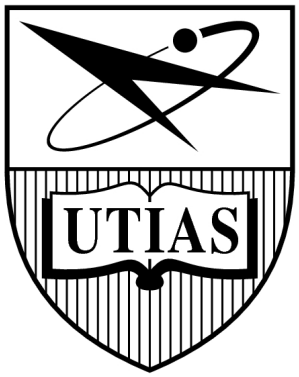

Development of a Regularized Gaussian Moment Closure for Three-Dimensional Micro-Scale Flows

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1 Introduction and Motivation

Generalized fluid behaviour is commonly described through the Navier-Stokes equations and has proven itself to be accurate when modeling typical problems encountered in the aerospace industry. However, the underlying assumption that the fluid behaves as a continuum breaks down when the mean free path for collisions between the fluid molecules is comparable in size to the characteristic length of the problem. At the other end of the dimensional spectrum, the modeling of rarefied flows is governed by the Boltzmann equation, and, in this regime, is readily solved using a variety of particle simulation techniques. The advent of micro-scale technologies [**?**] and upper atmospheric aerospace research [**?**] has prompted a need to model fluid flow behaviour lying between these two regimes, where non-equilibrium effects are significant but particle simulation techniques become prohibitively costly. Proper modeling of this transition regime is critical for understanding the behaviour of various macroscopic properties used in the overall design and function of these technologies.

Evaluation of non-continuum fluid flow behaviour is based on a statistical description of fluid particle movement, either through numerical approaches, such as a direct discretization of the Boltzmann equation and particle simulation methods, or through approximate techniques for the Boltzmann equation. Approximate techniques based on kinetic theory involve using a coupled set of non-linear partial differential equations that describe the transport of various macroscopic quantities. The classical mechanics concerning particle collisions are fully incorporated into these equations and the evolution of the particle distribution functions can be obtained. The resulting formulations can not only be used to derive the governing equations used in continuum flow, but can also provide the key to describing fluid flow behaviour in the non-equilibrium transition regime.

2 Scope of Research

This thesis will apply the Gaussian moment closure techniques to the modeling of three-dimensional non-equilibrium micro-scale flows by extending an existing two-dimensional formulation and numerical solution procedure developed originally by McDonald and Groth [**?**], and will investigate the incorporation of heat transfer terms inherently missing in the Gaussian closure via a regularization technique proposed by McDonald and Groth [**?**]. A finite-volume method with block-based adaptive mesh refinement (AMR) developed for solving the generalized transport equations of the Gaussian-based closures on a multi-block body-fitted hexahedral mesh will be accelerated with Newton-Krylov methods for steady-state flows and time-varying flows. The latter will make us of a dual-time stepping formulation. Verification and assessment of the capabilities of the approach will be conducted by considering its application to a number of canonical three-dimensional flow problems. Potential original contributions of this thesis will involve: (i) investgation of three-dimensional solutions of the Gaussian closure for a variety of flow problems; (ii) solution of the moment equations using a parallel implicit Newton-Krylov-Schwarz method; and (iii) the incorporation

and full evaluation of heat transfer terms following from the proposed regularization procedure.

3 Kinetic Theory of Gases

subsectionBoltzmann Equation A complete statistical description of particles in a fluid medium can be provided by a six-dimensional phase space distribution function spanning three-dimensional physical space and velocity space. This mathematical description was first described by Maxwell in 1859 and subsequently expanded and developed by Boltzmann in 1877 [**?**]. The mathematical distribution function for a monatomic gas in thermal equilibrium is given by the Maxwell-Boltzmann distribution function, M, having the form

$$M(\vec{v}) = n\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{mv^2}{2kT}}, \tag{1}$$

where $\vec{v}$ is the velocity vector, m is the mass, T is the temperature, and k is the Boltzmann constant ($k = 1.3807\times10^{-23}J/K$). The time evolution of the distribution function, F, in the general non-equilibrium case is described as a function of time and location in the six-dimensional phase space through the Boltzmann equation given by

$$\frac{\partial F}{\partial t} + v_i\frac{\partial F}{\partial x_i} + a_i\frac{\partial F}{\partial v_i} = \frac{\delta F}{\delta t}, \tag{2}$$

where F is any general non-equilibrium distribution function, $\frac{\delta F}{\delta t}$ is the time rate of change of the distribution function due to collisions, and x_i, v_i, a_i are the particle position, velocity and acceleration vectors respectively.

