zones using particle controllers in each control bin.
   b. A Maxwellian particle distribution is imposed at the outer boundaries of each relaxation zone via a diffuse wall at the local continuum velocity and temperature.
2. DSMC is performed in each sub-domain. From each measurement bin, the time-averaged property fields are extracted. Also, from both near-wall micro elements, the velocity and temperature of the gas at the wall surface is extracted.
3. With the extracted velocity and stress fields, we can compute the shear and normal stress corrections across each sampling zone using Eqs. 11 and 12. Similarly, using the extracted heat-flux and temperature, we can compute the heat-flux correction across each sampling zone from Eq. 13.
4. For simplicity, linear interpolation is used between the sampling zones to obtain the full correction fields across the entire flowfield. Note that, for this 1D geometry, interpolation of the boundary information is not required.
5. With the full correction fields and updated boundary conditions, solving Eqs. 8, 9, and 10 gives new corrected property fields, u_{new}, T_{new}, p_{new}, and, $\rho_{new} = p_{new}/R\,T_{new}$.
6. Replacing the old property fields with the new corrected property fields, we repeat from Step 1 until we get convergence.

3.2 Test Case: Results

Maintaining simplicity, we consider a test case where the confined gas is monatomic argon. The separation between the walls $H = 1$ μm, and we use $N = 201$ macro nodes across the domain (giving a constant node spacing $\Delta y = 5$ nm). Both walls are maintained at a constant temperature $T_{wall} = 273$ K. The lower wall moves at $u_{lower} = -1550$ m/s, while the upper wall moves at $u_{upper} = +1550$ m/s. With $Ma \approx 5$, viscous heating will be significant and so the temperature of the gas is expected to be considerably greater than the wall temperature. The initial NSF solution for this problem indicates that the average temperature of the

gas will be 1294 K. Based on this, we assume a reference viscosity $\mu_r = 6.25\times10^{-5}$ kg/ms, and a reference conductivity $\kappa_r = 0.049$ W/mK (see Younglove, 1986). Assuming a Variable Hard Sphere (VHS) molecular collision model, we set the gas density to obtain a gas mean free path λ of 0.01 μm, and hence a global Knudsen number Kn $=\lambda / H = 0.01$.

The accuracy of our hybrid approach depends on the configuration (i.e. the position and size) of our DSMC sub-domains, as this will determine the ability to capture the true form of the correction fields across the flowfield. These 'true' correction fields are those that can be computed from a full-scale DSMC solution, using the measured property fields in Eqs. 11, 12, and 13. To validate our coupling method, we consider an example configuration where we have two near-wall sub-domains, and four bulk sub-domains. As non-equilibrium is more prominent close to the walls, we position the bulk sub-domains such that they are centered at $y = 0.1H$, $0.3H$, $0.7H$, and $0.9H$. We select an extent of 5 local mean free paths λ_l for each relaxation zone, as this should be sufficient to allow for full relaxation of the particle state. We also approximate that an extent of 5 λ_l for each sampling zone should enable us to construct a reasonable approximation of the three correction fields. Therefore, our near-wall sub-domains have an extent of 10 λ_l while our bulk sub-domains have an extent of 15 λ_l.

We use the same cell-size and time-step for the DSMC sub-domains and the full simulation. With a time-step $\Delta t = 1\times10^{-12}$ s, an initial start-up run of 3 million time-steps allowed all simulations to reach steady state. All simulations were run for a further 20 million time-steps to minimize the statistical scatter in the averaging of the property fields.

Convergence of the solution occurs within 5 iterations here. Along with the initial NSF and full DSMC solutions, the final converged property profiles are shown in Fig. 3. Presented in Fig. 4, the mean percentage error $\bar{\varepsilon}$ of these hybrid property profiles (in comparison with the full DSMC solution) provides a more visible measure of the hybrid's accuracy. For a property b,

$$\bar{\varepsilon}_b = \frac{1}{N}\sum_{i}^{N}\left[\frac{b_{Full}(i)-b_{new}(i)}{b_{ref}}\times100\%\right], \quad (14)$$

where $i = 0, 1, 2,\ldots N\text{-}1$, and b_{ref} is a constant reference value. For the velocity, temperature, and density (which vary considerably across the flowfield), b_{ref} is the property range of the full-scale solution, i.e. $b_{ref} = b_{Full,max} - b_{Full,min}$. For the pressure (which remains almost constant across the flowfield), b_{ref} is the average of the full-scale solution, i.e. $b_{ref} = p_{Full,av}$. Note that iteration $l = 0$ corresponds to the initial NSF solution.

