Shocks and Jets from the Laboratory Environment to the Astrophysical Regime: Transforming AstroBEAR Into an All Purpose MHD Simulation Package

by

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ABSTRACT

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Supersonic jets and shocks play an important role in numerous astrophysical phenomena, ranging from stellar formation to active galactic nebulae (AGN). Laboratory astrophysics opens up new avenues for research into these jets and shocks, and computer simulations show great promise in linking laboratory and astronomical data. To date, the most effective codes for the laboratory environment are not readily available and lack magnetic fields, a key component in astrophysical jets and future magnetized laboratory experiments. Also no 3D simulation code has had its non-local thermodynamic equilibrium (LTE) cooling, essential for generating emission maps for comparison with astronomical observations, rigorously tested against an accepted baseline. The focus of this dissertation research was to improve an existing magnetohydrodynamic code, AstroBEAR, to better model jets and shocks in laboratory and astrophysical environments, with the ultimate goal of developing a code that can link astronomical and laboratory data.
The work outlined in this dissertation facilitates the connection between astronomical and laboratory data in two areas. First, we added a multiple material and non-ideal equation of state capability into AstroBEAR to handle the high density ionized plasmas that characterize laboratory astrophysics experiments and now have the first working 3D MHD code capable of simulating the laboratory environment. We used AstroBEAR in 2.5 D hydrodynamic mode to simulate a series of experiments carried out on the OMEGA laser, and compared the simulations with experimental data.

Secondly, we improved AstroBEAR's handling of radiative cooling, specifically in the post-shock cooling zones prevalent in many astrophysical jets. The first ever validation tests of a 3D code against a fully non-LTE 1D radiative cooling atomic code show explicitly that AstroBEAR correctly models post-shock radiative cooling down to the resolution and micro-physics limits. We used this improved cooling to simulate the HH 110 jet and conclude from these simulations that any model of stellar jet formation must be able to produce precessing and pulsing outflow. Overall the improvements of AstroBEAR's ability to handle jets and shocks in the laboratory and astrophysical environments position it to potentially link observational data with magnetized laboratory experiments.
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Chapter 1

Introduction

1.1 Motivation

Supersonic jets and the complicated shock interactions they produce play an important role in a wide variety of astrophysical phenomena, ranging from stellar formation to supernovae to active galactic nebulae. Historically the main avenue for research into these phenomena has been astronomical observations and theoretical calculations. Recently, however, laboratory astrophysics and computer simulations have become increasingly important in astrophysical research. Laboratory astrophysics uses lasers to recreate conditions and structures found in many astrophysical regimes. Computer simulation codes can be an effective tool for linking the laboratory results with the observational data. In the laboratory regime, to date the most effective simulation codes are not readily available to the astrophysical community at large. Also these laboratory simulation codes lack magnetic fields, which are a key component of astrophysical jets and will be necessary to model future magnetized laboratory jet experiments. In the astrophysical regime, post-shock non-local thermodynamic equilibrium (LTE) cooling is necessary to generate accurate synthetic emission maps for comparison with astronomical observations and no 3D code has been rigorously tested in this area. The focus of my doctoral research was to improve upon an existing astrophysical code containing magnetic fields, AstroBEAR, towards the long-term goal
of an all purpose MHD code capable of linking laboratory and astrophysical data. This dissertation describes the work done to add the capability for AstroBEAR to handle jets and shocks in the laboratory environment as well as the improvements made to the code’s ability to simulate jets and shocks in the astrophysical regime.

1.2 Simulation Codes

Simulation codes divide into two main categories, Lagrangian and Eulerian. Lagrangian codes consist of a base grid of cells initialized with physical properties such as mass, temperature and velocity. These cells then move and change shape according to solutions to the Euler fluid equations. This approach essentially treats each cell as a particle that represents the average value for all the particles in that cell. Lagrangian codes can use grid cells of different shapes and sizes, allowing for large and geometrically complex initial grids. These codes work best when the flows are not overly complicated and confined to a single dimension. For example, 1D star formation simulations involving collapsing gas can be done very effectively with smoothed particle hydrodynamic (SPH) simulations, which are Lagrangian. However, as the flows become more complicated, cells may fold back onto themselves and the resulting tangled grid then requires a complicated regridding procedure. When non-trivial, multi-dimensional shocks occur, Lagrangian codes usually do not work effectively. Hence, most multi-dimensional codes designed to study stellar outflows and supernovae, where shocks play a key role in the hydrodynamics, are Eulerian.

Eulerian codes start with a similar base grid structure as Lagrangian codes except the control volumes remain static rather than moving with the flow. The fluxes of physical properties, such as mass density, are calculated for a system of conservation
laws. In a conservative Eulerian code the flux out of a cell corresponds to a flux into another cell. Thus the physical variables in question, generally mass, energy, and momentum densities, are conserved over the whole simulation.

Hydrodynamical codes have evolved over the past decades to simulate more complicated flow structures, achieve higher resolutions, lessen computation times, and include additional physics (1). For example, expanding from 2D to 3D simulations was necessary to deal with more complicated flow structures, and adaptive mesh refinement codes (AMR; e.g. FLASH (2), ENZO (3), and ORION (4)) achieved faster computational times, resolved fine spatial scales in areas such as gravitational collapse, and captured shocks better than non-AMR codes. AMR is based on the concept of a cell size that adapts during the simulation, with changes in the cell size confined to the portions of the grid where smaller scale physics occurs. The ability to have more cells only where needed increases the computational efficiency of AMR codes, and parallelization also leads to increased computational efficiency of these codes.

Another major challenge for hydrodynamical codes has been to include magnetic fields, which play an important role in the hydrodynamics of many astrophysical phenomena, such as magnetized outflows and accretion disks. Such situations motivated the addition of magnetic fields to hydrodynamics codes to create magneto-hydrodynamics (MHD) codes. Codes such as ZEUS (5) were among the first to expand to MHD. Finally, many astrophysical situations require additional physics, e.g. molecule formation for dust grains (6), relativistic physics (7), and complex radiation transport (8). MHD codes are constantly evolving to meet these challenges. AstroBEAR (9), developed at the University of Rochester, is an example of an Eulerian-based simulation package with MHD, 3D, AMR, parallelization and
micro-physics capabilities. Chapter 2 will discuss in detail the numerical methods utilized by this code.

1.3 Laboratory Astrophysics

High intensity lasers produce high energy densities like those present in astrophysics (10). Laboratory astrophysics uses these lasers to recreate a variety of astrophysical phenomena, including shock-clump interactions (11), deflected jets (12), magnetized jets (13; 14), supernova blast waves (15; 16), supernovae explosions (17), stellar interior opacities (18), and planetary interiors (19). There are numerous facilities around the country involved in this type of research, such as the National Ignition Facility (NIF), the Z machine at Sandia National Laboratory, and the Laboratory for Laser Energetics (LLE) in Rochester, NY.

Laboratory experiments serve as valuable code validation tool. Historically astrophysical codes relied mainly on observational data and theoretical calculations as validation tools. These astronomical observations, providing data only on radiating material, are greatly limited in their ability to verify simulation results. However, laboratory experiments generate more direct data about the hydrodynamics involved in the entirety of a flow. Therefore a code validated via laboratory experiments allows for greater confidence in the validity of many other simulations done using that code. However, the high density plasmas associated with these laboratory experiments are not well modeled by the ideal gas equations of state (EOS) associated with most astrophysical MHD codes. Instead, a non-ideal gas equation of state capability must be added. Chapter 3 will discuss the steps taken to successfully incorporate such a capability into AstroBEAR, for the purposes of simulating the laboratory environ-
ment. It will also show simulations of a specific laboratory experiment and compare experimental data, ideal EOS simulations, and non-ideal EOS simulations.

1.4 HH Objects

Herbig-Haro (HH) objects (20) were first observed in the early 1950s independently by Herbig (21; 22) and Haro (23; 24). These objects are characterized by forbidden line metal emission as well as strong hydrogen recombination lines. Since their discovery over 600 of these objects have been cataloged and they have become directly associated with the bipolar outflows generated by young stars. Outflows and collimated jets appear in many other astronomical phenomena, such as X-ray binaries, active galactic nuclei (AGN), and planetary nebulae. Hence, a deeper understanding of HH flows can also lead to a better understanding of a wide range of astrophysical phenomena (25).

Many HH jets are comprised of a series of compact knots either aligned with or with a small spatial dispersion relative to the jet axis. These jets are characterized by low-excitation spectra which indicate shock velocities only on the order of 30 km s\(^{-1}\) a much lower velocity than the bulk velocity of these flows which tend to be on the order of 200 km s\(^{-1}\). This discrepancy led to two competing theories, oblique shocks generated by hydrodynamic or magnetohydrodynamic instabilities (26; 27) or by internal variations in the flow velocity (28). Recent Hubble Space Telescope (HST) observations of HH flows support the latter theory, showing HH flows with bulk velocities of 300 km s\(^{-1}\) and internal velocity variations on the order of 40 km s\(^{-1}\) (29).

The launching mechanism for HH flows remains a source of debate. The two
competing models are the X-wind theory (30) and the disk launching theory (31). The X-wind theory proposes that the jet is launched by the interaction of the stellar magnetosphere and the inner boundary of the accretion disk, while the disk launching theory suggests that the jet is launched from the accretion disk itself. These launching mechanisms can be classified more specifically as static or dynamic in nature. A static launching mechanism generates a steady state jet whereas a dynamic mechanism would consist of variation in properties of the jet such as velocity.

Once these jets are launched the collimation process is also not well understood. A purely hydrodynamical collimation process would require the pressure of the ambient medium, i.e. the flared accretion disk surrounding the young star, to be greater than the ram pressure of the jet. However, the ram pressure of a jet is generally high near the star and decreases proportional to the square of the distance from the star which makes hydrodynamical collimation only possible at relatively large distances. Also, as seen in HH 30 (32), the shape of the accretion disk is much wider than the opening angle of the jet and makes purely hydrodynamical collimation improbable. As a result, magnetic fields have been suggested as a way to aid in collimation. Models of magnetic field collimation show possible alignment of the magnetic field with the rotational axis of the star at large distances as well as possible wrapping of the magnetic fields in a toroidal configuration above and below the star. These models have been supported by observational evidence of strong magnetic fields ~ 100 AU from young stars, though it is important to note that fields begin to weaken at larger distances (33).

HH 110 (34; 35) represents a unique HH flow characterized by shock interactions and is generally accepted to be the deflected portion of a stellar outflow jet (36).
Studying this HH object will allow us not only to gain a better understand of how shocks interact with each other and the background medium, but also more insight into the properties of the progenitor stellar outflow jet, HH 270. This progenitor flow comes directly from a young star, so the flow’s properties will aid in the understanding of stellar formation as well as the generation and collimation of HH jets.

The AstroBEAR code was used to generate simulations of HH 110 with the purpose of further refining our understanding of the origin of HH jets. To accurately simulate HH 110 the code needed to get not only the flow dynamics correct but also the post-shock radiative cooling. The energy lost in these cooling zones has a dramatic effect on the hydrodynamics of the flow. These cooling zones are non-LTE and therefore require explicit tracking at each step in the code. Chapter 4 discusses the changes made to the code to better model the post-shock radiative cooling as well as the conclusions drawn from subsequent simulations of HH 110. Chapter 4 also compares the results of 1D simulations of radiative cooling shocks with an accepted baseline and for the first time shows explicit validation of an MHD code’s ability to handle post-shock radiative cooling.
Chapter 2

AstroBEAR Numerical Methods

The AstroBEAR code is an Eulerian, 3D, AMR, and MHD simulation code and is based on BEARCLAW (Boundary Embedded Adaptive Refinement Conservative Laws). This chapter will detail the underlying numerical methods behind the AstroBEAR code.

The Euler equations for use with pure hydrodynamics without magnetic fields are given by:

\[
\frac{\partial Q}{\partial t} + \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z} = 0
\]  

(2.1)

where \( Q \) and the flux matrix \( f_z \) are given by:

\[
Q = \begin{bmatrix} \rho & \rho v_x & \rho v_y & \rho v_z & E & \rho_T \end{bmatrix}
\]  

(2.2)

\[
f_x = \begin{bmatrix} \rho v_x & \rho v_x^2 + P & \rho v_y v_x & \rho v_z v_x & (E + P)v_x & \rho_T v_x \end{bmatrix}
\]  

(2.3)

\[
f_y = \begin{bmatrix} \rho v_y & \rho v_x v_y & \rho v_y^2 + P & \rho v_z v_y & (E + P)v_y & \rho_T v_y \end{bmatrix}
\]  

(2.4)

\[
f_z = \begin{bmatrix} \rho v_z & \rho v_x v_z & \rho v_y v_z & \rho v_z^2 + P & (E + P)v_z & \rho_T v_z \end{bmatrix}
\]  

(2.5)

where \( \rho \) is the mass density, \( E \) is the total energy density per unit volume, \( v_x \) is the fluid velocity along the x coordinate direction, \( v_y \) and \( v_z \) are the velocity components in the transverse direction \( P \) is the gas pressure and \( \rho_T \) is a passive flow tracer.

Advancing the conserved variables \( Q \) in time and space requires three basic steps: flux
upwinding, temporal integration, and spatial integration. There are many different methods that can be used when implementing these steps and full description of these steps and the different methods available when operating in pure hydrodynamics mode are found in §2.1.

In addition to pure hydrodynamics AstroBEAR can include magnetic fields for MHD simulations. This requires adding new conserved variables to the Euler equations. Solving these MHD equations requires a series of constraint conditions to make the solutions consistent with Faraday’s law. These constraints as well as the constrained transport method implemented for maintaining zero B divergence are described in §2.2.

AstroBEAR also has adaptive mesh refinement (AMR) capability. AMR allows for different levels of resolution in different regions of the grid structure. The idea behind AMR is that the code can identify areas where physics is happening at a smaller scale than the base grid resolution and, where necessary, increase the resolution to capture the smaller scale physics. This localized refinement can greatly increase the efficiency of a simulation when there are large areas with no small scale structures and where a coarser resolution is possible. The details of AstroBEAR’s patch based AMR implementation is discussed in detail in §2.3.

In order to increase the ability of the code to handle large scale problems, AstroBEAR has been parallelized. AstroBEAR parallelization is a physical approach as opposed to a task oriented approach. The code was designed to physically decompose the initial grid structure into smaller domains and for each sub-domain to be assigned to a different processor. When AMR is active the reassignment of cells from one processor to another can continue through the entire simulation. On each pro-
cessor however the code is essentially operated serially, with all operations required for a specific cell remaining on the cells host processor. The parallelization details are explained fully in §2.4.

Finally the code has the ability to handle a variety of microphysics. As with MHD, including microphysics will require an adjustment to the form of the Euler equations. In the case of additional physics, Euler equations are no longer homogeneous and require a source term, \( S(Q) \). Each different microphysics module will require a different type of source term and possibly a different method for solving the equations. Currently the microphysics available in AstroBEAR are cooling, heat diffusion, and gravity. The source terms and methods required for each of these modules is described in detail in §3.6.