3.1 Maxwell's Equation of Change

Macroscopic properties of the gas are essentially expected values of functionals of velocity space $W(\vec{v})$, and can be found by multiplying these functionals with the probability distribution and integrating over velocity space as follows:

$$\psi = \psi(\vec{x}, t) = m\left\langle W(\vec{v})F\right\rangle = m\iiint\limits_{\infty} W(\vec{v})Fd\vec{v}, \tag{3}$$

where ψ is the macroscopic property of interest

The Boltzmann equation also provides a description of the time evolution of the macroscopic moments, and thus their transport behaviour. Moment equations describing the transport of the macroscopic quantities can be obtained by weighting the Boltzmann equation and integrating term by term. Neglecting external forces, the resulting moment equations arising from the Boltzmann equation, Maxwell's equation

of change, can be written as

$$\frac{\partial}{\partial t}(m\langle W(\vec{v})F\rangle) + \frac{\partial}{\partial x_i}(m\langle v_i W(\vec{v})F\rangle) = \Delta\left[mW(\vec{v})F\right], \tag{4}$$

$$\Delta\left[mW(\vec{v})F\right] = m\iiint_{\infty} W(\vec{v})\frac{\delta F}{\delta t}d\vec{v} \tag{5}$$

where $\Delta\left[mW(\vec{v})F\right]$ represents the production and destruction of the moment produced by interparticle collisions. Note that the evaluation of each moment equation requires evaluating its flux i.e. the next higher order moment. This implies that the exact representation of the evolution of the distribution function requires the evaluation of an infinite set of coupled moment equations.

3.2 Moment Methods

The Boltzmann equation (2) in its original form is a non-linear, integro-differential equation with seven independent variables in time, physical space and velocity space. The complexity in solving this equation or its resultant infinite set of coupled moment equations in non-trivial cases has led to the use of approximate solution methods for the Boltzmann equation based on the stipulation of a specific form of the distribution function and approximate expressions for the collision term. The approximate form for the distribution function results in a closing expression for the moment equations.

3.2.1 Collision Term Approximations

In many theoretical studies, the five-dimensional integral expression for the exact collision term is frequently approximated by the Bhatnagar-Gross-Krook (BGK) or relaxation time approximation [**?**]. In this mathematical simplification, the collision term is replaced by the expression

$$\frac{\delta F}{\delta t} = -\frac{F - M}{\tau}, \tag{6}$$

where F is a general phase space distribution, M is the Maxwell-Boltzmann distribution function reached at equilibrium, where both F and M share the same moments, and τ is a relaxation time representative of the collisional processes. For systems with only small perturbations from equilibrium, the simplicity of the BGK approximation makes it an effective tool for modeling the behaviour of the distribution function [**?**].

The BGK approximation enforces a Prandtl number $Pr = 1$ for all flows, whereas considerations towards adding heat transfer terms into the Gaussian closure will require a more flexible Prandtl number. The ellipsoidal statistical model (ES) for the collision operator proposed by Holway [**?**] includes a relaxation time and relaxed distribution dependent on a prescribed Prandtl number while maintaining the simplified form of the BGK model. The model can be expressed as

$$\frac{\delta F}{\delta t} = -\frac{F - G_{ES}}{\tau_{ES}}, \tag{7}$$

where

$$G_{ES}(t, x_i, v_i) = \frac{\rho}{m(2\pi)^{\frac{3}{2}}(\det T_{\alpha\beta})^{\frac{1}{2}}} \exp\left(-\frac{1}{2} T_{ij}^{-1} c_i c_j\right), \quad T_{ij} = (1-\nu)\, RT\delta_{ij} + \nu\Theta_{ij} \tag{8}$$

and ν is a parameter that allows for the control of the Prandtl number via the relation $(1-\nu)Pr = 1$.

3.2.2 10-Moment Gaussian Closure

To resolve the problem of evaluating an infinite number of coupled moment equations, the distribution function can be assumed to have a particular form, where undetermined coefficients associated with this approximate form can be related to a set of velocity moments of interest. In doing so, the highest order moment of interest can be expressed as a function of a set of lower-order moments, thus providing closure for the equation set. Early moment closure hierarchies by Grad [**?**] provide transport equations for non-equilibrium quantities, but are prone to a loss of hyperbolicity even for benign flows and do not guarantee a physically realistic particle distribution function for all flows. More recently, Levermore [**?**] has proposed a hierarchy of maximum-entropy closures that remain hyperbolic with physically realizable solutions, though only the two lowest order members of the hierarchy can be solved for analytically. The 10-moment member of this hierarchy is the Gaussian closure, where the distribution function is assumed to take the form

$$F \approx G(t, x_i, v_i) = \frac{\rho}{m(2\pi)^{\frac{3}{2}}(\det\boldsymbol{\Theta})^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\Theta_{ij})^{-1} c_i c_j\right), \tag{9}$$

where Θ is a symmetric tensor defined by $\Theta_{ij} = P_{ij}/\rho$, P_{ij} is the generalized pressure tensor and ρ is the density. The Gaussian distribution function, G, is a function of the density, velocity and generalized pressure tensor and these may be obtained by solving the set of moment equations arising from Maxwell's equation of change with $F = G$. The moment equations of the Gaussian closure are equivalent to those arising from the Grad 10-moment closure [**?**], and similarly do not take into account heat transfer.

