Unified Solver for Rarefied and Continuum Flows in Multi-Component Gas Mixtures

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Abstract. A Unified Flow Solver (UFS) has been developed for simulations of rarefied, transitional and continuum flows based on direct numerical solution of the Boltzmann equation coupled to kinetic schemes of gas dynamics. The UFS uses dynamically adaptive mesh and automatic domain decomposition into kinetic and continuum domains based on continuum breakdown criteria. This paper describes UFS extensions to mixtures of atomic and molecular gases. Results of simulations for selected benchmark problems are presented including shock wave structure in a binary mixture of atomic gases and a rotationally excited molecular gas, supersonic flows of gas mixtures around cylinder. Challenges and future plans are discussed.

Keywords: Unified Flow Solver, Boltzmann Equation, Rarefied Gas Dynamics, Molecular Gas Mixtures, Internal Degrees of Freedom.
PACS: 51.10+y, 05.20Dd

INTRODUCTION

A Unified Flow Solver (UFS) has been developed for simulations of rarefied, transitional and continuum flows by solving the Boltzmann and continuum equations in appropriate parts of computational domain [1,2]. In the kinetic domains, direct numerical solution of the Boltzmann equation is obtained following [3,4]. In the continuum domains, the Euler or Navier Stokes equations are solved using kinetic schemes of gas dynamics [5,6]. The domain decomposition and coupling algorithm are based on the adaptive mesh and algorithm refinement procedure. The computational mesh in physical space is dynamically adapted to the solution and geometry using a tree-based data structure [7]. The UFS separates non-equilibrium and near-equilibrium domains using continuum breakdown criteria and automatically select appropriate continuum and kinetic solvers. Parallelization of the UFS has been achieved with dynamic load balancing among processors. The UFS can automatically introduce or remove kinetic patches to maximize accuracy and efficiency of simulations.

The present paper discusses basic UFS architecture and extensions to gas mixtures. We analyze the choice of continuum breakdown parameters for the domain decomposition in gas mixtures. The current UFS capabilities are demonstrated for a shock wave structure in a mixture of atomic gases, and in a molecular gas with rotationally excited states. Benchmark problems of gas flows around a cylinder at different Mach and Knudsen numbers are discussed. Challenges related to UFS extension to vibrationally excited molecules and chemical reactions, and mixtures of gases with disparate mass are briefly mentioned.

UFS ARCHITECTURE

The basic UFS architecture is shown in Figure 1. The Boltzmann solver is the main component of the UFS. The direct numerical solution of the Boltzmann equation rather than statistical particle simulation has been selected for the UFS. Another component of the UFS is a continuum (Computational Fluid Dynamics) solver implemented using kinetic schemes of gas dynamics. The remaining components of the UFS include continuum breakdown criteria for domain decomposition into kinetic and continuum parts and algorithms for coupling kinetic/continuum solvers at the interface. We briefly describe the key features of the UFS below referring for further details to [8,9].

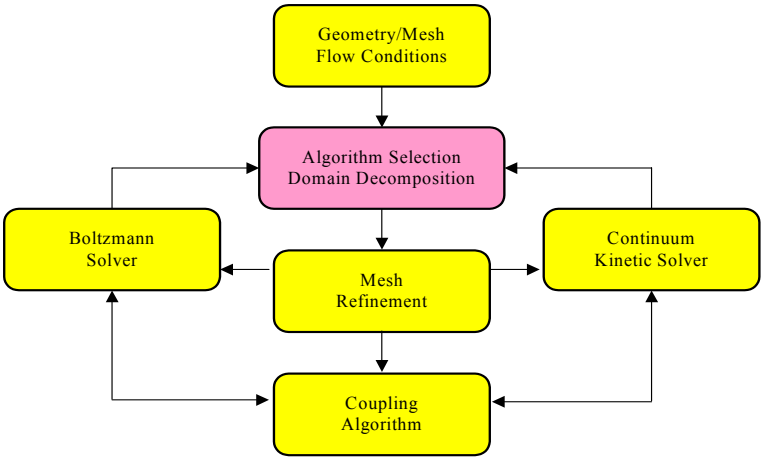

FIGURE 1. Key UFS Components

Boltzmann Solver

For the numerical solution of the Boltzmann equation, a Cartesian mesh in velocity space is introduced with a cell size $\Delta\xi$ and nodes $\boldsymbol{\xi}_\beta$. Using this velocity grid, the Boltzmann equation for each gas component is reduced to a system of linear hyperbolic system of transport equations in physical space with a nonlinear source term

$$\frac{\partial f_\beta}{\partial t} + \nabla_{\mathbf{r}} \cdot (\boldsymbol{\xi}_\beta f_\beta) = I(f_\beta, f_\beta) \tag{1}$$