### 2.1 Pure Hydrodynamics - No Magnetic Fields

#### 2.1.1 Spatial Reconstruction

AstroBEAR uses the finite volume method to integrate the Euler equation described by Eqns. 2.1-2.3. Discretizing the Euler equations yields the following formula used to advance the conserved variables in time and space:

\[
Q_{i,j,k}^{t+\Delta t} = Q_{i,j,k}^t + \frac{\Delta t}{\Delta x} (F_{x,i,j,k}^n - F_{x,i+\frac{1}{2},j,k}^n) + \frac{\Delta t}{\Delta y} (F_{y,i,j,k}^n - F_{y,i,j+\frac{1}{2},k}^n) + \frac{\Delta t}{\Delta z} (F_{z,i,j,k}^n - F_{z,i,j,k+\frac{1}{2}}^n)
\]

Where \( F_x^n, F_y^n, \) and \( F_z^n \) are the calculated volume and spatially averaged inter-cell fluxes in each dimension and \( \Delta t, \Delta x, \Delta y, \) and \( \Delta z \) are the temporal and spatial intervals by which the equations are advanced. A variety of different methods can
be used to calculate these intercell fluxes. The methods available in AstroBEAR are described below.

The first step in flux calculation is reconstructing the volume averaged cell quantities to the cell interfaces. This is done via:

\[ P_{L,i-\frac{1}{2}} = P_{i-1} + \frac{1}{2} \phi_{-,i} \]

\[ P_{R,i+\frac{1}{2}} = P_{i+1} + \frac{1}{2} \phi_{+,i} \]

where \( P_L \) and \( P_R \) represent the left and right restricted states of the primitive variables and \( \phi \) is the flux limiter, which is used to constrain spatial derivatives to physically meaningful values. The corresponding conserved variable restricted states are given by:

\[ Q_{L,i-\frac{1}{2}} = L_p^{-1}(P_{L,i-\frac{1}{2}}) \]

\[ Q_{R,i+\frac{1}{2}} = L_p^{-1}(P_{R,i+\frac{1}{2}}) \]

where \( L_p \) is the operator that converts conserved variables into primitive variables that are better for interpolation. There are currently three possible methods for implementing this reconstruction. Through a process of trial and error these processes have proven to be the most successful for the problems currently modeled by the code.

The monotone upstream-centered scheme for conservative laws (MUSCL) first put forth by Van Leer (37) is the first option. The flux limiter, \( \phi \) used in this method is known as a minmod limiter. This limiter, which maintains monotonicity, is defined by:

\[ \phi_{\pm,i} = \text{minmod}(P_i - P_{i-1}, P_{i+1} - P_i) \]
\[
\text{MINMOD}(x, y) = \begin{cases} 
\text{MAX}(0, \text{MIN}(x, y)) & \text{if } y > 0 \\
\text{MIN}(0, \text{MAX}(x, y)) & \text{else} 
\end{cases}
\] (2.6)

The second available method is local hyperbolic harmonic variation of the piecewise hyperbolic method (PHM) first introduced by Donat and Marquina (38). In this method the flux limited \( \phi_{\pm,i} \) is given by:

\[
\phi_{\pm,i} = \begin{cases} 
0 & \text{if } |\delta_L| < 10^{-14} \text{ and } |\delta_R| < 10^{-14} \\
 d \Delta x \eta_{\pm} & \text{else} 
\end{cases}
\] (2.7)
where

\[ \eta_{\pm} = \begin{cases} 1 & \text{if } |\kappa| < 10^{-5} \\ 2\kappa^{-2} \left( \log(\frac{3\pi}{2\pi}) \pm \frac{2\pi}{2\pi} \right) & \text{else} \end{cases} \]

\[ \kappa = 2 \begin{cases} \sqrt{\frac{2}{1+dx}} - 1 & \text{if } |\delta_L| < 10^{-14} \text{ or } (\delta_L,\delta_R \geq 0 \text{ and } \delta_R \leq \delta_L) \\ 1 - \sqrt{\frac{2}{1+dx}} & \text{if } |\delta_R| < 10^{-14} \text{ or } (\delta_L,\delta_R \geq 0 \text{ and } \delta_L \leq \delta_R) \\ \sqrt{\frac{d}{\delta_L}} - 1 & \delta_L \leq \delta_R \\ 1 - \sqrt{\frac{d}{\delta_R}} & \text{else} \end{cases} \]

\[ d = 2 \begin{cases} \delta_R \left( \frac{dx^2}{1+dx^2} \right) & \text{if } |\delta_L| < 10^{-14} \text{ or } (\delta_L,\delta_R \geq 0 \text{ and } \delta_R \leq \delta_L) \\ \delta_L \left( \frac{dx^2}{1+dx^2} \right) & \text{if } |\delta_R| < 10^{-14} \text{ or } (\delta_L,\delta_R \geq 0 \text{ and } \delta_L \leq \delta_R) \\ \frac{\delta L_{\delta}}{\delta\kappa + \delta L} & \text{else} \end{cases} \]

\[ \delta_L = \frac{P_i - P_{i-1}}{dx} \]

\[ \delta_R = \frac{P_{i+1} - P_i}{dx} \]

Thirdly the piecewise parabolic method (PPM) described by Colella (39) is available. A more detailed description of this method can be found in Miller and Colella (40) and Mignone (41). However as opposed to method described in Mignone we maintain monotonicity through the use of the minmod flux limiter instead of the Van Leer limiter. This choice was made based on trial and error with both methods. We also do not include the dissipation mechanisms found in §B.1 of Mignone.

The PPM and PHM methods are less diffusive, which can be important advantage when dealing with shocks, and more accurate than the MUSCL method. The main
draw back of these methods is robustness, that is the codes ability to handle small scale deviations without crashing the simulation. Specifically, the MUSCL method tends to be much more robust due to its ability to more readily handle small scale oscillations that lead to negative pressure cells in the PPM and PHM methods.

2.1.2 Upwinding Flux

Once the spatial reconstruction is done to determine the restricted states at the cell edges, these values are then used to calculate the upwinded fluxes needed to advance the Euler equations. AstroBEAR calculates the upwind fluxes via a decomposition of the system matrix of the conservative form of the Euler equations. The approximate linearized Riemann solver of Ryu and Jones (42) is used to decompose the cell edge states into eigenmodes. The same terminology as that found in Ryu and Jones is used, eigenvalues $a_m(Q)$, left and right eigenvectors $L_m(Q)$ and $R_m(Q)$, where $m$ denotes the number of the eigenmode. There are three available methods for determining the flux, the Roe solver, the Marquina solver, and an adapted Marquina solver.

The Roe solver calculates the flux by:

$$F_{x,i-\frac{1}{2}} = \frac{1}{2} (F_x(Q_{L,i-\frac{1}{2}}) + F_x(Q_{R,i-\frac{1}{2}})) -$$

$$\frac{1}{2} \sum_{m=1}^{N} L_{m,i-\frac{1}{2}} (a_{m,i}(Q_{R,i-\frac{1}{2}} - Q_{L,i-\frac{1}{2}}) R_{m,i-\frac{1}{2}})$$

(2.8)

where $N$ is the total number of waves present in the system. $N$ is typically 5 for a 3D pure hydro simulation and $N$=8 for a MHD simulation, one wave for each conserved variable in the system. The Roe solver can usually be approximated using what is called the Roe average state, which is the average state of the left and right
restricted states of a cell edge, and is symbolized by \(< Q_{L,i-\frac{1}{2}}, Q_{R,i-\frac{1}{2}} >\). Using this approximation the eigenvalues and vectors needed for Eqn. 2.6 are given by:

\[
\alpha_{m,i-\frac{1}{2}} = a_m(< Q_{L,i-\frac{1}{2}}, Q_{R,i-\frac{1}{2}} >) \\
L_{m,i-\frac{1}{2}} = L_m(< Q_{L,i-\frac{1}{2}}, Q_{R,i-\frac{1}{2}} >) \\
R_{m,i-\frac{1}{2}} = R_m(< Q_{L,i-\frac{1}{2}}, Q_{R,i-\frac{1}{2}} >)
\]

(2.9)

(2.10)

(2.11)

The Marquina solver uses the flux function:

\[
F_{x,i-\frac{1}{2}} = \sum_{m=1}^{N} \alpha_{m,i-\frac{1}{2}} L_{m,i-\frac{1}{2}}^L + \alpha_{m,i-\frac{1}{2}} R_{m,i-\frac{1}{2}}^R
\]

(2.12)

\[
\alpha_{L,i-\frac{1}{2}} = \begin{cases} 
\sum_{m=1}^{8} L_{m,i-\frac{1}{2}}^L F(Q_{L,i-1/2}) & \text{if } a_{m,i-1/2}^L a_{m,i-1/2}^R > 0 \text{ and } a_{m,i-1/2}^L > 0 \\
0 & \text{if } a_{m,i-1/2}^L a_{m,i-1/2}^R > 0 \text{ and } a_{m,i-1/2}^L \leq 0 \\
\frac{1}{2} \sum_{m=1}^{8} \text{MAX} \left(|a_{m,i-1/2}^L|, |a_{m,i-1/2}^R|\right) L_{m,i-1/2}^L Q_{L,i-1/2} & \text{else}
\end{cases}
\]

(2.13)

\[
\alpha_{R,i-\frac{1}{2}} = \begin{cases} 
\sum_{m=1}^{8} L_{m,i-\frac{1}{2}}^R F(Q_{R,i-1/2}) & \text{if } a_{m,i-1/2}^L a_{m,i-1/2}^R > 0 \text{ and } a_{m,i-1/2}^L > 0 \\
0 & \text{if } a_{m,i-1/2}^L a_{m,i-1/2}^R > 0 \text{ and } a_{m,i-1/2}^L \leq 0 \\
\frac{1}{2} \sum_{m=1}^{8} \text{MAX} \left(|a_{m,i-1/2}^L|, |a_{m,i-1/2}^R|\right) L_{m,i-1/2}^R Q_{R,i-1/2} & \text{else}
\end{cases}
\]

Unlike the Roe solver the Marquina method uses upwinded fluxes to both the left and right sides of a cell. This upwinding leads to eigenvalues and vectors for both sides of a cell and eliminates the need for so called average states. The eigenvalues
present in the Marquina method are:

\[
\begin{align*}
\alpha_{m,i-\frac{1}{2}}^L &= a_m(Q_{L,i-\frac{1}{2}}) \\
\alpha_{m,i-\frac{1}{2}}^R &= a_m(Q_{R,i-\frac{1}{2}}) \\
L_{m,i-\frac{1}{2}}^L &= L_m(Q_{L,i-\frac{1}{2}}) \\
L_{m,i-\frac{1}{2}}^R &= L_m(Q_{R,i-\frac{1}{2}}) \\
R_{m,i-\frac{1}{2}}^L &= R_m(Q_{L,i-\frac{1}{2}}) \\
R_{m,i-\frac{1}{2}}^R &= R_m(Q_{R,i-\frac{1}{2}})
\end{align*}
\]

The final method is an adapted Marquina method. This method employs some of techniques found in the Roe method and introduces a small amount of numerical diffusion into the code. This adapted Marquina method uses the average value states defined in the description of the Roe solver above and redefines the eigenstates as such:

\[
\begin{align*}
\alpha_{m,i-\frac{1}{2}}^L &= a_m(Q_{L,i-\frac{1}{2}}) \\
\alpha_{m,i-\frac{1}{2}}^R &= a_m(Q_{R,i-\frac{1}{2}}) \\
L_{m,i-\frac{1}{2}}^L &= L_m\left(<Q_{L,i-\frac{1}{2}}, Q_{R,i-\frac{1}{2}}>-\right) \\
R_{m,i-\frac{1}{2}}^L &= R_m\left(<Q_{L,i-\frac{1}{2}}, Q_{R,i-\frac{1}{2}}>-\right)
\end{align*}
\]

For the average states described above the codes uses an arithmetic average found in
Ryu and Jones, namely that:

\[ \langle \mathbf{P}^{IJ}_{i-\frac{1}{2}} \rangle = \left( \mathbf{P}^{IJ}_{L,i-\frac{1}{2}} + \mathbf{P}^{IJ}_{R,i-\frac{1}{2}} \right)/2 \]

The Roe solver tends to be a more robust and less diffusive solver than the Marquina solver. Also in the pure hydrodynamic limit talked about in this section the Roe solver can be used with exact formulas for the decomposition of the system matrix instead of an approximation.

2.1.3 Temporal Integration

First order integration of the cell centered values can be achieved by replacing \( n \) with \( t \) in Eqn. 2.8. AstroBEAR also has available four schemes for 2nd order integration that use the Eqn. 2.8 with estimates of the time-centered values for numerical flux.

The first of the schemes is the MUSCL-Hancock predictor-corrector temporal discretization method, which achieves 2nd order accuracy with a 1D predictor method and integrating cell-edge interpolated states by \( \Delta t/2 \). The predictor method is described by:

\[
Q_{L,i+1/2}^{t+\Delta t/2} = Q_{L,i+1/2}^t + \frac{\Delta t}{2\Delta x} \left( F_x(Q_{R,i-1}^t) - F_x(Q_{L,i+1}^t) \right) + \frac{\Delta t}{2} S(Q_i)
\]

\[
Q_{R,i-1/2}^{t+\Delta t/2} = Q_{R,i-1/2}^t + \frac{\Delta t}{2\Delta x} \left( F_x(Q_{R,i}^t) - F_x(Q_{L,i+1}^t) \right) + \frac{\Delta t}{2} S(Q_i)
\]

(2.14)

where \( F_x \) is the cell-centered and volume averaged flux.

The MUSCL-Hancock corrector method generates a 2\( ^{nd} \) order and time centered numerical flux based on the upwinding methods describe in §2.2.2. For this step
$Q_{L,i+1/2}^{t-\Delta t}$ and $Q_{R,i-1/2}^{t+\Delta t}$ serves as the left and right states used by the Riemann solver. Finally the MUSCL-Hancock method integrates Eqn. 2.8 with the time centered fluxes at $n=\Delta t/2$.

A characteristic tracing predictor-corrector temporal discretization method is also available in AstroBEAR. This method uses the characteristic information contained in the family of waves originating at a cell center and carried to a cell edge. The average effect of each wave on the primitive field is done using the piecewise parabolic method described in Colella (39):

\[
P_{L,i+1/2}^m = P_{L,i+1/2} - \frac{\Delta t}{2\Delta x} \text{MAX}(a_{m,i}, 0)
\]

\[
\left( P_{L,i+1/2} - P_{R,i-1/2} - \left[ 6 \left( 1 - \frac{2\Delta t}{3\Delta x} \text{MAX}(a_{m,i}, 0) \right) \left( P_i - \frac{1}{2}(P_{L,i+1/2} + P_{R,i-1/2}) \right) \right] \right)
\]

\[
P_{L,R-1/2}^m = P_{R,i-1/2} - \frac{\Delta t}{2\Delta x} \text{MAX}(-a_{m,i}, 0)
\]

\[
\left( P_{L,i+1/2} - P_{R,i-1/2} - \left[ 6 \left( 1 - \frac{2\Delta t}{3\Delta x} \text{MAX}(-a_{m,i}, 0) \right) \left( P_i - \frac{1}{2}(P_{L,i+1/2} + P_{R,i-1/2}) \right) \right] \right)
\]

The time-centered zone edge states are then generated using on the characteristic waves affecting the left and right averaged states using the following upwinding method:

\[
Q_{L,i+1/2}^m = L^{-1}(P_{L,i+1/2}^m)
\]

\[
Q_{R,i-1/2}^m = L^{-1}(P_{R,i-1/2}^m)
\]

\[
Q_{L,i+1/2}^{t+\Delta t/2} = Q_{L,i+1/2}^+ - \sum_{a_{m,i} > 0} \left[ L_{m,i} \left( Q_{L,i+1/2}^+ - Q_{L,i+1/2}^m \right) \right] R_{m,i} + \frac{\Delta t}{2} S(Q_i)
\]
\[ Q_{R,i-1/2}^{t+dt/2} = Q_{R,i-1/2}^- - \sum_{l,m,s} \left[ L_{m,s} \left( Q_{R,i-1/2}^m - Q_{R,i-1/2}^l \right) \right] R_{m,s} + \frac{\Delta t}{2} S(Q_i) \]  

(2.16)

where the + and - superscripts refer to the characteristic waves with the highest and lowest eigenvalues respectively.

