2011

Unsteady 3D Rarefied Flow Solver Based on Boltzmann-ESBGK Model Kinetic Equations

Sruti Chigullapalli
Purdue University

Alina A. Alexeenko
Purdue University - Main Campus, alexeenk@purdue.edu

Follow this and additional works at: <http://docs.lib.purdue.edu/aaepubs>

Part of the [Engineering Commons](#)

Recommended Citation

Chigullapalli, Sruti and Alexeenko, Alina A., "Unsteady 3D Rarefied Flow Solver Based on Boltzmann-ESBGK Model Kinetic Equations" (2011). *School of Aeronautics and Astronautics Faculty Publications*. Paper 24.
<http://dx.doi.org/10.2514/6.2011-3993>

This document has been made available through Purdue e-Pubs, a service of the Purdue University Libraries. Please contact epubs@purdue.edu for additional information.

Unsteady 3D Rarefied Flow Solver Based on Boltzmann-ESBGK Model Kinetic Equations

Sruti Chigullapalli*, and Alina Alexeenko†

School of Aeronautics & Astronautics, Purdue University, West Lafayette, IN 47907

Formulation and verification of unsteady rarefied flow solver based on Boltzmann-ESBGK equations in arbitrary three-dimensional geometries is presented. The solver is based on the finite volume method in physical space and the discrete ordinate method in velocity space with an implicit time discretization. Verification is carried out for an unsteady approach to equilibrium, a steady one-dimensional Couette flow and a two-dimensional quasi-steady gas damping problem. Finally, the application of the full 3D parallel solver is considered to simulate unsteady microscale gas damping in a micro-electro-mechanical system switch.

I. Introduction

Further development of high-frequency microsystems such as resonators, RF MEMS, microturbines and pulsed-detonation microengines require improved understanding of unsteady rarefied gas dynamics at the microscale. Accurate computational simulation of such flows demands new approaches beyond the conventional formulations based on the macroscopic constitutive laws. This is due to the breakdown of the continuum hypothesis in the presence of significant non-equilibrium and rarefaction because of the large gradients and small scales, respectively.

The limits on the continuum gas-flow models are determined based on the Knudsen number, $Kn = \lambda/L$, where λ is the molecular mean free path and L is the characteristic length scale. Flow simulations based on the Navier-Stokes equations with the no-slip boundary conditions are typically accurate for $Kn < 0.01$. For flows at large Knudsen numbers, a widely used numerical approach is to solve the Boltzmann equation by stochastic simulations using the direct simulation Monte Carlo (DSMC) method. However, the DSMC method becomes prohibitively expensive for low-speed and unsteady flows because the probabilistic nature of DSMC also leads to noise charged solutions.

In general, the motion of molecules in a dilute gas is described by the kinetic Boltzmann equation which is valid for arbitrary Knudsen numbers. However, due to the multidimensionality of the phase space, numerical solution of the Boltzmann equation is very expensive in terms of computational time, especially due to the quadratic cost of the velocity discretization of the collision operator. An alternative approach that allows to reduce the computational cost is to consider simplified models of the collision relaxation integral term in the Boltzmann equation.

One of the widely used model equations is the Bhatnagar-Gross-Krook (BGK) equation. The phase density $f(x_i, t, c_j)$ is governed by

$$\frac{\partial f}{\partial t} + c_x \frac{\partial f}{\partial x} + c_y \frac{\partial f}{\partial y} + c_z \frac{\partial f}{\partial z} = S \quad (1)$$

The BGK equation with its relaxation type collision term $S = -\nu(f - f_\gamma)$ is easier to solve because of the more compact form of the integrals over the velocity space. It also satisfies the Boltzmann H-theorem which states that the production of entropy is always non-negative and gives a Maxwellian distribution at

*Graduate Student, AIAA Student Member.

†Assistant Professor, AIAA Senior Member.

equilibrium.

A version of BGK-type collision relaxation model is the ellipsoidal-statistical model (ESBGK) where f_γ in Eq. (1) is replaced by an anisotropic Gaussian. It has been suggested by Holway¹ as a model that can overcome a limitation of BGK on the fixed Prandtl number. This model can reproduce transport coefficients, corresponding to arbitrary Prandtl numbers (Pr) while the standard BGK model gives a $Pr = 1$. A two-dimensional explicit ESBGK solver was developed in Ref.² and it was shown that Boltzmann model equations can provide a practical modeling framework for a wide range of Knudsen numbers. For a recent review of ESBGK approach and applications please see Ref.³ and references therein. With the advent of petascale computing platforms, it becomes practical to solve full three-dimensional rarefied flow problems using the ESBGK equations.

The ESBGK solver presented here is built into the multiphysics finite-volume solver within MEMOSA (MEMS Overall Simulation Administrator) simulation platform. MEMOSA is developed as part of the PRISM project (NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems) at Purdue University and a detailed description of the general finite volume solver in MEMOSA has been given by Mathur et. al.^{4,5} The computationally-intensive kernels are written in a compiled language (C++) while the driving logic, parameter setting and user interfaces are implemented in Python. All the creation and manipulation of objects, invocation of methods on them, and coupling between different components is then controlled from the interpreter through scripts.