Introducing computational grid in physical space, the solution of (1) is split into two stages: free flow and relaxation. An explicit finite volume numerical technique is used with automatic selection of the time step. The boundary conditions specified at surfaces of solid objects imbedded in the computational domain provide the distribution function of the reflected particles as a sum of diffuse and specular reflection.

The calculation of the collision integral $I(f_\beta, f_\beta)$ is based on previous works [3,4]. The discrete analog of the collision integral pertains the following properties:

- The integral is equal to zero for a Maxwellian distribution, $I(f_M, f_M) = 0$.
- The distribution remains positive for all nodes in velocity space when the relaxation problem is solved.
- For the collision invariants, $\psi(\xi) = (1, \xi, \xi^2)$, the conservation laws are satisfied $\int_{\mathbb{R}^3} \psi I(f, f) d\boldsymbol{\xi} = 0$

The collision integral is implemented for different inter-molecular interaction potentials. The Boltzmann solver has been validated for several benchmark problems including shock wave structure, heat transfer between parallel plates, supersonic and subsonic problems around blunt bodies in monatomic gas.

Continuum Flow Solvers

Kinetic schemes are used for the continuum equations to facilitate coupling to the Boltzmann solver. Our kinetic Euler scheme follows the EFM Equilibrium Flux Method by Pullin (see [6] for details). The kinetic NS solver is a generalization of the scheme used for the kinetic Euler solver and the Kinetic Flux Vector Splitting method by Chou and Baganof with the distribution function at cell faces taken from the gas kinetic BGK scheme by Xu [5]. The Prandtl number correction is used to calculate the heat flux on cell faces using polynomial interpolation of the velocity distribution function defined at cell centers. The results of calculations using continuum kinetic solvers were compared with classical NS and Euler solvers for several benchmark problems.

Domain Decomposition and Coupling Algorithms

Domain decomposition into kinetic and continuum parts is based on the continuum breakdown criteria. As discussed in [10,11], the applicability of different criteria and the ways to choose the threshold value depends on the type of the problem. The simplest criteria has the form

$$S_\rho = Kn \frac{1}{\rho} \left| \nabla \rho \right|, \qquad (2)$$

where ρ is density, *Kn* is the *local* Knudsen number. If *S* is greater then a threshold value, then the kinetic solver is used. We have found that for supersonic external flows the criterion (2) gives correctly the non-equilibrium domain near shock wave and behind solid bodies at moderate Knudsen numbers. It should be noted that breakdown criteria derived from continuum solutions might not be appropriate for all cases, and more computationally expensive breakdown criteria derived from the kinetic solvers might be necessary for specific problems.

Parallelization

The parallel version of the UFS has been developed with automatic domain decomposition and dynamic load balance among processors. The procedure of domain decomposition is performed using space-filling curves (SFC). Different weights are assigned to kinetic and continuum cells depending on CPU time required for performing computations in the cells [12]. Figure 2 illustrates an example of a parallel run on a 7-processor Linux cluster for the Inflatable Reentry Vehicle Experiment (IRVE) [13] at a 91 km altitude, for $Kn = 0.01$ and $M = 3.94$. The streamlines, Mach number, and computational mesh are shown on the left part, the right part illustrates the gas temperature profile in the vertical plane, as well as kinetic (red) and continuum (blue) domains in the horizontal plane.