3.3 Extension for Diatomic Gases

The construction of the transport equations up to now have assumed that the gas is composed of monatomic particles with no internal degrees of freedom. Many practical flow applications, however, involve the use of diatomic particles such as atmospheric nitrogen and oxygen. Although at modest temperatures the energy associated with vibrational modes of diatomic particles can still be neglected, the energy of the internal rotational modes is significant and must be accounted for.

The method used by Hittinger [**?**], is used here to account for rotational energy of the two symmetric modes of rotation in a three-dimensional rotational model for the diatomic molecule. The BGK approximation for the source terms is modified to account for an additional relaxation time associated with the rotational degrees of freedom and an additional equation for rotational energy, E_{rot}, is added. The final

set of eleven transport equations in divergence form are then as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k}(\rho u_k) = 0, \tag{10}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k + P_{ik}) = 0, \tag{11}$$

$$\frac{\partial}{\partial t}(\rho u_i u_j + P_{ij}) + \frac{\partial}{\partial x_k}(\rho u_i u_j u_k + u_k P_{ij} + u_j P_{ik} + u_i P_{jk}) = -\frac{3P_{ij} - P_{kk}\delta_{ij}}{3\tau_t} - \frac{2\left(P_{kk} - 3E_{rot}\right)}{15\tau_r}\delta_{ij} \tag{12}$$

$$\frac{\partial E_{rot}}{\partial t} + \frac{\partial}{\partial x_k}(u_k E_{rot}) = -\frac{3E_{rot} - P_{kk}}{5\tau_r}, \tag{13}$$

where the time scale, τ_t, is sufficient for some non-equilibrium distribution, G_D, to relax to F_D whereupon the particles are in translational equilibrium, but their rotational degrees of freedom are not in equilibrium. The rotational time scale, τ_r, relaxes this intermediate state to complete equilibrium in both translational and rotational degrees of freedom representative of the Maxwell-Boltzmann distribution, M_D.

3.4 Incorporating Heat Transfer via Regularization Procedure

Due to the assumed form of the particle distribution function given in (9), the third-order velocity moment, $m < c_i c_j c_k G >$, corresponding to a heat flux tensor, Q_{ijk}, for the Gaussian closure involves an integration over an odd function and is identically zero. The term appears in the energy equation in the equation set (12) as $\frac{\partial Q_{ijk}}{\partial x_k}$, but its value of zero eliminates the energy equation's dependence on a higher order moment, and a natural closure for system is achieved. While mathematically convenient, this poses a serious problem in attempting to apply the Gaussian closure for micro-scale flows where heat transfer is of utmost importance.

A regularization procedure developed by Struchtrup and Torrilhon [**?**] for Grad's 13 moment system, and extended on by McDonald and Groth [**?**] [**?**] for the Gaussian closure is used here to incorporate the heat transfer terms. The regularization procedure is based on a perturbative expansion technique applied either to the kinetic or the moment equation themselves. After forming the transport equation for the heat flux tensor and focusing only on the first-order deviations, the thermal-diffusion corrected energy equation becomes

$$\frac{\partial}{\partial t}(\rho u_i u_j + P_{ij}) + \frac{\partial}{\partial x_k}(\rho u_i u_j u_k + u_k P_{ij} + u_j P_{ik} + u_i P_{jk} + Q^{(1)}_{ijk}) = -\frac{3P_{ij} - P_{kk}\delta_{ij}}{3\tau_t} - \frac{2\left(P_{kk} - 3E_{rot}\right)}{15\tau_r}\delta_{ij}$$

where

$$Q^{(1)}_{ijk} = -\frac{\tau}{\mathrm{Pr}}\left[P_{kl}\frac{\partial}{\partial x_l}\left(\frac{P_{ij}}{\rho}\right) + P_{jl}\frac{\partial}{\partial x_l}\left(\frac{P_{ik}}{\rho}\right) + P_{il}\frac{\partial}{\partial x_l}\left(\frac{P_{jk}}{\rho}\right)\right] \tag{14}$$

4 Finite Volume Solution Method

Work by McDonald and Groth [**?**] in previous studies has successfully applied the Gaussian closure to two-dimensional micro-channel flows, where a finite-volume method with AMR was developed and used

to solve the moment equations. In this thesis, a finite-volume scheme with block-based AMR is used in a similar fashion for application to three-dimensional non-equilibrium micro-channel flows. For the three-dimensional case, a multi-block body-fitted mesh with hexahedral cells will be used in place of the quadrilateral cells used in the two-dimensional code. The hyperbolic fluxes at cell boundaries will be evaluated using a Riemann-solver based flux function by Roe, though an HLLE solver is also implemented. A Newton-Krylov-Schwarz (NKS) algorithm implemented for two and three-dimensional Navier-Stokes equations by Charest, Groth and Gülder [**?**] and Northrup and Groth [**?**] will be employed for steady-state solutions and unsteady solutions as well using a dual-time stepping method. The formulation of the elliptic heat transfer term additions to the closure suitable for application to the NKS algorithm will be investigated.