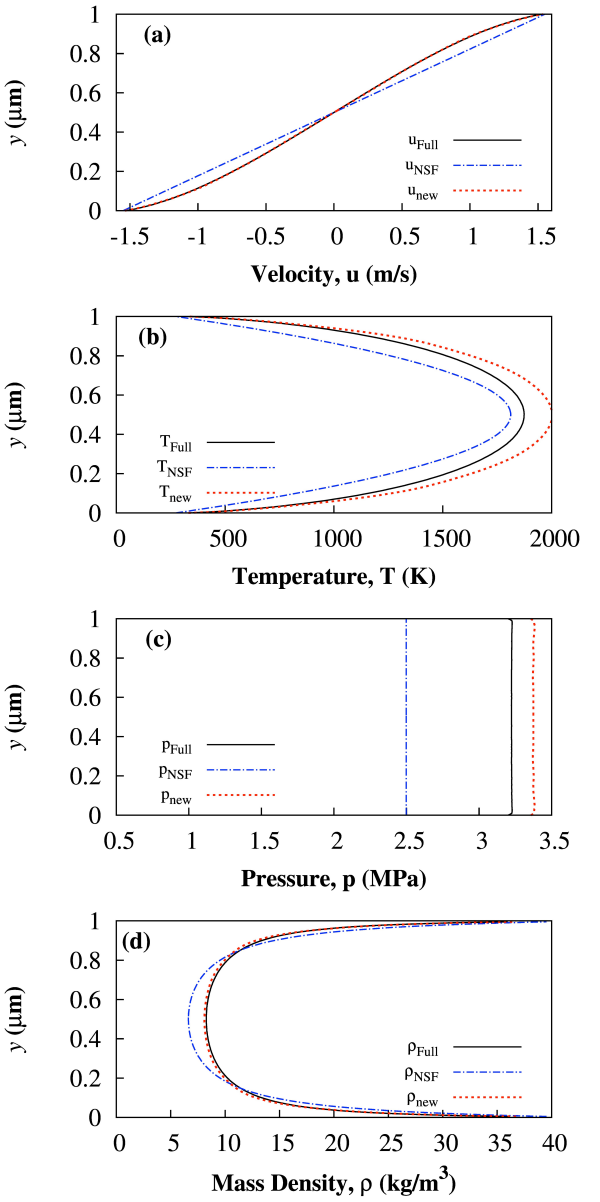

Fig. 3. NSF, Full DSMC, and final new hybrid solutions for (a) velocity, (b) temperature, (c) pressure, and (d) mass density.

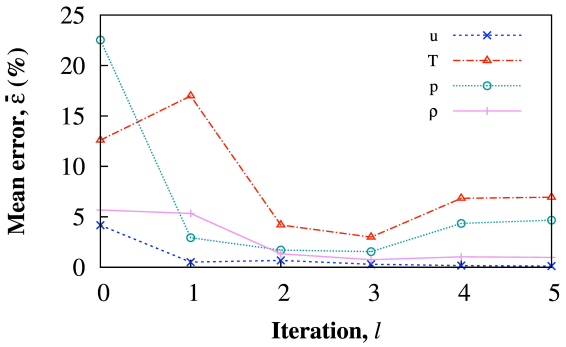

Fig. 4. Mean error in the hybrid velocity, temperature, pressure, and density solutions.

For all properties, this hybrid configuration provides a significant improvement over the initial NSF solution. The hybrid velocity field matches well to the full-scale solution, with a final error of 0.11%. The temperature and pressure profiles are less accurate, with final errors of 6.94% and 4.66%, respectively. This accuracy is a result of the approximated correction fields shown in Fig. 5.