A great advantage of the deterministic solution of kinetic equations is the possibility of direct coupling to other deterministic solvers. The common MEMOSA base ensures that no unnecessary translations and copying of data occurs while exchanging data between the two individual components. Therefore, it can be coupled with the well-known continuum equations to make a hybrid solver that solves the Navier-Stokes Equations in regions of equilibrium and the Boltzmann kinetic equations in regions of non-equilibrium.

The objective of this paper is to present the formulation and verification of the ESBGK solver in MEMOSA for unsteady and multidimensional problems. The remainder of the paper is organized as follows: In Section 2, we describe in detail the numerical method including physical and velocity space discretization, implementation of boundary conditions, algebraic multigrid solver and the conservative discretization of the collision term. Section 3 presents results from various verification tests for time discretization, diffuse-specular wall boundary and a 2d microscale damping problem. In section 4, we present some preliminary results for a full 3d damping problem and parallel performance of the solver.

II. Numerical Modeling Approach

The ESBGK solver consists of a finite volume method in physical space and discrete ordinate method in velocity space. The formulation of the conservative numerical method for the ESBGK equation with the implicit time integration is presented in this section.

II.A. Velocity Space Discretization

The velocity space discretization is implemented using both Cartesian type and spherical type meshes as shown in Fig. 1. The Cartesian type consists of discretization of c_x with uniform velocity abscissas $\tilde{c}_x(j_1) = \tilde{c}_{x,min} + (j_1 - 1)\Delta\tilde{c}_x$ where $\Delta\tilde{c}_x = \frac{(\tilde{c}_{max} - \tilde{c}_{min})}{N_1 - 1}$. The velocities c_y and c_z are discretized in a similar manner. It is to be noted that velocity is non-dimensionalized by $\sqrt{2RT}$ where R is the universal gas constant and T is the reference temperature. The spherical type consists of a 16th order Gauss-Hermit quadrature⁶ in velocity magnitude and both 3/8th rule and constant interval in angles. The velocity is then stored as an array of vectors, where $\vec{c}_j = (c_x, c_y, c_z)_j$ is the j^{th} element in the array. From here on, the subscript j will be dropped when referring to individual components of the vector $\vec{c}_j$ and will be referred to as c_x, c_y, c_z . Extents of the velocity domain $c_{max} = 7.5, 10.5$ were used in discretization of velocity mesh for all simulations in this paper. The macroparameters such as density, velocity and temperature are then calculated as:

$$\begin{aligned}
\rho &= \sum_j f_j w_j \\
\rho u &= \sum_j c_x f_j w_j \\
\rho v &= \sum_j c_y f_j w_j \\
\rho w &= \sum_j c_z f_j w_j \\
\frac{3}{2} \rho T &= \sum_j ((c_x - u)^2 + (c_y - v)^2 + (c_z - w)^2) f_j w_j
\end{aligned}$$

where w_j is the weight associated with the j^{th} ordinate in velocity space.

Figure 1. Velocity meshes a)Cartesian b)Gauss-Hermite.

II.B. Physical Space Discretization

The discretization in the physical space is based on arbitrary finite volume meshes. CuBit and Gambit were used to create the various meshes for the different tests. The solver has the capability to read in a Fluent cas file and the mesh partitioner automatically partitions the mesh.

The ESBGK equation for each velocity ordinate (1), upon discretization can be written in the form:

$$a_p f_p^{n+1} + \sum a_{nb} f_{nb}^{n+1} + S(f^n) = 0 \quad (2)$$

$$a_p f_p^n + \sum a_{nb} f_{nb}^n + S(f^n) = R_p^n \quad (3)$$

where superscript n corresponds to values from previous iteration, a_p is the coefficient of the p^{th} cell and a_{nb} are coefficients of the neighboring cells of p . S is the source term which is a function of f_γ , f from previous iteration and time levels respectively. The residual in each cell is R_p . Combining these two equations we get

$$a_p (f_p^{n+1} - f_p^n) + \sum a_{nb} (f_{nb}^{n+1} - f_{nb}^n) + R_p^n = 0 \quad (4)$$

Writing in to compact form

$$A \delta f + R = 0 \quad (5)$$

$$\delta f = f^{n+1} - f^n \quad (6)$$

An algebraic multigrid solver (AMG)^{5,7} is used for the solution of these linearized equations.⁴ Details for discretization of the convection term, algorithm for implementation of Dirichlet and Neumann conditions can found in Ref.⁴ The only difference for convection discretization formulation for the ESBGK equations is that the flux would be $(\vec{c}_j \cdot \vec{n})$ where n is the normal vector to the face. In the following section we

will describe the discretization of the time derivative and the collision terms only. Starting with the simple space-homogeneous equation

$$\frac{\partial f}{\partial t} = -\nu(f - f_\gamma) \quad (7)$$

On discretization gives

$$\frac{f^k}{\Delta t} - \frac{f^{k-1}}{\Delta t} + \nu(f^k - f_\gamma^k) = 0 \quad (8)$$