4.1 Newton-Krylov-Schwarz Solver

The NKS solution algorithm for the set of non-linear algebraic equations that result from the spatial and temporal discretization procedures uses Newton's method with a Krylov subspace approach for the solution of the linear system at each Newton step. An additive Schwarz preconditioner is used in the parallel implementation of the Krylov subspace method, and is fully compatible with the block-based AMR and domain decomposition procedure used in the parallel implementation of the solution method.

4.1.1 Newton's Method

For steady state solutions (the focus of the discussion here), at any iteration n, a residual vector $\mathbf{R}(\mathbf{U}^n)$ can be computed using the newly-computed solution vector. A steady state solution can be found by driving this residual vector to zero. Since this is only solution of interest, the semi-discrete form of the equations can be relaxed by using Newton's nonlinear solver. For a residual vector at time level n, the residual vector at time level $n+1$ can be subjected to a first-order Taylor series expansion and set to zero representative of a steady-state solution. A system of linear equations can be formed describing the change in the solution vector required.

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)^n \Delta \mathbf{U}^n = \mathbf{J}\left(\mathbf{U}^n\right) \Delta \mathbf{U}^n \approx -\mathbf{R}\left(\mathbf{U}^n\right) \tag{15}$$

The nonlinear system of equations has now been reduced into a linear one, which is then subjected to the following acceleration techniques to further reduce the computational cost of the model.

4.1.2 Krylov Subspace Linear Solver

Krylov subspace methods focus on the solution to linear systems of the form

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{16}$$

where $\mathbf{x} = \Delta\mathbf{U}^n$, $\mathbf{b} = -\mathbf{R}(\mathbf{U}^n)$ and $\mathbf{A} = \mathbf{J}(\mathbf{U}^n)$. A Krylov subspace for this non-singular system is a linear subspace defined as

$$\mathrm{K}_j(\mathbf{A}, \mathbf{b}) = \mathrm{span}\left\{\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, ..., \mathbf{A}^{j-1}\mathbf{b}\right\} \tag{17}$$

The usefulness of this subspace comes from the fact that the solution to the linear system lies somewhere within it. The Krylov method used in this thesis is the Generalized Minimum Residual Method (GMRES), which will define the spanning vectors and initiate a search through this subspace for a solution vector $\mathbf{z}$ that solves $\min_{\mathbf{z}\in\mathrm{K}_j(\mathbf{A},\mathbf{b})} \|\mathbf{b} - \mathbf{A}\mathbf{z}\|$.

GMRES constructs a set of orthonormal basis vectors for the Krylov subspace using Arnoldi's method, which in turn is an extension of the Gram-Schmidt process adapted to Krylov subspaces. Starting with the normalized vector $\mathbf{v}_1 = \mathbf{b}$, each iteration j through the Arnoldi algorithm recursively builds an orthonormal basis vector, $\mathbf{v}_{j+1}$, by a matrix-vector multiplication of the matrix $\mathbf{A}$ and the basis vector generated in the previous iteration, $\mathbf{A}^{j-1}\mathbf{b}$. Upon completion of the algorithm, a vector of the computed basis vectors, $\mathbf{V}_{j+1}$, and a Hessenberg matrix, $\mathbf{H}_j$, consisting of conjugate transpose multiplications used in the basis vector calculations can be be extracted. The decomposition process for each Arnoldi method iteration can be written as

$$\mathbf{A}\mathbf{V}_j = \mathbf{V}_{j+1}\mathbf{H}_j \tag{18}$$

with

$$\mathbf{V}_{j+1} = \begin{pmatrix}\mathbf{V}_j & \mathbf{v}_{j+1}\end{pmatrix}, \quad \mathbf{H}_j = \begin{pmatrix}\mathbf{H}_{j-1} & \mathbf{h}_j \\ 0 & \|\hat{\mathbf{v}}_{j+1}\|\end{pmatrix} \tag{19}$$

where $\|\hat{\mathbf{v}}_{j+1}\|$ is the magnitude of the non-normalized basis vector $\mathbf{v}_{j+1}$. The solution vector $\mathbf{z}$ is by definition a member of the Krylov subspace $\mathrm{K}_j(\mathbf{A}, \mathbf{b})$ and thus can be written as a linear combination of the orthonormal basis vectors as $\mathbf{z} = \mathbf{V}_j\mathbf{y}$, where $\mathbf{y}$ is some vector. With this relation, the minimization problem can be rewritten with

$$\mathbf{A}\mathbf{z} = \mathbf{A}(\mathbf{V}_j\mathbf{y}) = (\mathbf{V}_{j+1}\mathbf{H}_j)\mathbf{y}, \quad \mathbf{b} = \|\mathbf{b}\|\mathbf{v}_1 = \|\mathbf{b}\|\mathbf{V}_{j+1}\mathbf{e}_1 \tag{20}$$