The code also has a 2\textsuperscript{nd} order linear characteristic tracing predictor method. This method is a simplification of the previous method and is achieved by omitting the contents of the square brackets in Eqn. 2.17. The corrector predictor for this method is the same one that is used in the MUSCL-Hancock method already described.

The final available temporal integration scheme is the two-step Runge-Kutta operator found in Shu et al. (43). Step one of the Runge-Kutta method uses equation 2.8 with \( n=dt \) to calculate \( F_i^t \) and \( Q_i^{t+\Delta t} \). The second step uses the spatial reconstruction and upwinding methods described in §2.1.1 and §2.1.2 on the data to calculate \( F(Q_i^{t+\Delta t}) \). The time-centered fluxes are calculated to 2\textsuperscript{nd} order accuracy via:

\[ F_{x,i-1/2}^{t+\Delta t/2} = \frac{1}{2} \left( F(Q_{x,i-1/2}^{t+\Delta t}) + F(Q_{x,i-1/2}^t) \right) \]  

(2.17)

This Runge-Kutta method is somewhat more robust especially in non-linear problems than the MUSCL-Hancock method. However this method is more computationally expensive due to the multiple times the Riemann problem is solved for each cell.

Each time integration method has a \( \Delta t \) limited by the Courant stability condition:

\[ dt < \text{MAX} \left[ \left( \frac{a_{m,i-1/2,j,k}}{\Delta x} \right) + \left( \frac{a_{m,i,j-1/2,k}}{\Delta y} \right) + \left( \frac{a_{m,i,j,k-1/2}}{\Delta z} \right) \right] \text{ for all } i,j,k \]  

(2.18)

AstroBEAR allows the user to define the time step by using a user defined variable
CFL:

\[ dt = \text{CFL} \max \left[ \left( \frac{a_{m,i-1/2,j,k}}{\Delta x} \right), \left( \frac{a_{m,i,j-1/2,k}}{\Delta y} \right), \left( \frac{a_{m,i,j,k-1/2}}{\Delta z} \right) \right] \text{ for all } i,j,k \quad (2.19) \]

where CFL usually equal to 0.8 for 1D problems and 0.4 for 2D and 3D problems. These optimal CFL values are the maximum values for which the code will remain stable.

### 2.2 MHD

When dealing with magnetic systems, the Euler equation changes to:

\[
\frac{\partial}{\partial t} Q + \frac{\partial}{\partial x} F_x(Q) + \frac{\partial}{\partial y} F_y(Q) + \frac{\partial}{\partial y} F_y(Q) = S(Q)
\]
where

\[
Q = \begin{pmatrix}
\rho \\
\rho v_x \\
\rho v_y \\
\rho v_z \\
\epsilon \\
B_x \\
B_y \\
B_z
\end{pmatrix}
F_x = \begin{pmatrix}
\rho v_x \\
\rho v_x v_y - B_y(B \cdot v) \\
\rho v_x v_z - B_z(B \cdot v) \\
(\epsilon + P + B^2/2)v_x - B_z(B \cdot v) \\
0 \\
-E_x \\
E_y
\end{pmatrix}
\]

\[
F_y = \begin{pmatrix}
\rho v_y \\
\rho v_x v_y \\
\rho v_x v_z + P + B^2/2 - B_y^2 \\
(\epsilon + P + B^2/2)v_y - B_y(B \cdot v) \\
E_z \\
0 \\
-E_z
\end{pmatrix}
F_z = \begin{pmatrix}
\rho v_z \\
\rho v_x v_z \\
\rho v_y v_z \\
(\epsilon + P + B^2/2)v_z - B_z(B \cdot v) \\
-E_y \\
E_z \\
0
\end{pmatrix}
\]

with mass density \( \rho \), velocity \( v \), total energy density \( \epsilon \), thermal pressure \( P \), magnetic field \( B \), and electric field \( E \). Faraday’s law and Ohm’s law for a perfectly conducting medium were used to derive the above fluxes for the magnetic fields.

\[
\frac{\partial}{\partial t} B + \nabla \times E = 0
\]
\[ E = -v \times B \]

Solving the magnetic Euler equations also requires the magnetic field to be divergence free. The flux upwinding procedures described in the above section do not inherently preserve this field quantity. The fluxes used in the upwind procedure are simply second order approximations to the exact fluxes and thus the divergence and flux equations are as follows:

\[
\begin{align*}
F_x &= F_x + O(dx^3) \\
F_y &= F_y + O(dy^3) \\
F_z &= F_z + O(dz^3)
\end{align*}
\]

\[ \nabla \cdot B = O(dx^3) + O(dy^3) + O(dz^3) \]

These small scales divergences create an instability that will grow and ultimately corrupt the flow dynamics of the simulation (44). There are two prominent strategies used to modify Godunov-based MHD methods to explicitly maintain zero divergence. The first strategy involves devising a projection operator to remove all numerical divergences from the grid (Balsar 1998, Jiang & Wu 1999, Kim et al 1999, Zachary et al 1994, Ryu et al 1995). Unfortunately as the boundary condition become non-trivial this strategy fails. Since AstroBEAR is an AMR based code, non-trivial boundary conditions will be present in most simulations and thus this strategy is not a workable solution.

The second approach, known as constrained transport (CT), uses a conservative
form of the Stoke's theorem to represent magnetic field components at staggered collocation points. The basic approach of CT is to generate a face-averaged normal component of $\partial B/\partial t$ at each control volume interface. This component along with the average electric field component parallel to the control volume interface are used in the spatial discretization scheme to update the magnetic field components at each control volume interface. A complete description of the implementation of CT into AstroBEAR can be found in Cunningham et. al (9).

2.3 Adaptive Mesh Refinement

AstroBEAR is a patch based adaptive mesh refinement (AMR) code. A patch based scheme chooses regions of physical space in the grid to refine to a higher resolution as opposed to determining refinement on a cell by cell basis. In general AMR methods are designed to increase the efficiency of a simulation code by allowing for higher resolutions only where small scale structures exist. This varying resolution allows the portions of the mesh essential doing nothing to be left at a coarser resolution easily able to capture any large scale structures in these regions. Overall this leads to fewer overall computational cells than if the entire mesh were set to the highest resolution that will ever be needed throughout the entire simulation.

There are many different methods for determining where in the mesh a patch is needed to gain resolution. AstroBEAR tracks this process via an array that mirrors the mesh for each refinement level. When the code determines that a cell is in an area of need of refinement its value in the mirror mesh is set to 1 instead of 0. The code will then take all cells that have been marked for refinement and create a patch to cover these cells and a user defined area around these cells. The code has built in
checks for large density and pressure gradients. Above a set threshold these gradients will trigger a cell to be flagged for refinement. It is also possible for a user to write directly into the setup file for a particular simulation additional refinement checks, i.e. cells above a certain temperature or density etc.

The AMR algorithm is adaptive in time as well as space. In general, the update procedure starts by identifying on the coarser grid what areas of the mesh will be patched with a higher resolution mesh. Once these patches are determined all cells outside the patches are advanced one time step $\Delta t$ via the methods described in §2.1. The cells neighboring the patches are advanced with the zero flux from the patched regions. The code then handles the patched areas one level higher in resolution. On this level the code advances the cells two time steps each of $\Delta t / 2$. This advancement not only updates the quantities of the conserved variables on the finer level but also during the upwinding step on the finer level the fluxes along the patch edge are also calculated. Next the coarser grid is updated with the data from the finer grid. The finer level fluxes along the patch boundaries are then used to fully advance the coarser level cells that lie along the patch edge. During the next time step the patches are reevaluated to see if they are still necessary or if they needed to be moved. Cells that were in a patch that have been moved up one level of refinement are then prolonged back to the coarser resolution. The process described is a recursive process capable of handling multiple levels of AMR. In that case each level will follow the above process and continue refining until the used defined max refinement level is reached.

Specifically the first step on a particular level starts by initializing what are called ghost cells. These are cell that lie either outside of the computational domain or a patch. There are three types of ghost cells that arise in the code. The first type of
ghost cell is a physical ghost cell, one that lies outside of the computational domain of the entire base mesh. Secondly we have higher level ghost cells, these are cells that lie outside of a patched region but are one level coarser in resolution. Lastly we have same level ghost cells, these are cells that lie outside of a patched region but are on the same level of AMR and lie interior to another patched region. Physical ghost cells are set using one of three user selected boundary conditions: extrapolating, periodic, or reflecting. Same level ghost cells are set to the values of the cell interior to the neighboring patch. Higher level ghost cells are explained in detail later during the discussion of prolongation and restriction methods.

The next step is to determine what areas of the mesh are to be flagged for refinement. This step is where the setting of higher level ghost cells are initialized. The code will have the patched areas required for this timestep and the areas from the previous time step still in memory. Areas in the new patches that overlap with the patches from the previous timestep are simply filled by copying the values from the previous time step. The patchwork from the previous timestep is then released from memory. Ghost cells and interior cells that lie outside the previous patchwork are filled via a prolongation operator based on the interpolation of the values at the coarser level. In a non-MHD simulation this is a simple cell-centered average value interpolation. The prolongation operator necessary for MHD is described in §5.5.

Once the cells on the finer level have been initialized the code then advances in time the cells on the finer level two timestep \( \Delta t \). Since the ghost cells on the finer level are only initialized at time \( t \) and not \( t + \frac{\Delta t}{2} \), the ghost cells will only be synchronized every other timestep on the finer level. To overcome this obstacle the code adds an extended layer of ghost cells around a particular patch. Each patch will carry with
it ghost zones extending $r \times mbc$ where $r$ is the refinement ratio, usually 2, and $mbc$ is the number of ghost zones required by the spatial integration technique being used. This setup will allow the first ring of ghost zones to be used when integrating from $t$ to $\Delta t/2$ and out to the second layer when integrating from $t + \Delta t/2$ to $t + \Delta t$.

Once the finer level have been advanced in time the code must then synchronize the finer level with the coarser level. This process requires two main steps: updating fluxes and restricting the solution. The fluxes along the patch boundary calculated on the finer level are compared to those calculated during the advancement of the coarser level. The coarser level fluxes are then adjusted to have the same effective flux as the finer level. The conserved variables in the patch are the restricted to the coarser level grid. A volume weighted average is used for the restriction process. With all of the corrected fluxes and variables available on the coarser grid the cells that lie along the exterior edge of the patch can be properly updated. As mentioned above this is a recursive method and can be carried out with the "coarse" grid set to be any level of AMR except the max level.

2.4 Parallelization

AstroBEAR's parallelization scheme is an adaptation from the BEARCLAW method. It is a spatially based parallelization method as opposed to a task oriented one. Originally, AstroBEAR was a pure hydrodynamics code so the spatially based method makes sense. In general at the beginning of a simulation the code will decompose the base level mesh into sub domains and send all of the cells in a domain to a single processor. From that point on all calculations dealing with a particular cell are carried out on the processor on which it resides, essentially the code runs serially
on each processor. The domains can change and be shifted from one processor to
another at anytime if the code decides it would be more efficient. A task oriented
parallelization scheme would focus more on sending sets of tasks and calculations to
different processors to make maximum use of available cpu cycles. The advantage of a
spatially based scheme for a pure hydro code is that either increasing the physical size
or resolution of a particular simulation can be easily dealt with by adding additional
processors to handle the increased number of cells. With the continual addition of
more and more microphysics to the code, the number of calculations per cell is also
increasing. Work is currently being done to combine the spatial parallelization scheme
with a task oriented approach to allow for additional processors to handle extra tasks
as well as extra grid cells.

The parallel structure of the code is built around a single master processor with
multiple worker processors and uses the Message Passing Interface (MPI) paralleliza-
tion structure (45). MPI is a library of functions used for passing information between
multiple processors being concurrently used. The master processor controls the data
flow, keeps track of which parts of the mesh are on which processors, and determines
if a better configuration would be more efficient. At the beginning of a simulation
the master processor decides, based on a user set variable, how many sub domains
to decompose the bash mesh into and onto which processors these sub domains will
be sent. During this initial decomposition process, for example, if a user specifies
4 subdomains with no AMR but runs the simulation on 8 processors, four of the
processors simply will do nothing throughout the entire simulation. The addition
of AMR allows the master processor to load balance the distribution of cells across
processors. At each step the master processor well determine if moving a grouping
of higher level AMR cells from their original processor to one with more available processing time. If a grouping of cells is to be moved, the entire AMR structure will be moved. If at all possible children cells, i.e. cells at a high resolution AMR level, will always be kept on the same processor at their parent cells. Keeping the structure in tact greatly reduces the necessary communication between processors necessary to advance the hydrodynamic equations in time as this process requires information from both parent and children cells.

At the beginning of each time step the master processor sends a signal to each worker processor to advance one timestep the entire base level mesh. This advancement will result in an updating of the conserved variables for each base grid cell on all processors. After completing this step each worker processor sends a completion message to the master processor. The workers are then directed to determine where in their subdomain AMR refinement in necessary, this process is described in §3.1.2. The workers then generate the appropriate number of children cells based on the user defined refinement criteria, usually two children for one parent. The master processor then receives completion messages and children cell info from each processor. At this point the master processor can move cells from one processor to another if the load balancing criteria suggests it would be more efficient. This process is then repeated at the new refinement level where one timestep is smaller than the coarser grid by the refinement ratio, usually two. The process follows the AMR method described in §3.3 for advancing the conserved variables in time and space. The master processor can step in at each instance described above to rearrange cell placements based on load balancing criteria.

Currently work is being done in main areas for improving the efficiency of the par-
allelization. One of the main time consumers of this method involves the initialization of the ghost cells. As described in §3.2. There are three different types of ghost cells and each require initialization at every timestep for a particular AMR level. With multiple processors the information needed to initialize a ghost cell for region on one processor may lie on a different processor. As the number of processors and the number AMR patches increases, the amount information passing from worker to another also increases. Currently the code is set up so that the master processor is always the middle man between two worker communicating ghost cell information. Work is being done to simple allow two workers to talk directly to each other and cut out the extra communication overhead associated with the master processor. Secondly as described above work is being done to adapt the spatial nature of the parallelization scheme to one that is more task oriented and better able to handle increases in the type of additional physics included in the code. These changes will most likely involve designated one processor as the master processor for tasks, i.e. it will be able to shift particular tasks from one processor to another without having to move the cell these tasks are associated.

2.5 Additional Physics

Included in this section is a description of all of the additional physics currently available in AstroBEAR, i.e. radiative cooling and gravity. In addition a brief description of how the codes handles 2.5D simulations is included because the code treats this situation as a type of additional physics. To incorporate the additional physics desired the code must be able to handle advective tracers as well as source terms to the Euler equations.
Advective tracers are simply waves based on the multifluid advection method of Plewa & Muller (46). The code has mechanism called species tracking. With this switch turned on, at any given physical point in space the user may specify as many additional tracers as desired. These tracers are treated by the code as conserved densities and each is assigned a wave. The species tracking function requires that the density of the tracer materials must add up to the overall conserved density of a cell. By defining certain regions of space to be entirely one tracer initially, at later times one can determine what fraction of a given cell's mass density came originally from which region of the setup. Specifically in the area of radiative cooling, these tracers allow the different ionization states of different elements to be tracked and the cooling function to be determined accordingly.