where k is the current time step and $k-1$ is the converged solution from the previous time-step. It is to be noted that for every time step we perform a certain number of iterations by updating the equilibrium distribution function and the linear system of equations. To avoid confusion between solutions at different time-steps and solutions at different iterations for the current time-step, let $x_{N1} = f^{k-1}$ which is a known value from previous time level and $x = f^k$ which is the solution at current time. The equations at $n+1^{th}$ and n^{th} iterations can then be written as

$$x^{n+1}(\frac{1}{\Delta t} + \nu) - (\frac{x_{N1}}{\Delta t} + \nu x_\gamma) = 0 \quad (9)$$

$$x^n(\frac{1}{\Delta t} + \nu) - (\frac{x_{N1}}{\Delta t} + \nu x_\gamma) = R^n \quad (10)$$

Combining the two equations,

$$(\frac{1}{\Delta t} + \nu)(x^{n+1} - x^n) + R^n = 0 \quad (11)$$

This is of the form $A\delta x + R = 0$ where the diagonal term of matrix A and the residual are as follows:

$$A_{ii} = -\frac{1}{\Delta t} - \nu \quad (12)$$

$$R = -\frac{1}{\Delta t}(x - x_{N1}) - \nu(x - x_\gamma) \quad (13)$$

II.C. Conservative Discretization of the Collision Term

Following the discrete velocity approach suggested by Mieussens,⁸ the function $f_\gamma(x_i, t_k, c_j)$ for the BGK type equilibrium equation is chosen in the form

$$f_\gamma = \alpha_1 e^{\beta \cdot \mathbf{p}} \quad (14)$$

$$\beta = [-\alpha_2, \alpha_3, \alpha_4, \alpha_5] \quad (15)$$

$$\mathbf{p} = [((c_x - u)^2 + (c_y - v)^2 + (c_z - w)^2), (c_x - u), (c_y - v), (c_z - v)]^T \quad (16)$$

The coefficients (α s) can be found from the discretized versions of the following conservation equations: $\int mS \, dc = 0$, $\int mc_x S \, dc = 0$, $\int mc_y S \, dc = 0$, $\int mc_z S \, dc = 0$, $\int m((c_x - u)^2 + (c_y - v)^2 + (c_z - w)^2)S \, dc = 0$ where $S = (f - f_\gamma)$ is the collision term. The discrete set of mass, x-momentum, y-momentum, z-momentum and energy conservation equations shown below are solved iteratively using the Newton's method.

$$\begin{aligned} \sum_j f_\gamma w_j &= \rho \\ \sum_j c_x f_\gamma w_j &= \rho u \\ \sum_j c_y f_\gamma w_j &= \rho v \\ \sum_j c_z f_\gamma w_j &= \rho w \\ \sum_j (c_x^2 + c_y^2 + c_z^2) f_\gamma w_j &= \rho(u^2 + v^2 + w^2) + \frac{3}{2}\rho T \end{aligned}$$

Similarly, letting $c'_x = c_x - u$, $c'_y = c_y - v$, $c'_z = c_z - w$, the ES-BGK type equilibrium equation is of the form

$$f_\gamma = \alpha_1 e^{\beta \cdot \mathbf{p}} \quad (17)$$

$$\beta = [-\alpha_2, \alpha_3, -\alpha_4, \alpha_5, -\alpha_6, \alpha_7, \alpha_8, \alpha_9, \alpha_{10}] \quad (18)$$

$$\mathbf{p} = [(c'_x)^2, c'_x, (c'_y)^2, c'_y, (c'_z)^2, c'_z, c'_x c'_y, c'_x c'_z, c'_y c'_z]^T \quad (19)$$

Now there are 10 unknowns here and in addition to the conservation of mass and x, y, z-momentum equations, the following six conservation equations are used:

$$\begin{aligned} \sum_j c_x^2 f_\gamma w_j &= \rho(u^2 + T_{xx}) \\ \sum_j c_y^2 f_\gamma w_j &= \rho(v^2 + T_{yy}) \\ \sum_j c_z^2 f_\gamma w_j &= \rho(w^2 + T_{zz}) \\ \sum_j c_x c_y f_\gamma w_j &= \rho(uv + T_{xy}) \\ \sum_j c_y c_z f_\gamma w_j &= \rho(vw + T_{yz}) \\ \sum_j c_z c_x f_\gamma w_j &= \rho(wu + T_{zx}) \end{aligned}$$

where normal components are $T_{xx} = \frac{1}{\rho} \sum_j (c_x - u)^2 \left((1 - \frac{1}{Pr}) f_j + \frac{1}{Pr} f_{\gamma j, BGK} \right) w_j$ and the cross-terms are $T_{xy} = \frac{1}{\rho} \sum_j (c_x - u)(c_y - v) \left((1 - \frac{1}{Pr}) f_j + \frac{1}{Pr} f_{\gamma j, BGK} \right) w_j$. Pr is the Prandtl number and $f_{\gamma, BGK}$ is the BGK equilibrium distribution function. A tolerance limit of 10^{-14} in the calculation of α_i has been used with a Gaussian inversion for the Jacobian matrix. Further details can be found in Ref.²