$$\min_{\mathbf{z}\in\mathrm{K}_j(\mathbf{A},\mathbf{b})} \|\mathbf{b} - \mathbf{A}\mathbf{z}\| = \min_{\mathbf{y}} \|\|\mathbf{b}\|\mathbf{V}_{j+1}\mathbf{e}_1 - \mathbf{V}_{j+1}\mathbf{H}_j\mathbf{y}\| = \min_{\mathbf{y}} \|\|\mathbf{b}\|\mathbf{e}_1 - \mathbf{H}_j\mathbf{y}\| \tag{21}$$

where $\mathbf{e}_1$ is the first column of the identity matrix. Once the minimized vector $\mathbf{y}$ is obtained, the updated approximate solution is then found as $\mathbf{x}_j = \mathbf{V}_j\mathbf{y}$.

Additional iterations of the GMRES algorithm will expand the number of basis vectors in the Krylov subspace until $j = N$, wherein the exact solution of the system (16) will be found. but searching through the entire Krylov subspace can be computationally expensive. Krylov methods in general are instead used as iterative methods to accelerate solution convergence by prematurely terminating the number of iterations under two conditions: a limited number iterations $m < N$ as specified by the user, or if the residual norm $\|\mathbf{b} - \mathbf{A}\mathbf{x}\|$ is sufficiently small. In a restarted GMRES algorithm, also known as GMRES(m), computational improvements can be seen if modifications are made to the linear system to encourage an

accurate approximation within a small number of iterations, m.

4.1.3 Schwarz Preconditioning

Preconditioning a system of equations is any type of implicit or explicit modification done to a linear system that will make it easier to solve. Saad and Schultz [**?**] have shown that the size of the Krylov subspace is dependent on the minimal polynomial of $\mathbf{A}$. This phenomenon suggests that preconditioning the matrix into a more diagonal form has the potential to reduce the size of the searched subspace. Highly scalable parallel algorithms have been developed with this technique by Charest, Groth and Gülder [**?**] for the solution of radiative heat transfer and by Northrup and Groth [**?**] for unsteady laminar flames.

A right-preconditioning, additive Schwarz scheme is applied to the linear system in the form

$$\left(\mathbf{J}\mathbf{M}^{-1}\right)\left(\mathbf{M}\mathbf{x}\right) = \mathbf{b} \tag{22}$$

where $\mathbf{M}$ is the preconditioning matrix. An additive Schwarz global preconditioner is a domain decomposition method where the solution in each subdomain is updated only when the cycle of updates is completed for all subdomains. The domain decomposition aspect of the additive Schwarz and the independence of subdomain communication during temporal updates is exactly what is used in the parallel, block-based AMR scheme. A further block incomplete lower upper (BILU) local preconditioner is used in each subdomain as described by Saad [**?**]. The preconditioner with both global Schwarz and local BILU can be written in the form

$$\mathbf{M}^{-1} = \sum_{k=1}^{N_b} \mathbf{B}_k^T \mathbf{M}_k^{-1} \mathbf{B}_k \tag{23}$$

where N_b is the number of blocks, and $\mathbf{B}_k$ is a gather operator matrix for the k^{th} block, with the BILU preconditioning appearing in the local preconditioner, $\mathbf{M}_k$. Small overlaps between subdomains can be performed by a suitable exchange of data between blocks to increase the overall implicitness of the scheme, but care must be made to ensure that the cost of computing the preconditioner does not exceed the cost of not using a preconditioner at all.

Solving the right-preconditioned system in (22), the matrix-vector product $\mathbf{J}\mathbf{M}^{-1}\mathbf{x}$ is required. Numerical differentiation based on Fréchet derivatives yields an approximation to this product as

$$\mathbf{J}\mathbf{M}^{-1}\mathbf{x} \approx \frac{\mathbf{R}\left(\mathbf{U} + \varepsilon\mathbf{M}^{-1}\mathbf{x}\right) - \mathbf{R}\left(\mathbf{U}\right)}{\varepsilon} \tag{24}$$

where ε is a small scalar quantity representing a small perturbation in the solution state. The value for ε used here is derived from Neilsen *et al.* [**?**], and is presented as $\varepsilon = \varepsilon_o / \left\|\mathbf{x}\right\|_2^{1/2}$, where $\varepsilon_o \approx 10^{-8} - 10^{-7}$. Using this expression, the GMRES algorithm does not require an explicit definition of a global Jacobian $\partial\mathbf{R}/\partial\mathbf{U}$.