With source terms, the code uses the form of the Euler equation show in Eqn. 2.1. The source term, for a 3D simulation, can be expressed generally as:

$$ S(Q) = S_c + S_{grav} $$
\[
S_c = \begin{cases}
0 \\
0 \\
0 \\
0 \\
\end{cases} -\Lambda \\
\mu_{H_2}(R_{H_2} - D_{H_2}) \\
\mu_{H_i}(2(D_{H_2} - R_{H_2}) + D_{HI} - R_{HI}) \\
\mu_{HI}(R_{HI} - D_{HI}) \\
\mu_n(R_n - D_n)
\end{cases}
\]

\[
S_{\text{grav}} = \begin{cases}
0 \\
-x\rho \\
y\rho \\
z\rho \\
-pv_x x + pv_y y + \rho + v_z z
\end{cases}
\]

where \( S_c \) is the source term due to radiative cooling and \( S_G \) is the source term due
to gravity and \( n \) is the number of species the user has decided to track. \( R_x \) and \( D_x \) denote the recombination and ionization/dissociation rates for a given species and \( \mu_x \) denotes the molecular weight that species in amu. \( \Lambda \) is the overall cooling rate for a particular cell in units of erg cm\(^{-3}\) s\(^{-1}\). The full description of how \( \Lambda \) is calculated can be found in §4.1. Obviously if either gravity or cooling is turned off these source terms are simply set to zero. The conserved matrix \( Q \) and the flux matrix \( F \), also can be expressed in a general way:

\[
\begin{pmatrix}
\rho \\
\rho v_x \\
\rho v_y \\
\rho v_z \\
E_{kin} + E_{th} \\
\rho H_2 \\
\rho H I \\
\rho H II \\
\rho H III \\
. \\
. \\
. \\
\rho_n
\end{pmatrix}, \quad F = v_{tot} \begin{pmatrix}
\rho \\
\rho v_x \\
\rho v_y \\
\rho v_z \\
E_{kin} + E_{th} + P \\
\rho H_2 \\
\rho H I \\
\rho H II \\
. \\
. \\
. \\
\rho_n
\end{pmatrix}
\]

Simulating in 2.5D, otherwise known as cylindrically symmetric, is achieved by adding a geometric source term to the Euler equation. In this configuration \( Q, F \),
and $S_{\text{eql}}$ are given by:

$$
Q = \begin{bmatrix}
\rho \\
\rho v_r \\
\rho v_z \\
\rho v_\theta \\
E_{\text{kin}} + E_{\text{th}} \\
\rho H_2 \\
\rho H I \\
\rho H II \\
\rho_n \\
\end{bmatrix}, \quad F = v_{\text{tot}} = 
\begin{bmatrix}
\rho v_r \\
\rho v_z \\
\rho v_\theta \\
E_{\text{kin}} + E_{\text{th}} + P \\
\rho H_2 \\
\rho H I \\
\rho H II \\
\rho_n \\
\end{bmatrix}, \quad S_{\text{eql}} = 
\begin{bmatrix}
\rho v_r \\
\rho v_z \\
\rho v_\theta \\
\rho v_e^2 - \rho v_\theta^2 \\
v_r (E + P) \\
\rho H_2 \\
\rho H I \\
\rho H II \\
\rho_n \\
\end{bmatrix}
$$

With the source term switch on, the code still uses the method’s described in §3 to advance the source-term free portion of the Euler equation:

The source terms are integrated separately using an implicit fourth order Rosenbrock integration scheme for stiff ordinary differential equations. A scheme for dealing with stiff ordinary differential equations (ODE) is used due to the potentially highly variable effect the source terms can have on the solution. Ordinary differential equation schemes not suited for stiff ODE’s proved to be unstable when used on these source terms. The source term integration and the hydro integration are combined using a split operator approach. The detailed description of this split operator procedure can be found in Cunningham et. al (9).
Chapter 3

Laboratory Astrophysics and Non-ideal Equations of State

Incorporating a non-ideal equation of state into an astrophysical MHD code represents the next necessary step if simulations are to keep pace with the technological advancements in laboratory astrophysics studies and if the goal of connecting laboratory experiments with astronomical data is to be achieved. This chapter focuses on adding this capability to AstroBEAR(9), an Eulerian based code that has the 3D, MHD, AMR, and parallelization capabilities and is discussed in more detail in Chapter 2. Given AstroBEAR’s extensive use simulating the types of astrophysical flow structures that laboratory experiments are designed to reproduce and its inclusion of magnetic fields, it provides a good base code upon which to build a non-ideal gas EOS capability for simulating these laboratory experiments and future magnetized experiments.

This chapter will explore some differences between a non-ideal EOS and an ideal EOS framework. We will discuss the difficulties associated with incorporating a non-ideal EOS into an ideal EOS-based code and what changes were necessary to adapt AstroBEAR to a non-ideal gas code. We will also show the results from our first simulation of a laboratory experiment using AstroBEARs non-ideal EOS capability. We will compare ideal EOS simulations, non-ideal EOS simulations, and experimental results. These comparisons demonstrate AstroBEAR’s increased ability to accurately
simulate the laboratory environment.

3.1 Non-ideal EOS

Earlier versions of AstroBEAR had only ideal gas equation of state capability. For an ideal gas the energy density, \( \epsilon \), can be expressed by:

\[
\epsilon = \frac{F}{2} nk_b T
\]  

(3.1)

with degrees of freedom \( F \), temperature \( T \), number density \( n \), and Boltzmann’s constant \( k_b \). For an ideal gas the adiabatic constant \( \gamma \) and the pressure \( P \) are given by:

\[
\gamma = \frac{C_p}{C_v} = \frac{2 + F}{F}
\]  

(3.2)

\[
P = nk_b T = \frac{\rho k_b T}{\mu m_H}
\]  

(3.3)

where \( C_p \) and \( C_v \) are the specific heats of the gas at constant pressure and volume respectively, \( \rho \) is the mass density, \( m_H \) is the mass of hydrogen, and \( \mu \) is the mean molecular weight. For example the mean molecular weight of titanium is defined by \( \mu_{Ti} = m_{Ti} / (Z+1) \) with \( m_{Ti} \) equal to the molar mass of titanium and \( Z \) the ionization state of Ti, where \( Z = 0 \) is neutral Ti. Combining Eqns. 3.1, 3.2 and 3.3 yields the equation of state used by AstroBEAR when dealing with ideal gases:

\[
P = (\gamma - 1) \epsilon
\]  

(3.4)

To utilize equation 3.3 to generate an ideal EOS for titanium we must know how \( \mu \)
depends on density and temperature. For a fixed density, as the temperature increases
titanium becomes more ionized and $\mu$ decreases. For example, $\mu_{TII}=47.90$, $\mu_{TIII}=23.95$, $\mu_{TIII}=15.97$, etc. To approximate $\mu$ as a function of temperature and density
for the ideal case we use the Saha equation:

$$\frac{n_{i+1}n_e}{n_i} = 2 \left( \frac{2\pi m_e k_B T}{\hbar^2} \right)^{3/2} \frac{Z_{i+1}}{Z_i} \frac{e^{x_i/(k_B T)}}{1}$$

(3.5)

where $n_i$ and $n_{i+1}$ represent adjacent ionization states, $n_e$ is the electron number
density, $m_e$ is the electron mass, $T$ is temperature, $\hbar$ is Planck's constant, $x_i$ is the
ionization energy for the $i$th ionization state, and $Z$ is the partition function. However
at high temperatures the complicated level structure of a metal such as titanium
makes the calculation of partition functions non-trivial. For the purposes of our ideal
titanium EOS calculations we assumed the ratio of partition functions to be equal
to 1. These partition function are of order unity and should not have a significant
effect on the results generated using the Saha equation. For example, at a density
of 1.0 g cm$^{-3}$ and temperature of $10^5$ K, using our partition function assumption
yields a $\mu$ of 15.75 with TiII being the dominant ionization state. However if we set
$Z_{TIII}/Z_{TII}=2.0$, the Saha equation yields a $\mu$ of 14.95 only 5% change from our
previous result.

Fig. 3.1 compares the pressure-temperature dependence of this ideal EOS for
titanium with a non-ideal EOS obtained from the SESAME (47) tables, discussed in
more detail below. The dominant titanium species, from ideal calculations, is labeled
on each figure. As expected, these plots show that as the gas moves into a lower
density-higher temperature regime the ideal EOS and the SESAME EOS converge.
However, as the gas moves towards higher density-lower temperature regimes the SESAME EOS begins to deviate from the ideal EOS with the non-ideal nature of the gas most evident as the density approaches the solid density of titanium, $4.5 \text{ g cm}^{-3}$.

![image](image.png)

Figure 3.1: Real vs. Ideal EOS for titanium. The Roman numerals denote the dominant ionization state of the Ti, as determined from the Saha equation.

The basic assumption that underlies the ideal gas equation is that there are only collisional interactions between particles. However high-density plasmas contain charged particles in relatively close proximity, leading to non-collisional interactions and to non-ideal gas behavior. There are three main effects that cause a non-ideal gas EOS to differ from the ideal EOS: Coulomb interaction, ionization potential perturbation, and electron degeneracy gas pressure.

At low number densities the Coulomb interaction between particles is an overall attractive effect. Positively charged ions attract negatively charged free electrons,
known as Debye shielding. This attraction causes the ions to be more bound which in turn depresses the overall pressure of the gas. Debye shielding is significant so long as $n \ll 1.1 \times 10^5 (T/Z^2)^3 \text{ cm}^{-3}$, where $Z$ is the average ionization state of the gas (48). For a gas with $Z \sim 1$ at $T=5.0 \times 10^4 \text{ K}$, this condition is $n \ll 10^{19} \text{ cm}^{-3}$. In our experiments the number densities range from $10^{21} - 10^{22} \text{ cm}^{-3}$, so we can neglect the effects of Debye shielding in our calculations.

As the separation between ions decreases, Coulomb repulsion between the electrons bound to each ion increases. This interaction causes the electrons to become more loosely bound and results in an overall lower ionization potential at high densities. This ionization perturbation represents a major deviation from an ideal EOS for laboratory experiments and can be approximated by (48):

$$
\Delta I = 2(Z + 1)e^3 \left[ \frac{(\pi Z(Z+1)n)}{(kT)} \right]^{1/2}
$$

(3.6)

where $Z$ is the average ionization state of the ideal gas, $n$ is the number density, and $T$ is the temperature. For example, Ti gas with $\rho=4.5 \text{ g cm}^{-3}$ and $T=5.0 \times 10^4 \text{ K}$ has a change in average ionization potential of $\sim 35 \text{ eV}$. Given that the sum of the first 3 ionization energies of Ti is $\sim 45 \text{ eV}$ we can expect that this will effectively raise the average ionization state of Ti from 1.0 to $\sim 3.25$. This increase in ionization will lead to a decrease in $\mu$ and thereby an increase in pressure by a factor $\sim 3.25$. As the temperature increases the ionization perturbation decreases leading to convergence of the ideal number density and the non-ideal number density at high temperatures. This non-ideal effect is seen in Fig. 3.1(d).

Finally, as the density of the gas increases, so does the importance of electron
Electron degeneracy is important when the temperature is on the order of or smaller than the electron degeneracy temperature \( T_a = 4.5 \times 10^{-11} n^{2/3} \) K, where \( n \) (cm\(^{-3}\)) is the electron number density (48). Again using titanium as an example, for \( \rho = 0.1 \) g cm\(^{-3}\), \( T_0 = 5.0 \times 10^4 \) K while for \( \rho = 4.5 \) g cm\(^{-3}\), \( T_0 = 5.9 \times 10^4 \) K. As a result we can expect electron degeneracy pressure to have an effect for the high density gases at temperatures \( \lesssim 10^5 \) K. The minimum electron degeneracy pressure, \( P_d = (2.0 \times 10^{-11}) k_b n^{5/3} \) dyne/cm\(^2\) (48) where \( n \) is the electron number density (cm\(^{-3}\)) and \( k_b \) is Boltzmann's constant, for Ti gas at solid density and \( T = 5.0 \times 10^4 \) K is on the order of \( 2.0 \times 10^{11} \) dyne/cm\(^2\) for singly ionized Ti. This electron degeneracy pressure results in an increase in the pressure of a non-ideal gas relative to an ideal gas. As with the ionization potential, this effect will disappear at high temperatures well above the electron degeneracy temperature. The electron degeneracy pressure also vanishes at the lower temperatures when Ti is neutral. This non-ideal effect can be seen in Fig. 3.1(d).

The combination of Coulomb interactions, ionization potential perturbation and electron degeneracy will increase the pressure of a non-ideal gas relative to that of an ideal gas as the density of the gas increases. For example, at \( T = 5.0 \times 10^4 \) K, the factor 3.25 increase in pressure associated with the ionization potential perturbation and the \( 2.0 \times 10^{11} \) dyne/cm\(^2\) increase in pressure associated with electron degeneracy explain the difference between the non-ideal and ideal gas pressures plotted in Fig. 3.1. Given that our experiments involve vaporized solids at high densities, the expected non-ideal nature of these gases makes using an ideal EOS insufficient to accurately simulate the hydrodynamics.

Another example of the need for non-ideal EOS is the simulation of a solid ma-
A solid by its very nature implies that there are non-collisional interactions between particles. The strong bonding between particles restricts the ability of the particles to move freely. Therefore when energy is added to a solid this energy is used to break bonds before being used to increase kinetic energy, an obvious deviation from an ideal gas. Currently, AstroBEAR does not explicitly track the phase of a material; it instead relies on the SESAME tables which contain implicit phase behavior, mainly through the pressure derivatives. With solid materials, as with high-density plasmas, a non-ideal EOS must be used to model the laboratory experiments.

We used the SESAME tables, provided by Los Alamos National Laboratory (LANL), to determine the non-ideal EOS for the materials of interest. The SESAME tables are a collection of the data for many different elements and materials from a variety of sources, and these tables provide an array of physical properties. Since our code uses pressure and pressure gradients to determine flow we used the SESAME tables for pressure as a function of mass density and temperature. Energy density is a conserved variable and not temperature, so the SESAME table for energy density as a function of temperature and mass density had to be inverted to allow for the calculation of temperature. The tabular entries are derived from a combination of experimentally observed values, theoretically determined values, and interpolated values. These tables also include a series of FORTRAN routines for retrieving values and for interpolation.

The derivative of pressure with respect to energy density at constant mass density is contained in the SESAME tables and plays an important role in the computational scheme described in §3. For an ideal gas, this derivative can be easily calculated from
Eqn. 3.4 as:
\[ \kappa = \frac{\partial P}{\partial \epsilon} \bigg|_{\rho} = \gamma - 1 \] (3.7)
which is equal to 2/3 for both monatomic and non-relativistic electron degenerate gases. Therefore we expect that in the low density-low temperature and high temperature limits a gas will behave like an ideal gas and that \( \kappa \) will asymptotically approach 2/3. We also expect that at the highest densities when electron degeneracy is dominant \( \kappa \) will remain 2/3. In the non-ideal gas regime the energy is partitioned between increasing kinetic energy and ionization. In this sense ionization acts as an additional degree of freedom and decreases \( \gamma \) in much the same way that the rotational and vibrational modes of a molecule decrease \( \gamma \). Therefore we expect \( \kappa \) to decrease in the \( \rho - T \) regions where ionization is important. As a simple example, Fig. 3.2 shows a plot of \( \kappa \) as function of temperature and mass density for H. As expected at low temperatures \( \kappa \) goes to 2/5, \( \gamma - 1 \) for a diatomic gas, and at high temperatures it approaches 2/3, but at the intermediate temperatures \( \kappa \) decreases due to dissociation and ionization as the gas goes from H\(_2\) to H to H\(^+\).