II.D. Collision Frequency

The collision frequency in the non-dimensional form is

$$\nu = \begin{cases} \frac{P}{\mu} & BGK \text{ Model} \\ Pr \frac{P}{\mu} & ES-BGK \text{ Model} \end{cases} \quad (20)$$

where $P = \rho T$ is the non-dimensional pressure and viscosity is calculated from power-law $\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)$ with μ_{ref}, T_{ref}, w given by Bird.⁹ Note that the collision frequency is independent of the microscopic velocity, which might pose a limitation on the validity of this collision model for highly non-uniform flows.⁸

II.E. Boundary Conditions

Five different types of boundary conditions are incorporated into the solver. The first one is a fairly simple one called ‘ZeroGradBC’ which corresponds to no gradient in functional values and macroscopic properties. Two important boundary conditions are the fully diffuse wall boundary, used in the simulation of a moving wall for the Couette flow and the symmetry boundary, used to reduce the size of the computational domain. The solver also has the capability for specular-diffuse wall with given accommodation coefficient and far pressure inlet/outlet boundaries. For each boundary condition, the boundary distribution function is calculated and stored in the ghost-boundary cell. Finally for each linear system in the velocity space, Dirichlet and extrapolation type of boundary conditions are applied for incoming and outgoing directions respectively. The equations that follow are applicable to a boundary oriented in any arbitrary direction.

II.E.1. Symmetry boundary

The values of f incoming to the surface are flipped to include a reflection from the boundary. During initialization, a map of incident and reflected directions $[j_i, j_r]$ is created for each symmetry boundary group. For each incident discrete velocity vector $\vec{c}_i = \vec{C}(j_i)$, the reflected velocity vector $\vec{c}_r$ is found from

$$\vec{c}_r = \vec{c}_i - 2(\vec{c}_i \cdot \vec{n})\vec{n} \quad (21)$$

Finally, the index j_r associated with the reflected velocity vector is found from the minimum of the product $[(\vec{c}_r - \vec{c}_j) \cdot (\vec{c}_r - \vec{c}_j)]$ over for all directions j . Therefore,

$$f(j_r) = f(j_i) \quad \text{for all} \quad \vec{C} \cdot \vec{n} < 0 \quad (22)$$

II.E.2. Wall boundary

Given a wall at a temperature T_w and moving with velocity $\vec{V} = (u_w, v_w, w_w)$ where $\vec{n}$ is the outward pointing normal to wall, the f values in outgoing direction ($\vec{C} - \vec{V} \cdot \vec{n} \geq 0$) are updated using extrapolation from interior cells. The wall number density is calculated from the conservation of mass flux:

$$\sum_{(\vec{C}-\vec{V}) \cdot \vec{n} \geq 0} \vec{C} \cdot \vec{n} f = - \sum_{(\vec{C}-\vec{V}) \cdot \vec{n} < 0} \vec{C} \cdot \vec{n} \frac{n_w}{(\pi T_w)^{\frac{3}{2}}} e\left(-\frac{(c_x - u_w)^2 + (c_y - v_w)^2 + (c_z - w_w)^2}{T_w}\right)$$

The values of f for a fully diffuse wall boundary in the incoming direction are then calculated as

$$f_j|_{(\vec{C}-\vec{V}) \cdot \vec{n} < 0} = \frac{n_w}{(\pi T_w)^{\frac{3}{2}}} e\left(-\frac{(c_x - u_w)^2 + (c_y - v_w)^2 + (c_z - w_w)^2}{T_w}\right) \quad (23)$$

and stored in the boundary cell.

The specular-diffuse boundary condition allows the user to specify an accommodation coefficient σ for the wall. The distribution function in the incoming direction is then calculated as

$$f = \sigma f_{wall} + (1 - \sigma) f_{symmetry}$$

II.E.3. Far-Pressure Inlet

The values of f incoming to the domain are set to a Maxwellian at given inlet pressure, temperature and zero velocity.

$$f_{inlet}|_{\vec{V} \cdot \vec{n} < 0} = \frac{n_{inlet}}{(\pi T_{inlet})^{\frac{3}{2}}} e\left(-\frac{c_x^2 + c_y^2 + c_z^2}{T_{inlet}}\right) \quad (24)$$

where n_{inlet} is the inlet density found from the ideal gas relation.