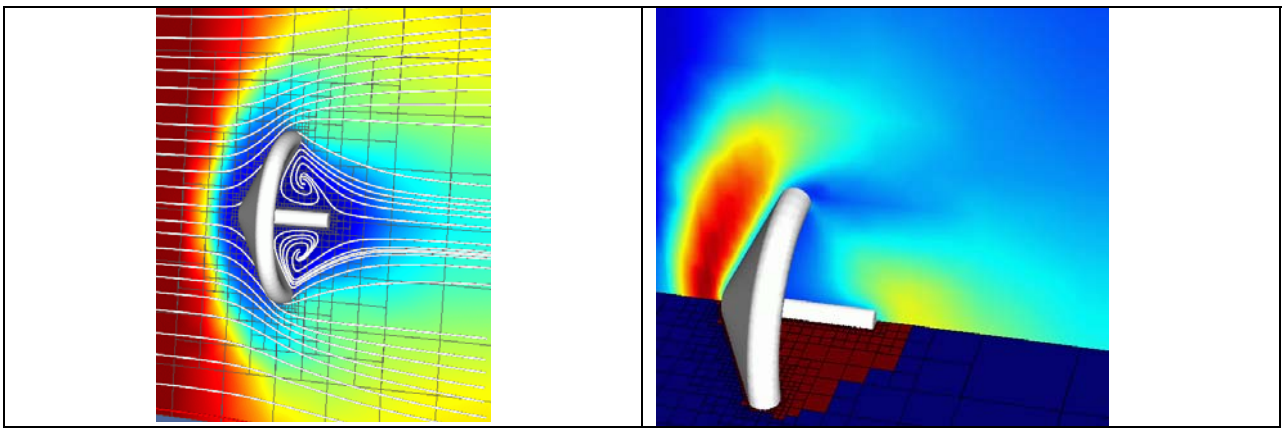

FIGURE 2. Streamlines, Mach number, and computational mesh (on the left). Gas temperature in the vertical plane, kinetic (red) and continuum (blue) domains in the horizontal plane (on the right).

UFS EXTENSIONS TO REACTIVE GAS MIXTURES

Mixtures of atomic gases

We have extended UFS to multi-component gas mixtures. Initial testing was performed for a 2-component gas using the BGK-type collision integral described in [14]. Furthermore, collision integral based on HS model for multi-component mixtures [15] was implemented using momentum space rather than velocity space. We have carried out calculations for the shock wave structure in a mixture of two gases with mass ratio ¼, the upstream density of heavy component 0.9 and M=2. The HS model is used with equal molecular diameters. Figure 3 shows the velocity distribution functions (averaged over y- and z-directions) of both species on the common momentum space and at different locations in the shock wave. Figure 4 shows the distribution of normalized densities $[(n_i(x)-n_{i-})/(n_{i+}-n_{i-})]$ and parallel and perpendicular temperatures of both gas species. The results are in close agreement with [15]. One can see that parameters of the heavy component react to shock wave with a delay compared to those of the light component. The "overshoot" of the heavy component temperature is also a well-known phenomenon [15]. We have found that with increasing the mass ratio, the computational time increases rapidly. Using different velocity mesh for different components and simplifying collision integral for mixtures with disparate mass [16] should increase the efficiency of simulations. We plan to explore this option in future work.

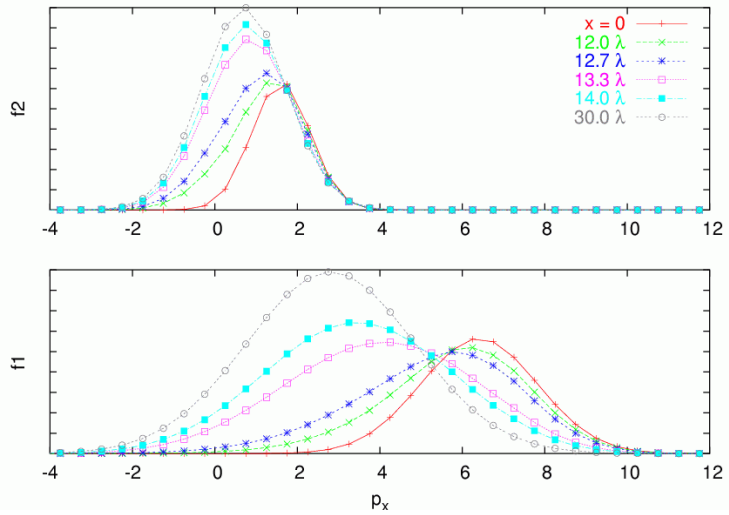

FIGURE 3. The velocity distributions of light (top) and heavy (bottom) species at different points of the shock wave for M=2 and mass ratio ¼. The species momentum space p_x is used as x-axis.