We expect Ti to have a more complex plot for \( \kappa \) due to its many ionization levels as well as different phases. Fig. 3.3 is a plot of \( \kappa \) for Ti obtained from the SESAME tables and clearly shows \( \kappa \) following the aforementioned trends. The lowest and highest densities asymptote to \( \sim 2/3 \) in low temperature limit and all densities asymptote to 2/3 in the high temperature limit. For the intermediate temperatures \( \kappa \) clearly drops as the gas begins to ionize and then returns to 2/3 when the gas becomes fully ionized. There is also a bump occurring at temperatures \( \sim 8.0 \times 10^4 \) K which corresponds to the transition from TiIV to TiV as the dominant ionization species.
Figure 3.2: Plots of $\kappa$ for H
This increase is expected because TiV is an Ar-like closed shell and much more difficult to ionize. Hence, the partition of energy is shifted back towards increasing kinetic energy and thereby raising $\gamma$. The final feature to note in Fig. 3.3 is the rise of $\kappa$ at low temperatures for densities where Ti is expected to be solid but not fully degenerate, these values of $\kappa$ represent the phase information implicitly contained in the SESAME tables.

Another aspect of laboratory experiments that differs from many astrophysical situations is the need to simulate multiple materials (see §3.3). Previously AstroBEAR had no capability to handle multiple non-ideal materials. Since each material in a simulation will have a unique EOS, any modification to the code to include non-ideal EOS also necessarily requires multiple non-ideal material capability. The computational approach to multiple materials used here will be discussed in the following two sections.

3.2 Numerical Methods

The Euler equations solved by AstroBEAR are given in Eqn. 3.8 in §2. For the present study we have updated the implementation of the hydrodynamic Riemann solver of Roe (49) for an arbitrary equation of state. The Roe approach considers the Euler equations in an approximate linearized form,

$$\frac{\partial Q}{\partial t} + A_x \frac{\partial Q}{\partial x} + A_y \frac{\partial Q}{\partial y} + A_z \frac{\partial Q}{\partial z} = 0$$

(3.8)

The AstroBEAR code implements several integration schemes for advancing of conservation law systems as described in §2.1.1 and §2.1.2. The code is implemented so
Figure 3.3: Plots of $\kappa$ for Ti
that the system of conservation laws under consideration are specified by the eigenvalues, right eigenvectors and left eigenvectors of the system matrix $A_{x\ ij} = \frac{\partial f_i}{\partial Q_j}$.

The linearized Euler equations are specified by the system matrix

$$A_x(Q) = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
\chi - v_x^2 + \kappa \nu^2 / 2 & -(\kappa - 2)v_x & -\kappa v_y & -\kappa v_z & -\kappa & 0 \\
-v_x v_y & v_y & v_z & 0 & 0 & 0 \\
-v_x v_z & v_z & 0 & v_x & 0 & 0 \\
\chi - v_z H + \kappa v_x v^2 / 2 & -\kappa v_z^2 + H & -\kappa v_y v_z & -\kappa v_z v_z & \kappa v_z & 0 \\
\rho_T v_z / \rho & \rho_T / \rho & 0 & 0 & 0 & v_z
\end{bmatrix}$$ (3.9)

where $v=$velocity, $H=$enthalpy per unit mass. Following the approach described by Mottura (50), we have defined the system matrix in terms of the pressure derivatives

$$H = \frac{P + E}{\rho}$$ (3.10)

$$\chi = \frac{\partial P}{\partial \rho} \epsilon$$ (3.11)

$$\kappa = \frac{\partial P}{\partial \epsilon} \rho$$ (3.12)

to implement arbitrary equation of state capability where $\epsilon = E - \rho v^2 / 2$ is the thermal energy per unit volume. In terms of the pressure derivatives, the sound speed is defined as

$$c = \sqrt{\chi + \kappa \left( H - \frac{1}{2} \nu^2 \right)}.$$ (3.13)
The desired eigenvalues are given as the components of the vector

$$\lambda = \left[ \begin{array}{c} v_z - c \\ v_x \\ v_x \\ v_x \\ v_x + c \end{array} \right]$$

the corresponding right eigenvectors are the columns of the matrix

$$R = \left[ \begin{array}{cccc} 1 & 0 & 0 & 1 \\ 0 & v_x - c & 0 & 0 \\ 1 & 0 & v_y & 0 \\ 0 & 1 & v_z & 0 \\ v_x - c & v_y & v_z & 0 \end{array} \right]$$

and the corresponding left eigenvectors are the rows of the matrix

$$L = \left[ \begin{array}{ccccc} \frac{c^2 + c v_x + \kappa (u^2 - H)}{2c^2} & -\frac{\kappa v_x}{2c^2} & -\frac{\kappa v_y}{2c^2} & \frac{\kappa}{2c^2} & 0 \\ -v_y & 0 & 1 & 0 & 0 \\ -v_x & 0 & 0 & 1 & 0 \\ \frac{\kappa (u - v)}{c^2} & \frac{\kappa v_x}{c^2} & \frac{\kappa v_y}{c^2} & \frac{\kappa}{c^2} & 0 \\ \frac{\kappa (H + v^2)}{c^2} & \frac{\kappa v_x}{c^2} & \frac{\kappa v_y}{c^2} & \frac{\kappa}{c^2} & 1 \end{array} \right]$$

The Marquina (38) flux function implemented in the code calls for the computation of the above eigen decomposition of fluid states that are interpolated to the left, $Q_L$ and right edge, $Q_R$, of each computational cell interface. The Roe (9) flux option
in the code, on the other hand, calls for the decomposition of a suitably averaged interfaces state. The density, fluid velocity and enthalpy are given by

\[ \rho = \sqrt{\rho_L \rho_R} \quad (3.17) \]
\[ \mathbf{v} = \frac{\mathbf{v}_L \sqrt{\rho_L} + \mathbf{v}_R \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (3.18) \]
\[ H = \frac{H_L \sqrt{\rho_L} + H_R \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (3.19) \]
\[ \rho_T = \frac{\rho_T \sqrt{\rho_L} + \rho_T \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (3.20) \]

and for a general equation of state, an interface average of the pressure derivatives is also required. For the present work we have used the arithmetic average

\[ \kappa = \frac{\kappa_L + \kappa_R}{2} \quad (3.21) \]
\[ \chi = \frac{\chi_L + \chi_R}{2}. \quad (3.22) \]

Because the code utilizes the arithmetic averaged linearized Riemann solver of Ryu & Jones (42) for magnetohydrodynamical problems, we expect this choice of pressure derivative averaging will allow simpler extension for MHD problems.

### 3.3 Validation Testing

Once the non-ideal EOS framework was in place, we tested it with a van der Waals EOS and series of four shock tube problems named WV1, DG1, DG2, and DG3 by Guardone and Vigevano (51). The van der Waals EOS gives pressure and its
derivatives as:

\[
P = \frac{\delta (E + a \rho^2) - a \rho^2}{1 - b \rho}
\] (3.23)

\[
\chi = \frac{b(E - a \rho^2) + 2a \rho}{(1 - b \rho)^2} - 2a \rho
\] (3.24)

\[
\kappa = \frac{\delta}{1 - b \rho}
\] (3.25)

where \(a\) and \(b\) are the van der Waals constants, \(E\) is thermal energy density, \(\rho\) is mass density, \(\delta = (R)/(\mu_o c_v)\), \(\mu_o\) is the mean molecular weight, \(c_v\) is the specific heat at constant volume, and \(R\) is the universal gas constant.

Figs. 3.4 and 3.5 shows the shock tube test problem results and Table 3.1 shows the initial conditions for the four tests, where pressure and density are defined relative to the critical values \(P_{\text{crit}} = a/27b^2\) and \(\rho_{\text{crit}} = 1/3b\). These 1D simulations contained 400 cells from \(x=0\) to 1.0 with the density and pressure jumps initially occurring at \(x=0.5\).

In each plot, the results obtained from AstroBEAR’s ideal EOS are plotted against the results from AstroBEAR’s van der Waals EOS. In all four cases AstroBEAR’s non-ideal Roe implementation scheme shows excellent agreement with the results found in Guardone and Vigevano (51).

<table>
<thead>
<tr>
<th>Test</th>
<th>(P_i)</th>
<th>(\rho_i)</th>
<th>(P_r)</th>
<th>(\rho_r)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WV1</td>
<td>1.60770</td>
<td>1.010</td>
<td>0.8967</td>
<td>0.594</td>
</tr>
<tr>
<td>DG1</td>
<td>3.00</td>
<td>1.818</td>
<td>0.5750</td>
<td>0.275</td>
</tr>
<tr>
<td>DG2</td>
<td>1.09</td>
<td>0.879</td>
<td>0.8850</td>
<td>0.562</td>
</tr>
<tr>
<td>DG3</td>
<td>1.09</td>
<td>0.879</td>
<td>0.5750</td>
<td>0.275</td>
</tr>
</tbody>
</table>

Table 3.1: van der Waals shock tube initial conditions
Figure 3.4: Comparison between AstroBEAR (left) and G&V (right) of van der Waals tests WV1 at t=0.2
Figure 3.5: Comparison between AstroBEAR (left) and G&V (right) of van der Waals tests DG1 at $t=0.15$
Figure 3.6: Comparison between AstroBEAR (left) and G&V (right) of van der Waals tests DG2 at $t=0.45$
Figure 3.7: Comparison between AstroBEAR (left) and V & G (right) of van der Waals tests DG3 at t=0.2
3.4 Experimental Setup

The experiments were conducted on the OMEGA Laser at the Laboratory for Laser Energetics (LLE) in Rochester, NY. The target schematic depicted in Fig. 3.8 is the target used in the experiments as well as the simulations. The entire target chamber is kept under high vacuum and the hohlraum is irradiated by lasers from the left of the diagram. This irradiation causes the cavity to heat to temperatures on the order of $1.0 \times 10^6$ K. At these temperatures the peak black body radiation is x-ray, which is then deposited into the adjacent titanium not covered by the gold shield. This laser deposition drives an ablation front off of the titanium from right to left, driving a shock to the right and through the titanium. The vaporized titanium then expands into the vacuum inside the washer hole. While passing through this vacuum the vaporized titanium accelerates until it hits the CH foam at the end of the vacuum tunnel. This collision and subsequent propagation of the titanium into the foam leads to jet formation in the foam. Experiments were conducted both with and without obstruction, i.e. CH ball, present in the foam.

The experimental data are radiograph images of the target at various times after the driving laser pulse. These images are generated by pin-hole backlighter irradiated by a separate laser pulse. The heating of this back lighter generated x-rays, which were channeled through a pin-hole so that the x-ray source had a well defined shape. The x-rays then passed through the target and the transmitted radiation was captured by either a photographic plate or CCD camera. The radiograph generation process is depicted in Fig. 3.9.
Figure 3.8: Laser target schematic

Figure 3.9: Radiograph Generation Process
3.5 Experimental Summary

I was a member of a large collaboration of researchers from Rice University, University of Rochester, Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL), Atomic Weapons Establishment (AWE), and General Atomics. The goal of our experiments was to produce jets and shocks in the laboratory environment that are analogous to astrophysical phenomena such as HH jets. These experiments so far consist of two experiment days per year on the OMEGA laser at the Laboratory for Laser Energetics (LLE) in Rochester, NY. We have had a total of 9 shot days beginning in May 2005 with the last being in February of 2009. This project is ongoing with another 3 more shot days already scheduled. The radiographs produced from the first 5 shot days can be found in Appendix A and the details of each shot can be found in Tables 3.2 and 3.3.

First, we studied the reproducibility of these experiments. Since each laser shot destroys the target and only one image of the jet at one point in time is produced from each shot, we needed to determine if these experiments were even possible or if we would be limited by target manufacturing capabilities. With this problem in mind, we used our first shot day in May 2005 (S05) to generate images at the same time using the same backlighters of targets that were as identical as possible. Fig. 3.10 which shows radiographs of similar targets at similar times and demonstrates the reproducibility of the experiments. While generally we were able to achieve a reproducible result, it was also obvious that target alignment and fabrication issues can have a large effect on the results of the experiment and thus precise manufacturing was of the utmost importance.
Next we explored the different types of backlighters, V, Fe, Zn, Ti, and Ni, that could be used to generate the radiographs. Each of these backlighters produces x-rays at different energies and thus has a different penetration depth. With the higher energy backlighters the more dense regions will show more detail while washing out the less dense regions and vice versa for the lower energy backlighters. These different exposure energies allow us to more thoroughly probe the results of our laser experiments. The difference in backlighter choice is evident when looking at the radiographs from our second shot day in August 2005, labeled F05. For example, in Fig. 3.11 the radiographs generated by Ti show considerably more penetration than those generated by Zn.

After exploring reproducibility and backlighter choice, we modified the target design to better model the deflected astrophysical jet HH 110. To achieve this goal we added an obstruction into the foam section of the target. This obstruction was
of the form of a CH ball placed at differing impact parameters with respect to the flow axis of the jet. We then explored the effect of impact parameter by generating radiographs at similar times in the evolution but by increasing or decreasing the impact parameter. The results of this study, shown in Fig. 3.12 were as expected, the smaller the impact parameter the more the jet bores into the ball and the larger the impact parameter the smaller the angle of deflection. Our shot days in August 2005 (F05), February 2006 (S06) and August 2006 (F06) were used for the impact parameter study.

We also studied the time evolution of the jets by taking radiographs of similar targets at varying times. The time variability of the laboratory experiments is a significant advantage over observational data, which is usually only available for a very small portion of an object’s evolution. This study combined with RAGE simulations give a clear picture of the evolution of the jet with time, shown in Fig. 3.13. At
Figure 3.12 : Impact Parameter: (a)325 μm; (b)352 μm; (c)405 μm; (d)492 μm. Smaller impact parameters generate more ball penetration and more lateral deflection.

Figure 3.13 : Time evolution: Time increases from 50 to 200ns from left to right. The plug shape is evident in (a) and the flute-like structure is evident in (c) and (d) early times, 50 ns, the jet has a flat top shaped that is a result of the Ti plug that has been accelerated into the foam. This plug then produces the bow-shaped shock that is evident at later times. At approximately 100 ns a secondary jet forms and remains uncollimated until approximately 200ns. This secondary jet and its flute-like structure are caused by the collapse of the hole in the Ti washer at late times. After the plug has passed, the low pressure region left behind causes the vaporized titanium washer to collapse and subsequently rebound. The expansion of the material after the rebound generates the characteristic flute like structure of the secondary jet.

Finally we checked to see if the pore size or the foam material was a significant
factor in the morphology of the jets produced. To this end, we tested four different materials, RF, large-pore RF, TPX, and large-pore TPX. Our shot day in February of 2007 (S07) was dedicated to this study and the results showed that neither pore size nor foam type had a significant impact on the experimental data.

After February 2007 we refocused our experiments to examine more closely the interaction of shocks with clumpy media. These shots required a complete redesign of the target and are not covered in this Chapter. A more detailed description of the experiments and results can be found in Hartigan et al. (12)

3.6 Scaling

The lengths, times, and velocities present in laboratory experiments are quite different than those seen in the astronomical objects these experiments are designed to model. However, the hydrodynamics can be scaled from the laboratory regime to the astrophysical regime, with certain restrictions, through the Euler equations for a polytropic gas:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (3.26)
\]

\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) + \nabla P = 0 \quad (3.27)
\]

\[
\frac{\partial P}{\partial t} + \gamma P \nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla P = 0 \quad (3.28)
\]

where \( \rho \) is mass density, \( \mathbf{v} \) is the velocity, and \( P \) is the gas pressure. These equations are invariant under the following transformations as shown by Ryutov et. al (52):

\[
r' = ar; \quad \rho' = b\rho; \quad P' = cP \quad (3.29)
\]
where \( r \) is the length scale, and the scaling factors are the constants \( a, b, \) and \( c. \) This transformation requires that time and velocity also be similarly scaled by:

\[
t' = a \sqrt{\frac{b}{c}} t; \quad \mathbf{v}' = \sqrt{\frac{c}{b}} \mathbf{v}
\]  

(3.30)

Using these transformations the Euler equations will have identical solutions in the different regimes.