II.F. Algebraic Multi Grid Solver

The AMG solver along with the Navier-Stokes solver in MEMOSA has been developed by Mathur et. al. and details can be found in Ref.⁷ For a simple Couette flow problem, the size of matrix for the linear system is only 800×800 . The number of equations is essentially the number of cells, $80 \times 10 = 800$. For the 3d damping problem, the size of the mesh is $60 \times 60 \times 40 = 144000$. The use of multigrid methods is very effective in accelerating convergence in such cases where the convergence of simple relaxation methods such as the Gauss-Seidel method stalls. The general procedure for multi-grid has been described by Trottenberg et. al.¹⁰ We use an algebraic multigrid technique wherein the coarse level system is derived purely from the fine level system without reference to the underlying grid geometry or physical principle that led to the fine level system. Starting with the finest linear system, n_1 number of relaxation sweeps are performed at each level. The residual is then transferred to the next coarse level where it forms the source. This is repeated recursively till the coarsest level on which the solution can be obtained easily because this level typically has only a few equations. Corrections from the coarse level are then propagated to the solution at the next fine level which is then further improved by n_2 relaxation sweeps. This constitutes one V cycle, with each level being visited twice, once during the down leg and once during the up leg. The solver has the capability to do V, W and F types of cycles.

III. Solver Verification

The model kinetic equations are applied to three problems. The solver was verified by comparison with both analytical solution and solution from a steady 2D ESBGK solver.

III.A. Verification - Space homogeneous relaxation

The first test case was chosen to test the time discretization. A space homogeneous relaxation of a weighted Maxwellian to a single Maxwellian was selected for this purpose. This is a 0D problem with the distribution function initialized to a weighted Maxwellian of two flows. The first has a non-dimensional velocity $u_1 = 1.0$ and weight $w_1 = 0.75$ while the second is described by $u_2 = 4.0, w_2 = 0.25$. They both have the same density ρ and temperature T . The initial distribution is

$$f_0(c_j) = w_1 \frac{\rho}{(\pi T)^{\frac{3}{2}}} e^{\frac{(c_x - u_1)^2 + (c_y)^2 + (c_z)^2}{2T}} + w_2 \frac{\rho}{(\pi T)^{\frac{3}{2}}} e^{\frac{(c_x - u_2)^2 + (c_y)^2 + (c_z)^2}{2T}}$$

The exact solution can be found by solving the following differential equation:

$$\frac{\partial f}{\partial t} = -\frac{(f - f_\gamma)}{\tau} \quad (25)$$

where τ is the relaxation time, i.e. $\nu = 1/\tau$ is the collision frequency.

The solution for f at any given time t is thus given by

$$f(t) = f_\gamma + (f_0 - f_\gamma) \exp\left(\frac{-t}{\tau}\right). \quad (26)$$

The final solution is a Maxwellian with a non-dimensional velocity $u = 0.75u_1 + 0.25u_2 = 1.75$. Figure 2 shows the iso-surfaces of the distribution function at level $f = 0.001$ using Cartesian-type velocity meshes of size 14^3 and 26^3 with extent of $c_{max} = 10.5$. A non-dimensional time step of $\Delta t = dt/H * \sqrt{2RT} = 1e^{-3}$ was used for all these simulations. These two show good agreement with the exact solution at 3 different instances in time where $\tilde{t} = \frac{t}{\tau} = 0, 0.85$ and 4.26 . Also shown is the solution from a Cartesian-type velocity mesh of size 20^3 with an extent of only 7.5 . Notice how the right end of the iso-surface is sliced off at both times $\tilde{t} = 0.0$ and $\tilde{t} = 0.85$. This shows that extent of $c_{max} = 7.5$ for the velocity domain is not sufficient to capture the entire iso-surface. This difference does not show up in the L_2 norm ratio in Fig. 3. Therefore, visualization of the distribution function can be useful in determining the correct extent of the velocity mesh for a particular problem.

Figure 3 shows that L_2 norm ratio is lower for a coarser velocity grid and eventually decreases to 0 with time for all the velocity meshes. L_2 norm ratio is a quantitative measure of the deviation from equilibrium solution and defined as:

$$\frac{\|f - f_\gamma\|_{L_2}}{\|f_\gamma\|_{L_2}} = \frac{\sum_j (f - f_\gamma)^2 w_j}{\sum_j f_\gamma^2 w_j} \quad (27)$$

The expression for translational entropy in terms of the velocity distribution function f can be derived (Eq. (37) in Ref.¹¹) as

$$S_{tr} = k \int_{-\infty}^{\infty} f(\vec{c}) \left[1 - \ln \left(\frac{h^3 f(\vec{c})}{m^3} \right) \right] d\vec{c} \quad (28)$$

where h is the Planck constant, m is the atomic mass of gas and c is the molecular velocity.

The entropy generation rate obtained using the collision term is given by $\dot{S}_{coll} = -\nu \int_{-\infty}^{\infty} (f(\vec{c}) - f_\gamma(\vec{c})) (1 - \ln \left(\frac{h^3 f(\vec{c})}{m^3} \right)) d\vec{c}$. More details on the formulation and use of discrete version of H-theorem for analysis of numerical accuracy of rarefied flow simulations can be found in Ref.² In discretized form, $\nu \sum_j (f_j - f_{\gamma,j}) w_j = 0$ from conservation of mass and entropy generation rate reads

$$\dot{S}_{coll} = \nu \sum_j (f_j - f_{\gamma,j}) \ln \left(\frac{h^3 f_j}{m^3} \right) w_j \quad (29)$$

Figure 2. Iso-surface at level $f=0.001$ of the distribution function from solver and exact solution at different times.