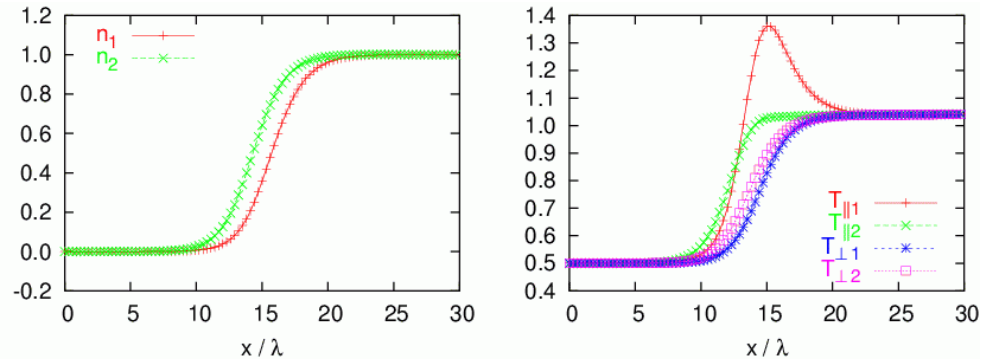

FIGURE 4. Profiles of normalized density and parallel and perpendicular temperatures for the shock wave in a binary gas mixture for M=2 and m_1/m_2 = ¼.

The Euler-Boltzmann coupling for multi-component gas mixtures has been implemented. Figure 5 shows results for supersonic flow of binary mixture over a cylinder at M=2, for 3 Knudsen numbers. Two species with masses of

3.2 and 1.6 (reference mass = 10), with no chemical reactions were considered. The HS model has been used for the Boltzmann solver. For the domain decomposition, continuum breakdown criterion (2) was used with the total density $\rho_t = \sum m_i \rho_i / \sum m_i$. The temperatures of species become different in kinetic domains (while they are equal in the continuum domains).

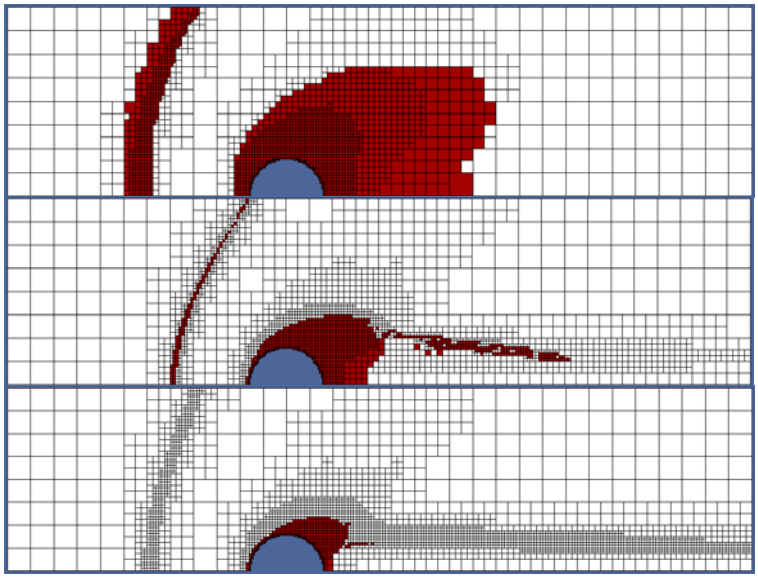

FIGURE 5. The computational mesh and kinetic/continuum domains for binary mixture of monatomic gases at *M*=2, for *Kn* numbers 0.125, 0.025, and 0.0125

Molecular Gases

We have extended kinetic solver to molecular gases with internal degrees freedom following the work by Tcheremissine [17]. Figure 6 (left part) shows distributions of gas density, translational and rotational temperatures obtained in our simulations for *M*=12.9. The right part of Figure 6 shows rotational spectrum for 25 levels at several points along the wave front. The center of SW is located at X=0. On the x-axes is the rotational number, on the y-axes is the population of the rotational levels. It is clearly seen that the rotational equilibrium inside the SW doesn't exists for this high Mach number. Further details can be found in [18].