For the purposes of the simulations shown in §3.9 the experimental data can be separated into the jet and the working surface, where the jet interacts with the ambient medium. Estimates for the pressure, density, and velocities in these two regions show how well the experimental data scale to the astrophysical regime.

For the jet region, astrophysical jets, such as HH 270, have a typical \( r \) on the order of \( 10^{15} \) cm and \( \rho \) on the order of \( 10^{-20} \) g cm\(^{-3}\) with a gas pressure of \( 10^{-8} \) dyne cm\(^{-2}\). In the laboratory experiments, \( r \sim 0.02 \) cm and \( \rho \) is on the order of \( 1 \) g cm\(^{-3}\) with a gas pressure of \( 3 \times 10^{10} \) dyne cm\(^{-2}\). Thus, the scaling parameters become \( a \sim 5 \times 10^{16}, b \sim 2 \times 10^{-20}, \) and \( c \sim 3 \times 10^{-19}. \) Using these scaling parameters the time scales well, with 80 years in the astrophysical regime corresponding to 200 ns in the laboratory environment. The velocity scaling yields \( 10 \) km s\(^{-1}\) in the laboratory corresponding to \( 40 \) km s\(^{-1}\) in the astrophysical regime, which is a factor of four smaller than the velocities observed in HH objects. The velocity scaling discrepancy comes from the radiative cooling that is present in HH objects that is not present in the laboratory environment. This radiative cooling effectively raises the Euler number in the astrophysical jets, \( \sim 20, \) compared to the laboratory experiments, \( \sim 6. \)

However it is important to note that in both regimes the jets are highly supersonic.
For the working surface between the jet and the ambient medium, the most important factors are time scales, Mach numbers in the shocks, and density contrast between the jet and the ambient medium in front of the working surface. Based on above calculations the time scales well. The Mach numbers found in HH objects typically range from 20-200, and in the experimental jets the Mach numbers are ~ 200. The ratio of the mass density of the jet to the ambient medium, $\eta$, has a large effect on the morphology of the working surfaces. For typical stellar jets, $\eta \sim 10$, and for the experiments, over the time period from 50-200 ns, $\eta$ ranges from 8 to 1 and is in good agreement with stellar jets.

In order for this scaling to be valid, factors such as viscosity, heat conduction, mean free path, and radiative energy flux must be considered. Since the Reynolds number, which measures viscosity, and the Peclet number, which measures heat conduction, are much larger than unity in both the astrophysical and laboratory environments, these effects are negligible and can be ignored. For the Euler equations to applicable, the jet must act as a fluid. That is, the mean free path must be short when compared with the size of the system. This condition is easily met in both the astrophysical and laboratory regimes. The importance of radiative energy flux is given by the Boltzmann number, is $\gg 1$ in both regimes and thus can be ignored as a negligible effect.

Overall, the hydrodynamics of the experimental jets scale well with regards to the astrophysical regime, with the working surfaces tending to scale more accurately than the jet region of the experiments. However, due to the large difference in the number density between the laboratory and astrophysical regimes, effects from radiative cooling will not scale. A more complete discussion of scaling from the laboratory
environment to the astrophysical regime can be found in Hartigan et al. (12).

### 3.7 Problem Setup

The code utilizes advective tracers to track how different materials move. The advection equation:

\[
\frac{\partial \rho_T}{\partial t} + \frac{\partial \rho_T v_x}{\partial x} + \frac{\partial \rho_T v_y}{\partial y} + \frac{\partial \rho_T v_z}{\partial z} = 0
\]

sets up an advected density for each different material. Initially all cells are defined to be a single material, and each different material involved in the simulation is assigned its own tracer. At any point in the simulation a combination of the conserved variable of mass density and the value of each materials tracer define the mass percentage of each material in that cell. These percentages combined with the total mass density flux of a particular cell determine the flux for each material in that cell. For example, a pure titanium cell at a density of 4.5 g cm\(^{-3}\) has a titanium tracer value of 4.5, while other tracers are assigned value of 0.0. The fractional energy density of each material is also necessary. The fraction of each cells energy that is assigned to a particular material is determined by using a weighted average. The mass fraction of a material combined with its molar mass is used to calculate the molar fraction of that material for that cell. The energy density fraction is defined to be the same as the mole fraction of a material in a cell. After determining the mass fraction and energy fraction for a material in a particular cell, these values are used to look up the values for pressure, \(\chi\), and \(\kappa\) from the SESAME tables. The final \(\chi\) and \(\kappa\) for an entire cell are the weighted averages of the \(\chi\)'s and \(\kappa\)'s of each material in the cell, based on their molar fraction of the material. The mixed material cells are assumed
to be fully mixed gases. The total pressure for the cell is defined to the sum of the SESAME pressure for each material.

The simulation of laboratory experiments also should include a treatment of the laser used to drive the experiment. As an astrophysical based code, AstroBEAR was not designed with any type of laser deposition capability. The code does not currently have the physics necessary to simulate laser deposition. Therefore, we approximated the pressure drive from the laser using the hydro code RAGE (53) out of LANL, which does have ablation simulation capability. RAGE was able to generate a pressure profile as a function of time along the laser deposition surface. This pressure profile allowed us to calculate energy densities necessary to generate the proper pressure in the deposition layer of the titanium surface. These cells are specifically defined as a function of time to have the necessary energy density needed to recreate the pressure profile provided by LANL. Fig. 3.14 is a plot of the pressure profile used in the simulation. The x-axis shows time in ns after the beginning of the laser pulse. The y-axis shows the pressure inside the deposition layer in dyne cm\(^{-2}\).

Fig. 3.8 shows the schematic of the target used in designing the simulation’s initial conditions, with all material boundaries initially mesh aligned. The titanium plate and washer are defined to be initially at 300K at a density of 4.4467 g cm\(^{-3}\) using SESAME table 2961. The foam is defined using the CH SESAME table 7592 at a temperature of 300K and a density of 0.1 g cm\(^{-3}\). The vacuum space inside the washer was defined using the dry air SESAME table 5030 at a temperature of 300K and a density of .001 g cm\(^{-3}\). Simulations are 3.0mm by 2.0mm with a resolution of 8 \(\mu\)m, using a 360x240 mesh. Extrapolating boundaries were used for the left, right and top boundaries and a reflecting boundary was used for the bottom. The 2nd order
accurate MUSCL-Hancock integration method was used. The linearized Roe solver was used for solving the flux function as described earlier. Simulations were run for approximately 150 ns. The non-ideal simulations took approximately 1 hour to run on 4 processors at this resolution.

3.8 Synthetic Radiographs

Before comparing AstroBEAR simulations with experimental results, we converted the AstroBEAR output into synthetic radiographs similar to those produced by the laboratory experiments. As a hydrodynamics code, Fig. 3.15 shows a sample of raw AstroBEAR output where the total mass density is depicted.

To generate simulated radiographs we converted the 2.5D cylindrically symmetric output of AstroBEAR into 3D data by rotating the 2.5D data around the axis of
symmetry and filling in the 3D space with the appropriate values. The tracer variables provided the mass fraction of the different materials, i.e. Ti, CH, or dry air. We used these mass fractions to generate 3D mass density data for each material in the simulation. We then calculated the radiation transmission through each material along the line of site and then multiplied these values to get the total transmission:

\[
T_{\text{material}} = \frac{I_{\text{trans,material}}}{I_0} = e^{-L\rho_{\text{material}}\sigma_{\text{material}}}
\]

\[
I_{\text{trans,total}} = \left( \sum_{\text{materials}} T_{\text{material}} \right) I_0
\]

where \( I_0 \) is the incident intensity from the back-lighter, \( T \) the percent transmission, \( \sigma \) is the opacity, \( L \) is the column length along the line of site, \( \rho \) is the column density for a particular material, and \( I_{\text{trans}} \) is the transmitted x-ray intensity that reaches the
film. Currently the sensitivity of the photographic plate or CCD actually used in the experiment has not been taken into account when generating these radiographs.

3.9 Results and Analysis

Fig. 3.16 shows a comparison of 2.5D (cylindrically symmetric) AstroBEAR simulations and experimental data at 100 ns after the laser drive. Panel (a) depicts a simulated radiograph from an ideal EOS setup containing only neutral hydrogen, using the drive pressure profile provided by LANL. Panel (b) is a simulated radiograph from a simulation using the same setup, but with the newly implemented SESAME based non-ideal EOS with multiple materials instead of the single material ideal EOS. Panel (c) is actual experimental data. Features of note in the experimental data include the shock front position, shock width, and the presence of an interior flute-like jet. This interior jet is caused by the collapse and subsequent rebounding of the walls of the titanium washer after vaporized titanium has accelerated through the vacuum (12).

Fig. 3.17 plots the position of the jet head as a function of time in the experiment and the simulations, where distance is measured from the face of the titanium washer. Both the ideal and non-ideal simulations are in reasonably good agreement with the experimental data, although the position of the head is approximately 35% ahead of the experimental data. This discrepancy is most likely caused by the approximation of the laser pulse using the pressure profile in Fig. 3.14. Small changes to the pressure profile affected the position of the head with respect to time without significantly affecting the morphology of the jet.

The ideal EOS radiograph shows obvious inaccuracies in simulating the laboratory
environment. While the position of the shock front is similar to the experimental data, the ideal radiograph bears almost no morphological resemblance to the experiment. In contrast, the non-ideal EOS simulation shows dramatic improvement in modeling the overall morphology of the experiment. The non-ideal simulation reproduces both the lateral shock and a flute-like shape for the interior jet, key factors missing from the ideal simulation. Remaining differences between the non-ideal simulation of the interior jet and that seen in the experiment arise in part because of the ideal treatment of cells with mixed materials (§3). These mixed cells occur as the jet forms from the collapse of the washer, and are important for determining how the jet evolves.

3.10 Summary

A non-ideal EOS and a capability to handle multiple non-ideal materials was successfully added to the astrophysical MHD code, AstroBEAR. Redefining the flux function in terms of pressure and its derivatives proved to be more successful than forcing a non-ideal EOS into an ideal EOS framework. Our first non-ideal EOS simulations from AstroBEAR show that a non-ideal EOS framework is clearly preferable to an ideal EOS for the simulation of laboratory experiments.

While the basic capability for using non-ideal EOS has been achieved, plenty of room exists for further improvement. For example, including the physics necessary to properly simulate the laser drive will lead to better models of the jet’s evolution. The calculation of mixed cells involving solids and gases may be improved, and a more sophisticated treatment of energy splitting for mixed cells can be implemented, taking into account a mixed cell with different states of matter. AstroBEAR now has stable basic implementation of a non-ideal EOS capability upon which these improvements
Figure 3.16: Simulation Comparison

can be added.
Figure 3.17: Jet head position vs. time comparison for AstroBEAR with SESAME EOS, AstroBEAR with ideal H EOS, and experimental results.
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Table 3.3: Summary of Experiment Parameters for OMEGA laser laboratory experiments. F06-August 2006, S07-March 2007.
Chapter 4

HH 110 Simulations and Radiative Shock Cooling

This chapter focuses on HH 110, a unique HH jet in Orion that contains numerous knots and complicated shock interactions. HH 110, shown in Figs. 4.1 and 4.2, appears as a well collimated jet that expands to a maximum opening angle of $\sim 12^\circ$. The lack of an obvious stellar source for HH 110 led to a search for the explanation of its origin. Reipurth et. al (36) proposed that HH 110 was in fact the result of the deflection of HH 270 based on H$\alpha$ and S II observations of this region of the sky. The HH 270 jet (54) also contains knots, however these knots remain more collimated than those observed in HH 110. Proper motion data from these HH objects supports the proposed deflection origin for HH 110 (35).

Noriega-Crespo et. al (55) investigated the H$_2$ emission from HH 110 as a possible probe of the jet-cloud interaction. These observations showed H$_2$ emission coincident with H$\alpha$ and S II emission at the beginning of HH 110 but offset towards the molecular cloud further along the flow. This separation is consistent with a boundary layer between the HH 110 flow and the molecular cloud and also supports the proposed deflection origin of HH 110. Recent observations by Hartigan et. al have also supported the cloud deflection theory (12).

With this origin theory in mind, we use AstroBEAR, discussed in detail in Chapter 2, to investigate what types of variations in the progenitor jet could explain the clumpy morphology of HH 110 and to generate synthetic emission maps for future
Figure 4.1 : HH 270-HH110 Deflection: HH 270 Begins in the NW corner and deflects off the molecular cloud. This deflection generates HH 110 flowing towards the SE and depicted in more detail in Fig. 4.2. The triangle denotes the stellar source of HH 270.

comparisons with observational data. To generate a physically valid simulation we must model both flow dynamics and radiative cooling. The flow dynamics of the jet are handled by solving the Euler equations, a well tested section of the code. However, for HH objects the morphology is heavily affected by post shock radiative cooling. This energy loss affects the post-shock pressure and thus the hydrodynamic flows.

Before being applied to the HH 110 simulations, the cooling function underwent a series of rigorous tests to determine its accuracy and limits. The baseline for these tests was the 1D shock code written by Raymond and Cox (56). This chapter will
compare analogous 1D shocks from the Raymond code and from AstroBEAR and will for the first time show explicitly that a MHD code is handling post shock cooling in a manner consistent with an accepted baseline. This chapter also discusses the methods used to implement radiative cooling, the assumptions made, and the limits where the cooling remains valid.

4.1 Cooling

AstroBEAR has three types of cooling: hydrogen cooling, metal cooling, and ionization/recombination cooling. In the astrophysical regime elements past Helium on the
periodic table exist only in trace amounts and are collectively referred to as metals. The first two categories represent cooling due to line emission from the excitation of either hydrogen or metal atoms by collisions with free electrons. AstroBEAR does not track individual emission lines, but rather tracks the total energy lost due to the combination of all lines. The third category comprises the energy lost from the system when a species ionizes due to electron collisions and energy lost when free electrons recombine with an ionized species.

4.1.1 Ionization and Recombination Rates

To properly account for the different types of cooling it is necessary to track more physical variables than the traditional conserved quantities used in the Euler equations. AstroBEAR currently tracks the mass density of up to five species, H I, H II, He I, He II, and He III in addition to the standard conserved quantities. To within a small error the sum of the mass densities of these species is equal to the total mass density tracked by the Euler equations. Tracking these species separately requires not only the calculation of their fluxes due to pressure gradients but it also requires additional functions that calculate the ionization and recombination coefficients of each of the species at each time step. These rates provide an additional source term used in solving the non-homogeneous form of the Euler equations. A full description of how these source terms are implemented can be found in Chapter 2.

The ionization coefficients are calculated from the following equation found in Mazzotta et al. (57):

\[ F = A(1 - x f_1) + B(1 + x - x(2 + x)f_1) + C f_1 + D x f_2 \]  

(4.1)
\[
\alpha_{\text{ion}} = 6.697 \times \frac{e^{-x}}{(kT)^{3x/2}} \times 10^{-7} \tag{4.2}
\]

where \(\alpha_{\text{ion}}\) is in \(\text{cm}^3 \text{s}^{-1}\), \(x = I/kT\) with \(I\) equal to the ionization potential, \(T\) the temperature, and \(k\) being Boltzmann’s constant. The constants \(I\), \(A\), \(B\), \(C\), and \(D\) are different for \(\text{H I, He I, He II, and He III}\) and are found in Mazzotta et al.