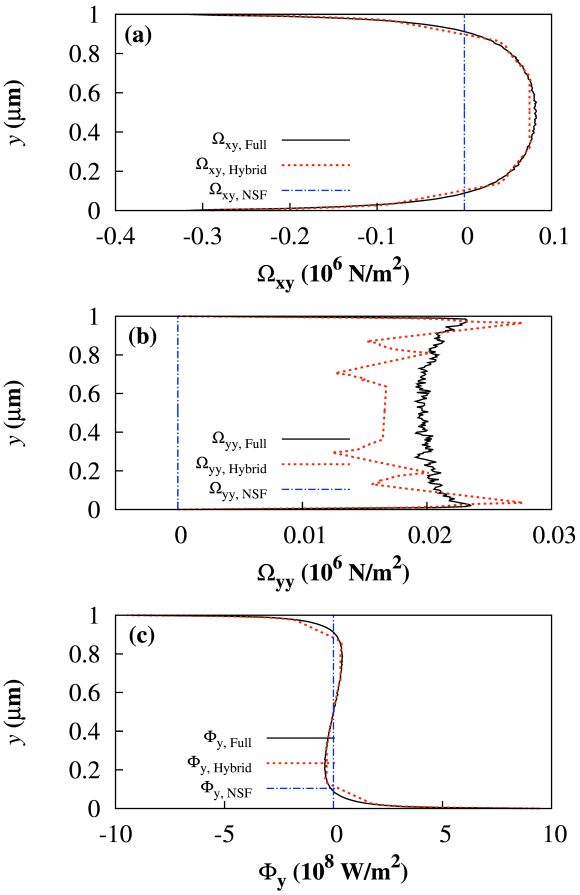

Fig. 5. The NSF, full-scale and hybrid (a) shear stress Ω_{xy}, (b) normal stress Ω_{yy}, and (c) heat-flux Φ_y correction fields. Note that the NSF solution provides no correction.

The accuracy of the temperature and pressure fields would likely be improved by increasing the molecular resolution close to the walls. This could be done by enlarging the sub-domains, by adding more bulk sub-domains, or both.

3.3 Computational Effort

A measure of the computational speed-up S is obtained here as the ratio of the total processing time of the full DSMC approach, to the total processing time of our hybrid approach. For each simulation, the total processing time is the total number of DSMC time-steps M × the average clock time per DSMC time-step t_c, i.e.

$$S = \frac{M_{Full} t_{c,Full}}{M_{Hybrid} t_{c,Hybrid}}. \qquad (14)$$

The total number of DSMC time-steps is the same for the full-scale and the hybrid sub-domain simulations, i.e. $M_{Full} = M_{Hybrid} = 23\times10^6$. The total average clock time per time-step for the hybrid approach $t_{c,Hybrid}$ is calculated as the sum of t_c for all micro sub-domains, over all iterations.

For this validation case, the degree of length scale separation is fairly small and so the required micro sub-domains occupy a significant portion of the domain. So, with five iterations, we see no computational speed-up at all for this one-dimensional test case, and $S < 1$. It is important to note, however, that this test case has been chosen simply to test and validate the hybrid methodology. Future simulations of larger, more realistic, 2D and 3D problems will highlight any computational advantages of our multiscale approach. The use of time scale separation may also increase computational savings.

4. Conclusions

Based on an HMM-FWC approach, we have proposed a hybrid method for microscale gas flows that couples a continuum-fluid solver with a DSMC particle method. The key advantage of this hybrid is that DSMC sub-domains of any size can be placed at any location, i.e. close to walls or in the bulk of the domain. The micro resolution can therefore be

adjusted for each problem to obtain the desired balance between accuracy and computational cost.

We have demonstrated our new method on a high-speed micro Couette flow problem, with coupling performed through momentum and energy. We have shown the hybrid method's ability to compensate for inaccurate boundary and constitutive information, and good agreement with the equivalent full-scale DSMC simulation was observed (with the exact level of accuracy determined by the micro sub-domain arrangement). Due to the small degree of scale separation in this test case, no computational speed-up was observed. However, significant speed-ups could be expected on larger, more realistic problems. Work is now focusing on application to complex 2D and 3D problems.

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