We have also extended kinetic solver for vibrationally excited molecules. For future development of the UFS, we plan to take into consideration that vibrational equilibration in VT and VV collisions occurs much slower compared to translational and rotational equilibration. As a result, in most cases, it is adequate to model computational domains where vibrational relaxation and chemical reactions take place using continuum models.

Chemical Reactions

We have implemented the multi-component kinetic Euler solver for reactive gas mixtures following the work [19]. Figure 7 shows an example of simulations for supersonic air flow around a cylinder at *M*=2, for the incoming gas density $\rho = 0.1$ kg/m^3. It is known that due to slow V-T relaxation, vibrational temperature lags behind translational temperature, in our case vibrational temperature remains high behind the cylinder and has different values for different molecules and for different incoming low gas densities.

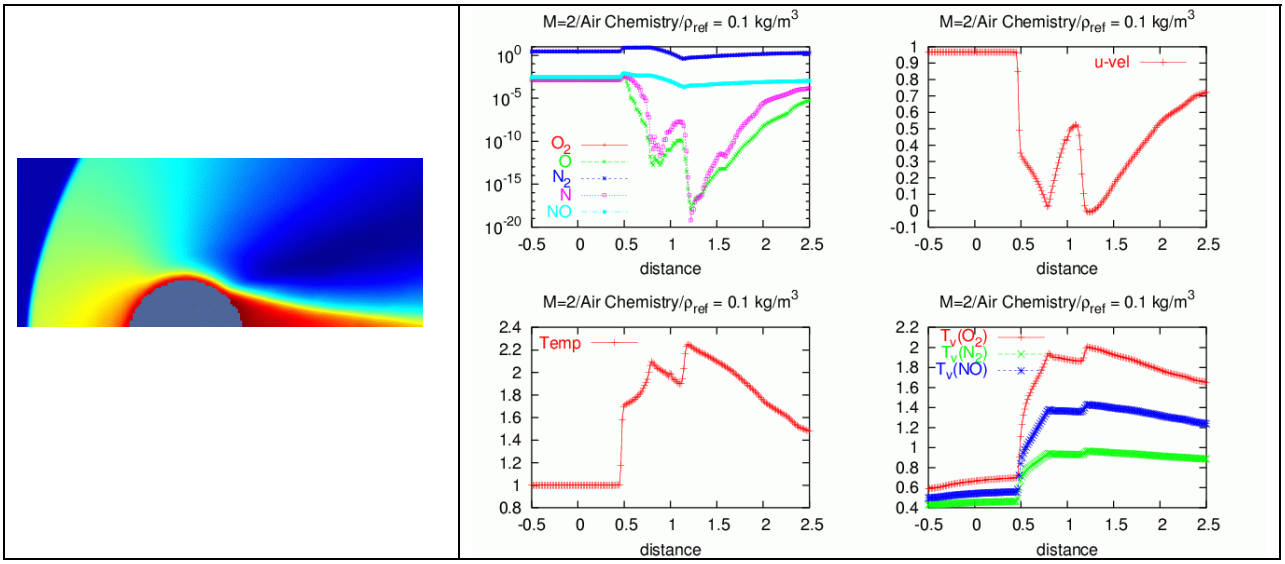

FIGURE 7. Translation temperature near the cylinder surface (left), species density, *u* component of velocity, translational and vibrational temperature of different molecules along a central stream line (on the right)

CONCLUSIONS

We have described the architecture of Unified Flow Solver (UFS) and the ongoing work towards UFS extensions to gas mixtures. It seems feasible to produce in the near future an efficient solver for unified simulation of practical problems involving reactive gas mixtures of different degrees of rarefaction.

ACKNOWLEDGMENTS

This work is supported by the US Air Force SBIR Project F33615-03-M-3326 and by the Russian Foundation for Basic Research, Grant N 04-01-00347. We thank Mr. Eswar Josyula for useful discussions and guidance.

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