Entropy can be a powerful parameter in verification of numerical solution to non-equilibrium flows. In this 0-D problem, non-dimensional entropy starts from an initial value of 31.25 and increases with time till equilibrium is reached at 31.85. The different types of velocity discretization converge to different equilibrium states as shown by the final entropy. The final entropy is lower for a coarser velocity grid and increases to reach the exact entropy as the velocity grid is made finer. The L_2 norm ratio on the other hand, shows that the convergence to equilibrium is exponential but fails to distinguish between the different final equilibrium states. Entropy generation rate decreases for all velocity meshes to reach equilibrium state with net $\dot{S}_{coll} = 0.0$.

One interesting thing to note is that the $20 \times 20 \times 20$ grid with extent of 7.5 has lower values for both initial and final entropy than the exact solution. These are also lower than the values for the coarser mesh with 14^3 velocity ordinates. This is because the extent of the domain is not enough to capture the entire weighted Maxwellian. But this difference between the extents of $c_{max} = 7.5$ and 10.5 does not show up in the L_2 norm ratio. Therefore, entropy can be a valuable tool to optimize the extent and size of the velocity mesh for a given problem.

III.B. Verification - Couette Flow:

The second test case considered is the one-dimensional plane Couette flow. Specifically this case was used to verify the implementation of the wall boundary condition, in particular the specular-diffuse Maxwellian model with given accommodation coefficient σ . The same data used by Bird⁹ is used. The gas, argon, lies between two plates $H = 1m$ apart maintained at a temperature of $T_w = T_0 = 273K$. The bottom wall is at rest while the top is moving with the velocity $u_w = 10$ m/s in the x direction. Initially the gas has a density $\rho = 9.28 \times 10^{-6}$ kg/m³, corresponding to a pressure $P_0 = 0.528$ Pa. For this data, Bird obtains the Knudsen number from his variable hard sphere model as 0.01. For the case $Kn = 0.1$, all conditions are same except

Figure 3. Variation of L_2 norm ratio from weighted Maxwellian at initial to equilibrium at final times.

the height of the channel is now $0.1m$.

The theoretical solution to the incompressible Couette flow is:

$$u(y) = \frac{u_w}{H \left(1 + 2 \frac{2-\sigma}{\sigma} Kn \right)} \left(y + \frac{2-\sigma}{\sigma} \lambda \right) \quad (30)$$

where σ is the accommodation coefficient and is defined to represent the fraction of diffuse reflections. $\sigma = 1$ represents a fully diffuse reflection and $\sigma = 0$ represents a purely specular reflection.

A linear profile of velocity is used as the initial condition for all the simulations. Figures 4(a) and 4(b) show the comparison between theoretical velocity profile and the profile obtained from the Boltzmann Kinetic Solver on a 10×80 mesh in physical space and a 10^3 Cartesian-type velocity mesh. The rms error for $Kn = 0.1$ and $\sigma = 1.0, 0.5, 0.0$ are 1.44%, 1.18% and 1.63% respectively.

Table 1 shows the rms error defined as $\sqrt{\frac{\sum (u_{memosa} - u_{analytical})^2}{N_y}}$ for meshes of different sizes. To determine the convergence of the solution on each mesh, a tolerance of 10^{-9} was used for the residual.

Figure 4. Couette flow. Velocity profile for $u_w = 10$ m/s at two different Knudsen numbers and different accommodation coefficients

Table 1. Rms error for different mesh sizes

No. of cells in y	% Rms error
10	19.26
20	7.27
40	2.81
60	1.78
80	1.44
90	1.36

The order of convergence [12, Eq.6],

$$p = \frac{\log\left(\frac{y(h_m) - y(h_c)}{y(h_f) - y(h_m)}\right)}{\log(r)}$$

can be found using solution from three meshes, coarse, medium and fine with refinement ratio r . Three meshes with refinement factor $r = 2$, i.e. meshes with 20, 40 and 80 cells in y direction were used here. Using rms error from meshes for the Couette flow problem, the apparent order is found to be $p = 1.8$. It should be noted that the boundary conditions implemented are still first order accurate.

III.C. Verification: 2D Squeeze-film damping

In microsystems involving moving microstructures, prediction of gas forces is increasingly important. This is because, as the device size decreases, the surface effects such as gas- damping become increasingly significant as compared to volumetric forces such as structural damping because of the increased surface to volume ratio. In particular, modeling of squeeze-film damping (SFD) for microstructures over a wide range of pressures is challenging due to the breakdown of conventional damping models in rarefied regime. The damping force is generated by a small pressure difference between the top and bottom surfaces of a moving structure close to the substrate. Figure 5 shows the parallel decomposition of computational domain and boundary conditions. The left, top, bottom, right boundaries are symmetry, pressure-inlet, pressure-inlet and wall boundaries respectively. Mesh and domain size convergence studies were performed for squeeze-film damping of a beam with width $w = 18\mu\text{m}$, thickness $t = 2.25\mu\text{m}$ and gap-size of $g = 1.4\mu\text{m}$. This specific case was picked out to verify the correctness of pressure-inlet and moving wall boundaries. The resulting damping force calculated from the simulation was compared with the 2d compact model by Guo et. al.¹³ and

the error was 5.8% for the 100×100 mesh. This error would be further reduced by increasing the velocity grid.