The recombination rates are divided into two categories, radiative and dielectronic. For Hydrogen-like radiative recombination the rates are given by:

\[
\alpha_{\text{rec,rad}} = a \left\{ \frac{T}{T_0} \left(1 + \frac{T}{T_1} \right)^{1-b} \left(1 + \frac{T}{T_1} \right)^{1+b} \right\}^{-1} \tag{4.3}
\]

where \(T\) is the temperature and the constants \(a\), \(b\), \(T_0\), and \(T_1\) are found in Verner and Ferland (58). The dielectronic recombination, found in Mazzotta et al. is given by:

\[
\alpha_{\text{rec,dt}} = T^{3/2} e^{-E/T} \tag{4.4}
\]

where \(T\) is the temperature, \(E=39.70\), and \(c=1.12 \times 10^{-9}\).

Using these ionization and recombination rates, the source term values are given by:

\[
\frac{dn_{\text{HI}}}{dt} = \mu_H (n_e n_{\text{HI}} \alpha_{\text{rec,HI}} - n_e n_{\text{HI}} \alpha_{\text{ion}}) \tag{4.5}
\]

\[
\frac{dn_{\text{HII}}}{dt} = \mu_H (-\frac{dn_{\text{HI}}}{dt}) \tag{4.6}
\]

\[
\frac{dn_{\text{HeI}}}{dt} = \mu_{\text{He}} (n_e n_{\text{HeI}} \alpha_{\text{rec}} - n_e n_{\text{HeI}} \alpha_{\text{ion}}) \tag{4.7}
\]

\[
\frac{dn_{\text{HeII}}}{dt} = \mu_{\text{He}} (n_e n_{\text{HeII}} \alpha_{\text{rec}} + n_e n_{\text{HeII}} \alpha_{\text{rec}} - n_e n_{\text{HeII}} \alpha_{\text{rec}} - n_e n_{\text{HeII}} \alpha_{\text{ion}}) \tag{4.8}
\]

\[
\frac{dn_{\text{HeIII}}}{dt} = \mu_{\text{He}} (n_e n_{\text{HeIII}} \alpha_{\text{ion}} - n_e n_{\text{HeIII}} \alpha_{\text{rec}}) \tag{4.9}
\]
where the subscripts $rec$ and $ion$ correspond to recombination and ionization, $n_e$ is the electron number density, $n_{X_i}$ is the number density for that particular species, and $\mu_{X_i}$ is its mean molecular weight. These values are essential for the cooling routines, because the total energy loss is dependent on the number density of each species as well as the overall ionization fraction.

### 4.1.2 Hydrogen Cooling

The cooling due to hydrogen excitation from electrons is one of the three components of the AstroBEAR cooling term. We consider the energy lost from all lines generated by the excitation of a ground state electron to the $n=2, 3, 4$ or 5 levels. We do not track specific emission lines and we neglect collisional de-excitation of $H$, hence the energy is subtracted from the system when the excitation of the ground state electron occurs. The path that electron takes back to the ground state is not necessary for total energy loss calculations. Only the energy difference from the ground state to each excited state and the collision strengths are required to calculate the cooling due to hydrogen excitation. The equation used to calculate the cooling function for hydrogen excitation is:

$$\Lambda_{\text{hydrogen}} = n_e n_{HI} \alpha$$

$$\alpha_{ij} = h\nu_{ij}(8.63 \times 10^{-6}) \frac{e^{-h\nu_{ij}/kT}}{g_i \sqrt{T}} Y_{eff}$$

$$\alpha = \sum_{j=2}^{5} \alpha_{ij}$$
where $\Lambda_{\text{hydrogen}}$ is the energy loss rate in ergs cm$^{-3}$ s$^{-1}$, $\alpha$ (ergs cm$^3$ s$^{-1}$) is the total rate coefficient for hydrogen cooling by collisional excitation, $\alpha_{ij}$ is the rate coefficient for the transition from the n=i to j level, $h\nu_{ij}$ is the energy difference between the i and j levels, $Y_{\text{eff}}$ is the effective collision strength for this transition and $g_i$ is the statistical weight of the n=i level. The effective collision strengths were obtained from Anderson (59).

4.1.3 Metal Cooling

Calculation of cooling due to the excitation of metals is a more complex problem. The code does not track the mass densities of each line-emitting metal, therefore metals were assumed to be present in solar abundances relative to hydrogen. We started with the cooling curve found in Dalgarno & McCray et al (DM) (60). However, this cooling curve makes many assumptions that are incorrect when used in the context of a post-shock radiative cooling gas. The DM curve assumes ionization equilibrium, which is far from a valid assumption in post-shock gas. The post shock material will have a quick increase in temperature relative to its change in ionization, leading to a hot gas with low ionization relative to the ionization equilibrium value. Assuming ionization equilibrium will lead an overestimation of the hydrogen ionization fraction and the number of free electrons available to excite metal atoms. This overestimation will lead to metal cooling term that is too high for the post-shock gas. The DM curve also includes hydrogen cooling, which is redundant based on our separate calculations for hydrogen excitation cooling described in § 4.1.2. To better adapt the DM cooling model to our situation we used the method described in § 4.1.2 to calculate the cooling term for hydrogen in ionization equilibrium as a function of temperature, $\Lambda_{H,\text{equi}}(T)$.
(ergs cm\(^{-3}\) s\(^{-1}\)):

\[
\Lambda_{H,\text{equil}}(T) = n_{e,\text{equil}}n_{H,\text{equil}}\alpha(T) = n_{H}^{2}X_{\text{equil}}(T)[1 - X_{\text{equil}}(T)]\alpha(T)
\]  

(4.13)

where \(X_{\text{equil}}\) is the ionization fraction in equilibrium and \(\alpha\) is the rate coefficient defined in § 4.1.2. The \(\Lambda_{H,\text{equil}}\) represents the portion of the DM cooling generated by the collisional excitation of \(H\). To calculate the metal cooling term, \(\Lambda_{\text{metal}}\), we subtracted \(\Lambda_{H,\text{equil}}\) from the original DM value, \(\Lambda_{DM}\). Figure 4.3 shows \(\Lambda/n_{H}^{2}\) for the original DM, hydrogen equilibrium ionization, and \(H_{\text{equil}}\)-subtracted DM curves.

![Figure 4.3: DM cooling curve, H ionization equilibrium curve, and DM-H ionization equilibrium](image)

However, even after subtracting the contribution due to \(H\) from the DM cooling curve, the curve still assumes ionization equilibrium. To solve this problem we renor-
malized the DM values to get the correct electron number density by multiplying these values by the ratio \( X_H / X_{H,\text{equil}} \) which is equivalent to \( n_e / n_{e,\text{equil}} \). Thus, the overall metal cooling term is given by:

\[
\Lambda_{\text{metal}}(T) = \left[ \Lambda_{DM}(T) - \Lambda_{H,\text{equil}}(T) \right] \times \frac{X_H}{X_{H,\text{equil}}(T)}
\]

(4.14)

where \( X_H \) is the ionization fraction tracked by the code and \( X_{H,\text{equil}} \) is the ionization fraction in equilibrium. Our renormalization correction gives a more accurate number of free electrons available for metal cooling but does not correct for the over ionization of the metals themselves. However we can ignore the difference in metal ionization because the different ionization species of the same element, e.g. \( \text{O I} \) and \( \text{O II} \), have similar fine structures with similar energy level differences and thus the overall cooling will be relatively insensitive to the metal ionization fraction as compared to the \( X_H \). Below 8000 K the cooling depends more heavily on the ionization fraction of the gas and our renormalization procedure is no longer a good approximation. Therefore metal cooling is only allowed for temperatures above 8000 K.

### 4.1.4 Ionization and Recombination Cooling

For a hydrodynamics simulation code the flows are influenced when either the thermal or kinetic energies are changed. So when discussing energy lost due to ionization it is important to clarify that it is energy that has been removed from the thermal energy of the gas and not necessarily lost from the system. When an atom is ionized electron thermal energy is converted to binding energy and is not actually lost from the system until that electron recombines and radiates the energy away. However, at
the moment of ionization the thermal energy, the temperature, and thus the pressure of the gas is reduced. It is for this reason that we remove energy from the simulation at the moment of ionization. The energy loss rate due to ionization, \( \Lambda_{\text{ion}} \) (ergs cm\(^{-3}\) s\(^{-1}\)), is the ionization energy multiplied by the ionization rate:

\[
\Lambda_{\text{ion}}^X = I^X \alpha_{\text{ion}}^X
\]

where \( I \) is the ionization energy, \( \alpha_{\text{ion}} \) is the ionization rate given in § 4.1.1, and \( X \) is the species involved, H I, He I, He II, or He III.

There is however additional energy lost when an electron undergoes recombination. We can assume that after a recombination event the electron will cascade back to the ground level and thereby radiate away the ionization energy, which has already been subtracted out of the system. The additional energy lost is in the form of kinetic energy. When an electron recombines with an ionized hydrogen atom for example, the electron has some kinetic energy as well as the 13.6eV of binding energy generated during ionization. To calculate the average amount of kinetic energy lost during each recombination, we used the Maxwellian distribution of kinetic energy as a function of temperature. The resulting average energy lost per recombination event is \( kT \).

Therefore the energy loss rate due to recombination, \( \Lambda_{\text{recomb}} \) (ergs cm\(^{-3}\) s\(^{-1}\)), is given by:

\[
\Lambda_{\text{recomb}}^X = kT \alpha_{\text{recomb}}^X
\]
\[ \Lambda_{\text{recomb}} = \sum_{X} \Lambda_{\text{recomb}}^{X} \]  

(4.18)

where \( \alpha_{\text{recomb}} \) is the recombination rate given in § 4.1.1 and \( X \) is the species involved: H II, He II, or He III. The total energy loss rate term is given by:

\[ \Lambda_{\text{total}} = \Lambda_{\text{hydrogen}} + \Lambda_{\text{metal}} + \Lambda_{\text{ion}} + \Lambda_{\text{recomb}} \]  

(4.19)

This \( \Lambda_{\text{total}} \) becomes the source term, \( dE/dT \), used in solving the non-homogenous Euler equations as described in Chapter 2.

### 4.2 Simulation Setup

The control simulation is based on the variable jet model found in Raga et al. (61), with dimensions of 0 to 5.0\( \times 10^{17} \) cm in the \( x \) and \( z \) directions and 0 to 10.0\( \times 10^{17} \) cm in the \( y \)-direction. The simulations were run at a resolution of 4 cells per jet radius or 1.5\( \times 10^{16} \) cm, corresponding to 128x256x128 cells at the highest level of refinement. Higher resolution runs were impossible due to hardware and time constraints on the SUGAR cluster. The simulation was set up with a base grid of 64x128x64 cells with one extra level of AMR refinement. The ambient medium was defined to be 10 cm\(^{-3} \) atomic hydrogen gas at 1000 K. The molecular cloud was defined to be 10000 cm\(^{-3} \) atomic hydrogen at 1K. The progenitor jet was defined to be 50 cm\(^{-3} \) atomic hydrogen gas at 1000 K. The jet was injected at (3.5,2.5,0)\( \times 10^{17} \) cm in the positive \( y \)-direction. The velocity of the jet was defined by:

\[ V_{1} = V_{0} + \delta V \sin(2\pi t/\tau_{1}) \]  

(4.20)
\begin{align}
V_x &= V_1 \sin(\alpha) \cos(2\pi t/\tau_2) \\
V_y &= V_1 \cos(\alpha) \\
V_z &= V_1 \sin(\alpha) \sin(2\pi t/\tau_2)
\end{align}
(4.21, 4.22, 4.23)

where $\tau_1$ is the pulsing period, $\alpha$ is the precession opening angle, and $\tau_2$ is the precession period. The control configuration, Model A, has $V_o=300$ km s$^{-1}$, $\alpha = 5^\circ$, $\tau_1=200$ yrs, and $\tau_2=400$ yrs. Model B decreases $\tau_1$ to 75 yrs and increases the number of clumps in the progenitor jet. Model C decreases $\delta V$ to 0 to generate a constant speed jet precessing at a $5^\circ$ opening angle. Model D changes $\alpha$ to $0^\circ$ to generate a non-precessing but speed variable jet injected in the $y$-direction. A synopsis of the different models is shown in Table 4.1. These four models will allow us to tell something about the effects of speed variation and precession on the morphology of the resulting spray.

<table>
<thead>
<tr>
<th>Model</th>
<th>$\delta V$</th>
<th>$\tau_1$</th>
<th>$\tau_2$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model A</td>
<td>300 km s$^{-1}$</td>
<td>200 yrs</td>
<td>400 yrs</td>
<td>$5^\circ$</td>
</tr>
<tr>
<td>Model B</td>
<td>300 km s$^{-1}$</td>
<td>75 yrs</td>
<td>400 yrs</td>
<td>$5^\circ$</td>
</tr>
<tr>
<td>Model C</td>
<td>0 km s$^{-1}$</td>
<td>0 yrs</td>
<td>400 yrs</td>
<td>$5^\circ$</td>
</tr>
<tr>
<td>Model D</td>
<td>300 km s$^{-1}$</td>
<td>200 yrs</td>
<td>400 yrs</td>
<td>$0^\circ$</td>
</tr>
</tbody>
</table>

Table 4.1 : Summary of Simulation Model Parameters

To utilize the radiative cooling, all gas in the simulation was set to be initially neutral and contain the solar abundance of 8.51 % He relative to H, i.e. the ambient medium was $100 \text{ cm}^{-3}$ H and $8.51 \text{ cm}^{-3}$ He. The He was allowed to exist only as He I or He II throughout the simulation and radiative cooling was allowed only for temperatures above 8000 K. The initial post-shock temperatures are on the order of...
$10^5$ K, so cooling to 8000 K covers over 90% of the initial post-shock temperature and should have very little effect on the hydrodynamics of the simulation.