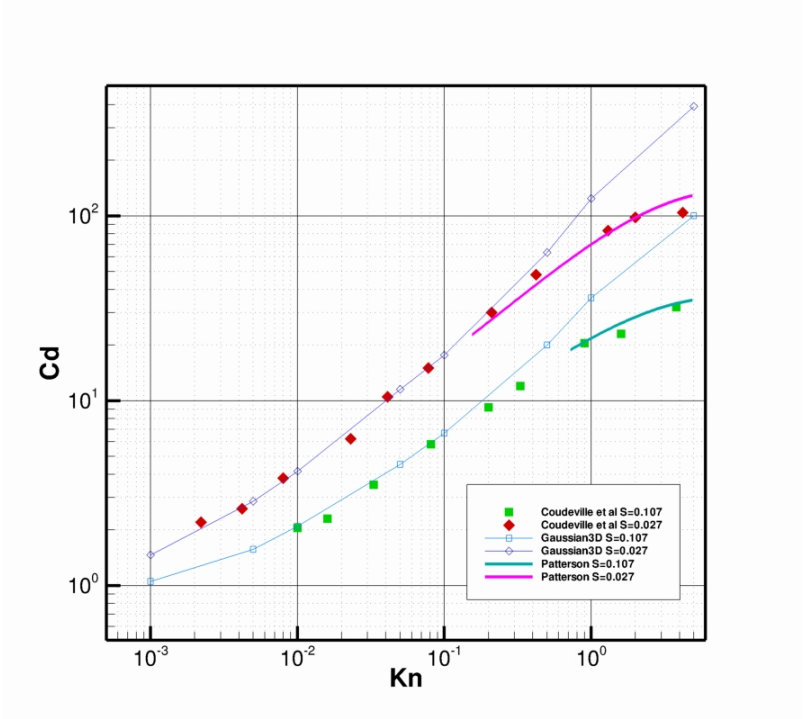


Figure 1: Drag coefficient for varying Knudsen numbers at two speed ratios: Gaussian closure vs. experimental results.

5 Preliminary Numerical Results and Validation

Preliminary results for a number of test flow problems have been computed using the Gaussian closure without heat transfer effects. The flow problems considered are useful in assessing the validity of the closure and solution method for predicting gaseous flows in both the continuum and transitional regimes. Results for three-dimensional subsonic immersed flow over a cylinder, flat plate boundary layer flow and Couette flow are shown in what follows.

5.1 Flow Past an Immersed Cylinder

The drag coefficient on a cylinder in immersed flow is plotted against the Knudsen number in Figure 1 for two different speed ratios S. The Gaussian closure is shown to be successful in duplicating experimental results by Coudeville *et al.* [**?**] in both the continuum and transition regimes, and is also in agreement with an analytical free-molecular solution by Patterson [**?**], though the over-predicted drag in the free-molecular region may be due to the lack of heat transfer terms. Velocity profiles shown in Figure 3 over continuum, transitional and free-molecular regimes show a clear separation of the flow with a recirculation area in the wake of the cylinder in the continuum regimes, and an increase in the boundary layer thickness and flow attachment with increasing Knudsen number as predicted by the larger mean free paths in kinetic theory.

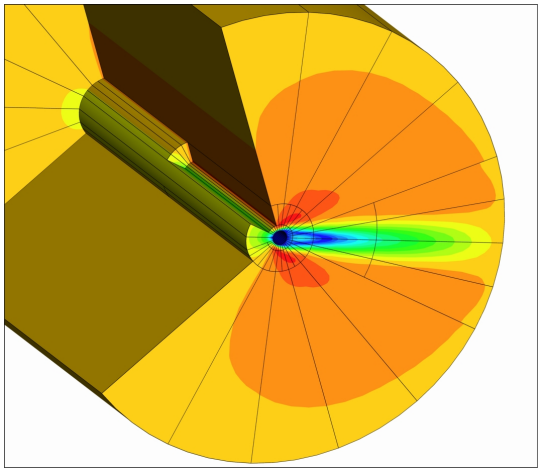
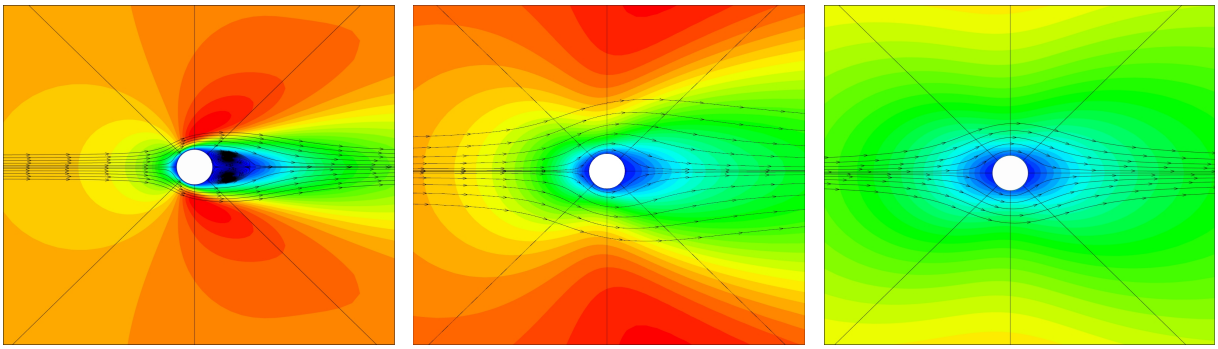