(a) Schematic

(b) Spatial Domain decomposition

Figure 5. Squeeze-film damping at $Kn = 0.389$ and velocity $V = -2.4m/s$ on 50×50 mesh.

IV. 3D Simulations: Preliminary Results and Discussion

Full three-dimensional ESBGK simulations were performed to simulate the flow and gas damping force on a RF MEMS switch during actuation. The description of the device and typical geometric and material properties can be found in Ref.¹⁴ The electroplated Nickel fixed-fixed beam has dimensions of $400\mu m$ length and $120\mu m$ width. The beam is about $2\mu m$ thick and situated $4.0\mu m$ above the electrodes. The gas damping simulations correspond to a situation near pull-in when the air gap between the bottom of the beam and the electrode has a value of about $0.8\mu m$. Figure 6 shows the beam deflection and velocity obtained from the PRISM coarse-grained beam dynamics model¹⁵ using a pull-in voltage of $100V$. The model uses Euler-Bernoulli beam deflection equations which are described as:

$$\mu \frac{\partial^2 u}{\partial t^2} + EI \frac{\partial^4 u}{\partial x^4} = F' \quad (31)$$

where μ is the mass, u is the deflection, x is the coordinate along the length of the beam, E is the Youngs Modulus, $I = \frac{wh^3}{12}$ is the moment of inertia and F' is the force per unit length which includes electrostatic force and damping force from compact model.¹³

A simple flat plate in a box type of geometry was created using CuBit. Then, the 3D spatial mesh was deformed using the 'Moving-mesh' with the given input deflection. The initial and deformed meshes are shown in Fig. 6a. The beam velocity is specified as a boundary condition for the ES-BGK solver.

ESBGK equations can be a valuable resource to solve for the gas-damping on the beam near pull-in. Figure 7(a) shows a map of the Knudsen number based on the gap-size calculated from the pressure profile

Table 2. Comparison of damping force for different domain sizes and mesh sizes

Mesh	Domain	Force	%error
20×40	18×9	0.0199	-
20×40	27×12	0.0195	-
20×40	36×18	0.0193	-
50×50	18×9	0.0217	3.23
50×50	27×12	0.0213	3.27
50×50	36×18	0.0211	3.29
100×100	18×9	0.0222	0.80
100×100	27×12	0.0218	0.82
100×100	36×18	0.0216	0.82
$RE(50 \times 50, 100 \times 100)$	18×9	0.0224	-
$RE(50 \times 50, 100 \times 100)$	27×12	0.0220	-
$RE(50 \times 50, 100 \times 100)$	36×18	0.0218	-

Figure 6. Deflection and velocity predicted by coarse-grain model

under the beam. It can be seen that most of the domain is in the transitional regime. A 2d domain has a constriction of freedom in the x direction and will predict a higher force than a 3d domain. From Fig. 8(d) it can be seen that the velocity of fluid along the beam are significantly higher than the velocity of the beam and therefore should not be neglected as we do so in a simple 2d calculation.

Figure 7. Full 3D simulations

Pure 2d simulations predict higher pressures on the bottom of the beam than a full 3d simulation and hence predict higher damping forces. Figures 8 show the normalized pressure and stream traces from a plain 2D simulation and a 2D slice from a 3D simulation located close to the center of the beam at $x = 40\mu m$. The pressure P_{yy} on the bottom of the beam from the 3d simulation at a particular x -location is significantly lower compared with the 2d simulation as shown in Fig 8(c). Stream traces are drawn at 3 locations and the effect of x -velocity under the beam can be clearly seen at slice with $x = 160\mu m$. The fluid is squeezed down at the center of the beam and flows towards the anchor. Counter-rotating vortices form around the edges of

the beam and all along the beam.

Figure 8. Comparison of pressure profiles on the bottom of the beam between 2d and 3d simulations.

The solver showed good parallel performance on HERA, a compute cluster at LLNL. All these simulations were performed on a physical mesh with $N_c = 144000$ cells and $N_v = 10^3$ velocity mesh. The total number of unknowns are f, f_0, f_γ which is $3 \times N_c \times N_v$ and this is approximately 0.4 billion. The estimate for memory requirement is $0.4 \times 10^9 \times 8 / (1024)^3 = 3.2Tb$. A scaling of 55 was reached from simulations on up to 512 processors. The average time per iteration on 128 processors was 9.8 seconds. The solver also has the capability to restart with the distribution function and coefficients for the equilibrium distribution function saved in hdf5 file format. This gives a file compression of about 4.5 when compared to ascii format. This is the first parallel unsteady full 3d solver to have been developed based on the model kinetic equations and shows tremendous promise for a wide variety of applications. Some MEMS applications include calculation of Knudsen force on a hot micro-beam close to a cold substrate and damping simulation of cantilever array in high-g silicon accelerometers. The solver can also be used in high rarefied systems such as thermal convection in a vacuum system used in pharmaceutical freeze-drying chambers.