Figure 2: A cutaway view of the two hundred eighty-eight radial mesh blocks created by the AMR algorithm for immersed cylinder flow in the continuum regime with Mach number contours, showing refined block structure at the surface of the cylinder and in the downstream regions



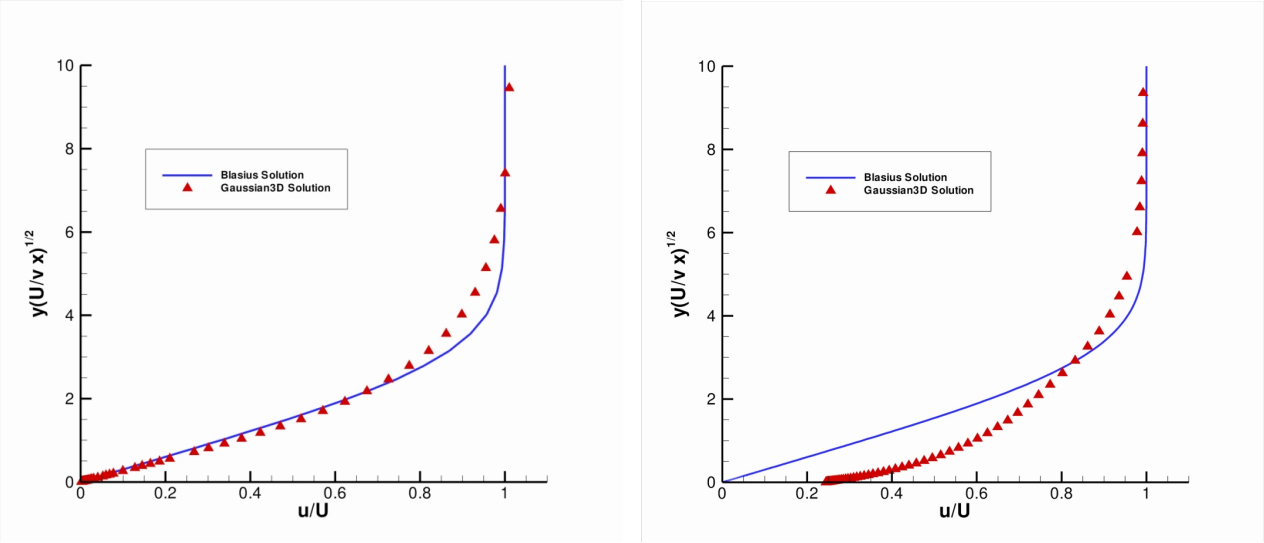
(a) (b) (c)

Figure 3: Comparison of x-directional velocity profile for immersed cylinder flow for various Knudsen numbers (a) $Kn = 1 \times 10^{-3}$, (b) $Kn = 1 \times 10^{-1}$, (c) $Kn = 1$.

5.2 Flat Plate Boundary Layer Development

The Gaussian closure's ability to model slip flows and its effect on the boundary layer is shown here through the modeling of boundary layer development over a flat plate. Figure 4 compares the boundary layer profiles between the Knudsen number-independent Blasius solution [**?**] and solutions from the continuous ($Kn = 2.6 \times 10^{-5}$) and transition regimes ($Kn = 2.6 \times 10^{-1}$). Blasius proposed a relation between a non-dimensionalized velocity u/U normalized to the free stream velocity, U, and a non-dimensional number $y\sqrt{\frac{U}{\nu x}}$ relating to the development of the boundary layer at a certain position above the plate. These non-dimensionalized numbers are calculated for both the continuous and transitional case for comparison purposes.

The continuum result from the Gaussian closure matches closely with the Blasius approximation with a zero slip velocity at the wall, while a transitional regime solution clearly shows a non-zero velocity at the



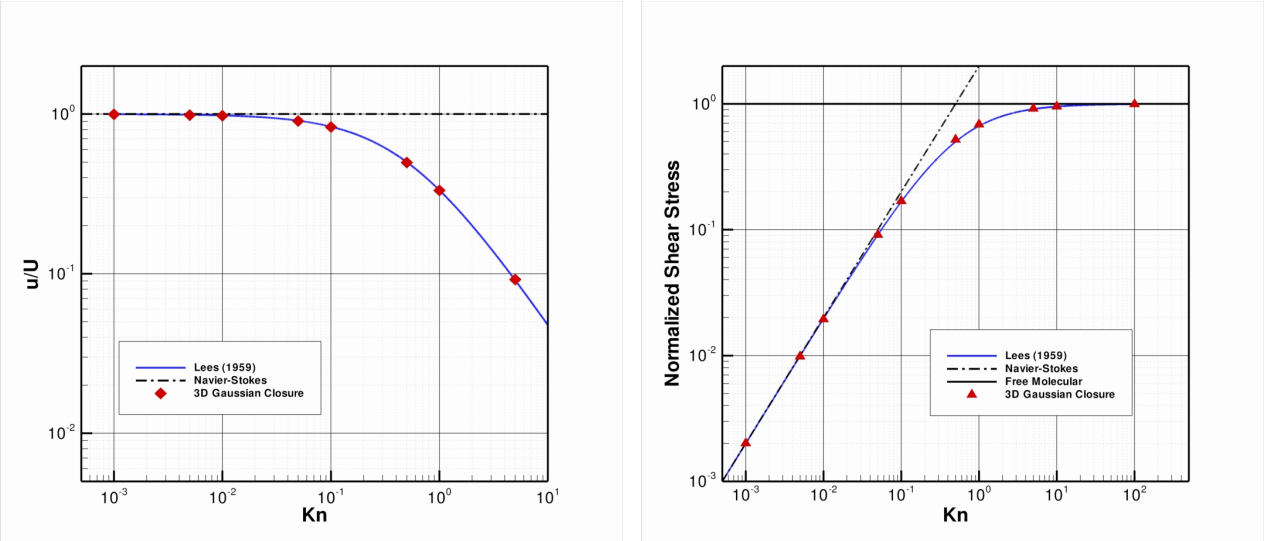
(a) (b)

Figure 4: Flat plate normalized velocity distribution in developing boundary layer at varying Knudsen numbers (a) Continuum Regime, $Kn = 2.6 \times 10^{-5}$, (b) Transition Regime, $Kn = 2.6 \times 10^{-3}$.

wall. The ability to model slip flow effects without changing the boundary conditions of the problem is a powerful tool that the Gaussian closure can provide.

5.3 Planar Couette Flow

Planar Couette flow is studied here to illustrate the Gaussian closure's ability to model boundary layer and shear stress evolution in various flow regimes. For this particular problem, the two plates are moving at 30 m/s in opposite directions in argon at 288k in standard pressure, and the setup is extruded in the z direction. Figure 5(a) shows the non-dimensionalized velocity $\frac{u}{U}$, where u is the fluid velocity at the wall and U is the wall velocity, versus the Knudsen number based on the separation of the two plates. The continuum solution using the Navier-Stokes equations with no extra treatment for slip flows calculates the fluid velocity at the wall to be equal to the velocity of the wall regardless of Knudsen number. The free molecular solution generates an infinite slip velocity at the wall, with the fluid velocity at the wall equal to zero for all flows. Lees solution (1959) [**?**] provides an analytical solution to this problem that predicts the slip velocity and shear stress at the wall, gradually transitioning from the continuum result to the free-molecular. The Gaussian solution is capable of modeling the formation of a slip velocity and follows Lees solution closely for a wide range of Knudsen numbers. The shear pressure profile for the same problem can be seen in Figure 5(b). For comparison purposes, the shear stresses are normalized to the free molecular solution as $\frac{\tau_{xy}}{\rho U \sqrt{\frac{2kT}{\pi m}}}$. Use of the continuum formulation predicts an ever-increasing shear stress with increasing Knudsen number, while the free-molecular shear stress remains constant regardless of Knudsen number. The Gaussian solution predicts a smooth transition between the continuum and



(a) (b)

Figure 5: (a) Normalized fluid velocity at the wall vs. Knudsen number. Note that the free-molecular solution gives $u = 0$ at the wall regardless of Knudsen number, (b) Normalized shear stress at the wall vs. Knudsen number.

free-molecular solutions and is in close agreement with the analytical solution by Lees.

6 Summary of Progress to Date and Future Work

6.1 Progress to Date

Task	Completion Date
Completion of 3D Gaussian moment closure code	October 2010
Completion of models for 3D Gaussian closure: immersed cylinder, flat plate boundary layer, couette	December 2010
Learning Newton-Krylov-Schwarz mathematical foundations	January 2011
Preliminary testing for immersed cylinder applied on NKS, no heat transfer	January 2011
Derivation of heat transfer terms for Gaussian closure	March 2011

6.2 Future Work

Task	Completion Date
Learning heat transfer incorporation into Gaussian closure and computational effects on solution	April 2011
Convective Heat Transfer (MIE1212); heat transfer for internal and external flows, developing boundary conditions, final paper	April 2011
Introduction to Modern Flow Control (AER1308); turbulence models, flow control techniques, final paper	April 2011
2D Gaussian moment closure code: example analysis for heat transfer effects, application towards 3D code	May 2011
AIAA Conference paper/presentation: NKS solver applied to Gaussian closure without heat transfer effects	June 2011
Adapting 3D Gaussian moment closure code for other mesh geometries	August 2011
Incorporation of heat transfer terms in 3D Gaussian moment closure code, testing and validation, comparison with experimental results	January 2012
Investigation of alternate regularization methods and their effect on computational time and accuracy	June 2012
Thesis write-up	March 2014

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