V. Conclusions

A 3D unsteady solver for the Boltzmann-ESBGK model kinetic equations has been developed with a goal of providing a framework for the simulation of rarefied gas flows in microsystems with realistic complex geometries. The solver was verified by comparison to analytical solutions for unsteady 0D and steady 1D problems as well as through solver-to-solver comparison for 2D problems. Preliminary results for a full 3d microscale gas damping simulation with half a billion unknowns on 128 processors were presented.

Figure 9. Parallel performance and spatial domain decomposition.

Acknowledgments: The authors are grateful for support from the Purdue PRISM center under Department of Energy (National Nuclear Security Administration) award number DE-FC52-08NA28617. The authors would like to thank Prof. Sanjay Mathur, Dr. Battalgazi Yildirim and Dr. Lin Sun of Purdue University for their assistance with the use of the MEMOSA-FVM solver suite including the parallelization framework and the Algebraic Multi Grid Solver.

References

- ¹Holway, L. H., "New statistical models for kinetic theory: Methods of construction," *Physics of Fluids*, Vol. 9, 1966, pp. 1658.
- ²Chigullapalli, S., Venkatraman, A., Ivanov, M., and Alexeenko, A., "Entropy considerations in numerical simulations of non-equilibrium rarefied flows," *Jou. of Comp. Phys.*, Vol. 229, 2010, pp. 2139–2158.
- ³Bhutta, B. A. and Lewis, C. H., "Investigation of the ellipsoidal-statistical BhatnagarGrossKrook kinetic model applied to gas-phase transport of heat and tangential momentum between parallel walls," *Physics of Fluids*, Vol. 23, 2011, pp. 030601.
- ⁴Mathur, S. R. and Murthy, J. Y., "A Pressure-Based Method for Unstructured Meshes," *Numerical Heat Transfer, Part B: Fundamentals*, Vol. 31, No. 2, 1997, pp. 195–215.
- ⁵Sun, L., Mathur, S. R., and Murthy, J. Y., "An unstructured finite volume method for incompressible flows with complex immersed boundaries," *Numerical Heat Trasfer, Part B*, Vol. 58, No. 4, 2010, pp. 217–241.
- ⁶Shizgal, B., "A Gaussian Quadrature Procedure for Use in the Solution of the Boltzmann Equation and Related Problems," *Journal of Computational Physics*, Vol. 41, pp. 309–328.
- ⁷Mathur, S. and J. Murthy, "Unstructured finite volume methods for multi-mode heat transfer, in: W. Minkowyz, E.M. Sparrow (Eds.)," *Advances in Numerical Heat Transfer 2*, Taylor and Francis, 2001, pp. 37–67.
- ⁸Mieussens, L. and Struchtrup, H., "Numerical comparison of Bhatnagar-Gross-Krook models with proper Prandtl number," *Physics of Fluids*, Vol. 16, No. 8, 2004, pp. 2797–2813.
- ⁹Bird, G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, New York, 2nd ed., 1994.
- ¹⁰Steuben, K. and Trottenberg, U., "Multigrid methods: fundamental algorithms model, problem analysis and applications, in: W. Hackbush, U. Trottenberg (Eds.)," *Multigrid Methods, Lecture Notes in Mathematics*, Springer-Verlag, Berlin, 1982, pp. 1–176.
- ¹¹Schrock, C. R., McMullan, R. J., and Camberos, J. A., "Continuum Onset Parameter Based on Entropy Gradients Using Boltzmann's H-Theorem," *43rd AIAA Aerospace Sciences Meeting and Exhibit*, AIAA 2005-967, Reno, Nevada, 2005.
- ¹²Hemez, F. M., "Uncertainty Quantification and the Verification and Validation of Computational Models in. D.J. Inman, C.R.Farrar, V.Lopes, and V.Steffen Jr." *Damage Prognosis for Aerospace, Civil and Mechanical Systems*, John Wiley and Sons Ltd., London, United Kingdom, 2004.
- ¹³Guo, X. and Alexeenko, A., "Compact model of squeeze-film damping based on rarefied flow simulations," *Journal of Micromechanics and Microengineering*, Vol. 19, No. 045026, 2009, doi:10.1088/0960-1317/19/4/045026.
- ¹⁴Alexeenko, A., Chigullapalli, S., Zeng, J., Guo, X., Kovacs, A., and Peroulis, D., "Uncertainty in Microscale Gas Damping: Implications on Dynamics of Capacitive MEMS Switches," *Reliability Engineering and System Safety*, Vol. 96, 2011, pp. 1171–1183, doi:10.1016/j.res.2011.01.002.
- ¹⁵Ayyaswamy, V. and Alexeenko, A., "Coarse-grained Model for RF MEMS Device," Aug 2010, <https://memshub.org/resources/36>.