### 4.3 Synthetic Emission Line Maps

The simulations produce data for the conserved variables mass density-$\rho$, momentum densities-$p_x, p_y, p_z$, total internal energy-$e$, and the mass densities of the tracked atomic species, $\rho_{H I}, \rho_{H II}, \rho_{He I},$ and $\rho_{He II}$. To compare our results with observational data we used post-processing routines to convert AstroBEAR output into temperature, H$\alpha$ emission, and S II emission maps. The temperature and ionization fraction, $X$, are calculated directly from the total internal energy and atomic species data:

\[
E_{\text{thermal}} = E_{\text{total}} - 0.5(p_x^2 + p_y^2 + p_z^2)/\rho \tag{4.24}
\]

\[
\mu = (n_{H I}\mu_{H I} + n_{H II}\mu_{H II} + n_{He I}\mu_{He I} + n_{He II}\mu_{He II})/n_{\text{tot}} \tag{4.25}
\]

\[
T = (E_{\text{thermal}}/\rho)(\gamma - 1)\mu \tag{4.26}
\]

\[
X = \frac{n_{H II}}{n_{H I} + n_{H II}} \tag{4.27}
\]

where the number density $n_X = \rho_X / \mu_X$, $\mu_X$ is the molecular weight of a species, and $\gamma$ is the thermodynamic variable for the ratio of specific heats. The ionization fraction and temperature are both necessary when generating the H$\alpha$ and S II maps.
4.3.1 Hα Maps

Hα maps are based on emission from recombination and collisional excitation of hydrogen atoms. These emission rates (ergs cm$^{-3}$ s$^{-1}$) are given by:

\[ \Lambda_{\text{rec}} = h \nu_{\text{rec}} n_e \alpha_{\text{eff,rec}} \]  \hspace{1cm} (4.28)

\[ \Lambda_{\text{coll}} = h \nu_{\text{coll}} n_e \alpha_{\text{eff,coll}} \]  \hspace{1cm} (4.29)

where

\[ \alpha_{\text{eff,rec}} = a \left[ \frac{T}{T_0} (1 + \frac{T}{T_0})^{1-b} (1 + \frac{T}{T_1})^{1+b} \right]^{-1} \]  \hspace{1cm} (4.30)

with \( a=7.982\times10^{-11} \text{ cm}^3 \text{ s}^{-1} \), \( b=0.7480 \), \( T_0=3.128 \text{ K} \), and \( T_1=7.03\times10^{-6} \text{ K} \). The rate \( \alpha_{\text{eff,coll}} \) is defined by:

\[ \alpha_{ij} = h \nu_{ij} \frac{8.63 \times 10^{-6}}{g_i \sqrt{T}} \sum \frac{P_l}{\Upsilon_{\text{eff},l}} \]  \hspace{1cm} (4.31)

\[ \alpha = \sum_{j=3}^{5} \alpha_{ij} \]  \hspace{1cm} (4.32)

where \( \Upsilon_{\text{eff},l} \) is the effective collision strength to the \( l \) shell in the \( j \) energy level and \( P_l \) is the probability that decay from this state will lead to Hα emission. Fig. 4.4 shows the value of \( P_l \) for the different \( l \) shells for energy levels \( n=3, 4, \) and 5. These calculations result in:

\[ \Lambda_{\text{Hα}} = \Lambda_{\text{coll}} + \Lambda_{\text{rec}} \]  \hspace{1cm} (4.33)

The Hα emission maps are generated by summing the \( \Lambda_{\text{Hα}} \) values along the line of sight, which is the z-axis for these simulations. This type of calculation assumes
4.3.2 Other Emission Maps

The emission due to lines other than $\text{H}\alpha$ from species such as $\text{O I, O II, N I, N II}$, and $\text{S II}$ is given by:

$$A_{i,j} = n_{i,sp}A_{i,j}(\nu_{i,j})$$

(4.34)

where $n_{i,sp}$ is the number density for the emitting species with the electron starting in the $n=i$ state, $A_{i,j}$ is the Einstein A value for line transition from $n=i$ to $j$, and $\nu_{i,j}$ is the energy associated with this transition. The code does not track the number density for each species and the relative number densities in each excited state, therefore emission maps rely on the assumption of statistical equilibrium and solar abundances to calculate $n_{i,sp}$. We can safely assume solar abundances because gas in the interstellar medium will be fully mixed and should have no compositional variation, neglecting dust formation, and since metals are only present in traces amounts, small variations from solar abundances will have very little effect on the overall emission.
maps.

Since we cannot directly calculate \( n_{i,Sp} \), we first calculate the ratio \( P_i = n_{i,Sp}/n_{Sp} \), where \( n_{Sp} \) is the total number density of a species including all excited states. For this calculation we balance the rates out of and into a specific excited state by solving the following equation for \( P_i \):

\[
\sum_{i=j} P_i n_e \alpha_{i,j} + \sum_{i>j} P_i A_{i,j} = \sum_{j>i} P_j A_{j,i} + \sum_{i=j} P_j n_e \alpha_{j,i}
\] (4.35)

\[n_{i,Sp} = P_i n_{Sp}\] (4.36)

From Eqn. 4.34 in addition to \( P_i \) we also must calculate \( n_{Sp} \). This number density depends on temperature, hydrogen ionization fraction, and solar abundances. The solar abundances relative to hydrogen, \( O_{sa} \) and \( N_{sa} \), give us \( n_X \), which is the total number density of an element like O or N including all ionization states, e.g.:

\[n_O = O_{sa} n_H\] (4.37)

The only term remaining to solve for is the relative abundance for each ionization state of a particular element. These relative abundances are determined through charge exchange, which couples the ionization fractions of O and N to \( X_H \). The 1st ionization energy for S is 10.36 eV and is \( \sim 3-4 \) eV lower than the 1st ionization energies of H, O, and N. This low ionization energy effectively leaves S unshielded by H to background radiation below 13.6 eV and thus S will never exist as neutral S in HH objects. Therefore we assume all S to exist as SII for the purposes of generating
S emission maps. The charge exchange relationship is given by:

\[
C = \frac{n_{SpI}}{n_{SpII}} = \frac{n_{HI} \cdot g_{SpI} \cdot g_{HI} \cdot I}{n_{HI} \cdot g_{HI} \cdot g_{SpII}} \cdot \frac{g_{SpI}}{g_{SpII}} \cdot \frac{(I_{Sp} - I_{HI})}{(kT)} \tag{4.38}
\]

\[
n_{SpII} = (1 + C)^{-1} n_X \tag{4.39}
\]

\[
n_{SpI} = C(1 + C)^{-1} n_X \tag{4.40}
\]

where \(n_{SpI}\) and \(n_{SpII}\) are the number densities of the element in its 1st and 2nd ionization states, \(n_X = n_{SpI} + n_{SpII}\), \(I\) is the ionization potential, and \(g\) is the statistical weight of the ground state of the species. Species are restricted to the 1st and 2nd ionization states because of the temperature ranges dealt with in the simulations.

With the above calculated values \(n_{i,Sp}\) can be defined as follows:

\[
n_{i,SpI} = P_i n_{SpI} \quad n_{i,SpII} = P_i n_{SpII} \tag{4.41}
\]

and the emission from each line for O I, O II, N I, N II, and S II is then calculated using Eqn. 4.32. The S II maps are of the line \(\lambda = 6731\AA\) and the transition from the 2nd excited state to ground. As with \(H\alpha\) these maps are sums along the line of sight.

### 4.4 Cooling Validation

The radiative cooling detailed in §4.1 was tested separately from the HH 110 simulations. 1D radiative cooling shocks were generated via AstroBEAR over a range of shock velocities and compared against similar 1D shocks generated by the Raymond
shock code. The 1D Raymond code calculates the cooling in a far more detailed manner than AstroBEAR. It tracks the energy lost due to a wide array of emission lines, including forbidden lines, hydrogen lines, and numerous metal lines, whereas AstroBEAR only tracks cooling as the total energy lost from all lines combined. As a result the Raymond code is considered to be the most accurate 1D shock code available and as close the "correct" answer achievable via simulation.

The pre-shock gas for the AstroBEAR simulations was defined to have \( n_H = 100 \) cm\(^{-3}\), \( n_{He}/n_H = 0.00851 \), and \( T = 1.0 \times 10^4 \) K. The shock velocities used for testing were 40, 60, and 80 km s\(^{-1}\). The Raymond initial conditions for these values was identical, however Raymond tracks the emission lines from many other elements such as Fe, N, etc. so these elements are present in the Raymond simulation at solar abundance levels relative to hydrogen. While the AstroBEAR simulations did not include magnetic fields, they are required for the Raymond code. To minimize this effect on the simulation the magnetic field was set to 0.1 \( \mu \)G in the Raymond code. As described above, the cooling functions used in AstroBEAR fail below 8000 K due to the increased importance of metal cooling and the presence of molecules. Taking this into account, the AstroBEAR simulations are not allowed to cool below 8000 K and comparisons with the Raymond code are only meaningful down to this temperature. Further work is currently being done to improve AstroBEAR’s cooling function to lower temperatures.

The resulting post-shock structure of the two codes was compared in four ways: temperature vs. distance behind the shock, hydrogen ionization fraction \( X_H \) vs. temperature, \( X_H \) vs. distance behind the shock, and \( n_H \) vs. distance behind the shock. Figs. 4.5, 4.6, and 4.7 compare the two codes for different shock velocities and
at different AstroBEAR resolutions.

Figs. 4.5, 4.6, and 4.7 show that the resolution of the AstroBEAR simulations is one of the limiting factors in the ability of AstroBEAR to handle post-shock radiative cooling properly. Specifically the upper right panel in Fig. 4.6 shows that the lower resolution simulations greatly over estimate the ionization fraction. This result is expected because a shock generated in AstroBEAR is not infinitely thin but rather is spread out over a few cells. This shock dispersion allows the pre-shock gas an intermediary state in which it can cool and ionize before it reaches post-shock conditions. This resolution effect thus becomes a function of shock velocity because the higher shock velocities generate higher initial post-shock temperatures. The higher post shock temperatures will lead not only to stronger cooling but also higher initial ionization rates. Thus at the higher shock velocities the more impact the intermediary state of the gas will have on the structure of the post-shock gas. As the resolution is increased the physical size of the shock is decreased and the less impact its dispersion will have on the simulation.

Another limiting factor in the ability of AstroBEAR to handle shocks involves radiation transport. Currently AstroBEAR has no capability to handle to emission of radiation from one section of the grid and reabsorption by another section. When shock velocities approach the 100 km/s range the post-shock gas is emitting radiation that travels upstream of the shock and can begin to pre-ionize the pre-shock gas. We therefore expect the cooling routines to remain valid only for shock velocities below $\sim 100 \text{ km s}^{-1}$.

Within these resolution and shock velocity parameters AstroBEAR shows remarkable agreement with the Raymond code in the overall post-shock gas structure. These
comparisons mark the first rigorous test of AstroBEAR’s handling of radiative shocks and give greater confidence in subsequent HH 110 radiative cooling simulations.

4.5 HH110 Simulations and Analysis

Figure 4.8 shows slices along the z=2.5e17 cm plane of the temperature profile for the four different models of HH 110 simulated at t=2500 yrs after the initial jet injection. For the purposes of this discussion the simulation will be broken down into three parts, the progenitor jet, the cloud, and the spray. Figure 4.9 shows the Hα emission and figure 4.10 shows the SII emission, both at t=2500 yrs.

The temperature profiles shown in figure 4.8 do not show a great deal of difference
in range amongst the four models. While Model D appears to show a significantly different morphology than the other models, these temperature profile suggest that the nature of the progenitor jet will not have much effect on the overall temperature of the spray. These morphology differences are more evident in the \( \text{H}\alpha \) and SII maps shown in figures 4.9 and 4.10.

One central aspect of HH 110 morphology is the clumpy nature of the spray. This feature is clearly visible in many observational images, such as those found in figure 4.2. In both emission lines shown in figures 4.9 and 4.10, model D clearly fails to reproduce this important HH 110 feature. Models A, B, and C produce varying numbers of clumps with different distributions but all three models more accurately reproduce HH 110 morphology. Model D differs mainly in the fact that the progenitor
jet lacks precession, but is instead a linear jet with a time-dependant speed. This result suggests that precession of the progenitor jet is likely to play a significant role in the spray morphology of HH 110.

Observations of the progenitor jet to HH 110 appear to show a series of shocks along the direction of flow. These shock fronts suggest that the progenitor jet was generated by a pulsing mechanism. Models A, B, and D all have pulsed jets and all depict the same type of structure observed in the progenitor jet to HH 110. These models are therefore consistent with the pulsed generation theory. While precession plays an obvious role in the spray morphology, a pulsed progenitor jet is important as well. The difference in spray morphology between Model B and C shows that the pulses cause the clumps in the spray to be more concentrated and observational data
on HH 110 clearly shows concentrated clumps in the spray. It can be concluded that the progenitor jet that produces the spray observed in HH 110 must be both pulsed and precessing nature. This conclusion also means that future models of jet formation by young stars must be able to produce a precession and pulsing jet.

4.6 Magnetic Fields

Magnetic fields are likely present in HH jets (62) but are not included in these simulations. In the presence of magnetic fields, gases can be differentiated as collisional or non-collisional. In a collisional gas the mean free path for particles is much smaller than the gyroradius from the magnetic field. Conversely, a non-collisional gas has a small gyroradius compared to the mean free path. In effect, a collisional gas will respond to phenomena such as shocks through particle-particle collision while a non-collisional gas will respond to these phenomena through magnetic field effects. In HH 110, we estimate the mean free path, \( l \), and the gyroradius, \( r \), through the following equations:

\[
\begin{align*}
  l &= (n\sigma)^{-1} \quad (4.42) \\
  r &= \frac{mv}{qB} \quad (4.43)
\end{align*}
\]

where \( n \) is the number density, \( \sigma \) is the cross-section, \( m \) is the particle mass, \( q \) is the particle charge, \( v \) is the particle velocity perpendicular to the field, and \( B \) is the magnetic field strength. For a typical HH object, if \( n=10 \, \text{cm}^{-3} \) and \( \sigma = \pi r_{\text{Bohr}}^2 \), then \( l \sim 10^{-2} \, \text{AU} \). For the gyroradius, \( q = e, m = m_{\text{proton}}, v = 100 \, \text{kms}^{-1}, \) and \( B = 50 \, \mu G \), which yields \( r \sim 10^{-6} \, \text{AU} \) (62).

HH 110 is at a distance of \( \sim 460 \, \text{parsecs} \) and the resolution of HST is on the order
of 0.1 arcseconds. This resolution corresponds to a physical resolution of ~ 50 AU. As evidenced by Eqns. 4.42 and 4.43, the gyroradius and the mean free path are much smaller than the best available telescopic resolution. As a result, we do not know if HH 110 is collisional or non-collisional based solely on observation. However, comparing the morphology of the jets produced by simulation with observational data can help to set limits on the collisional nature and level of magnetic effect on such jets. Comparison with laboratory experiments, which are certainly collisional, can still be made within such limits.

The general effect of magnetic fields on the morphology of a jet can be predicted. A shock will compress magnetic field lines and thereby strengthen the post-shock magnetic field. The strength of the magnetic field is directly related to the number density of the gas, and the magnetic pressure is directly related to the square of the magnetic field. Hence, even in situations with relatively small pre-shock magnetic fields, the square dependence on number density can lead to important magnetic pressures in the post-shock gas. This added pressure, which is not present in our simulations, should add an extra resistance to compression. Therefore, when magnetic fields were present, we would expect the knots in the HH 110 spray to be more extended and have less of a bullet-like shape. Observations of HH 110 do indeed shows knots that are more extended that those that appear in our simulations. This difference is an indication that magnetic fields are present in HH jets in a large enough quantity to effect post-shock regions of the jet. Future simulations of HH 110 will include magnetic fields to investigate these effects.
4.7 Conclusion

We were able to successfully introduce into AstroBEAR a radiative cooling capability for use with the simulation of astrophysical situations involving shocked material. This cooling capability was tested against the most accurate shock simulation code available and showed agreement limited only by the micro-physics included in AstroBEAR and by resolution.

Using this new cooling capability, we were able to simulate HH 110 and investigate which properties of the progenitor jet are most important in the morphology observed in the spray. We concluded that the both precessing and pulsing nature of the progenitor jet has significant impact on the clumpy nature of the spray and that any jet formation model must include both precession and pulsing. There are many other parameters spaces to explore to better define the important progenitor jet characteristics. In the future we plan on studying the impact parameter of the jet with respect to the cloud, cloud density and progenitor jet density, smooth vs. random pulsing, and precession opening angle.
Figure 4.8: Temperature profiles for the different simulation models
Figure 4.9: Hα emission maps
Figure 4.10: SII emission maps
Chapter 5

Conclusion

Great progress was made towards the goal of transforming AstroBEAR into an all purpose MHD simulation code capable of linking laboratory and astrophysical data by improving the code's ability to accurately simulate jets and shocks in both the laboratory and astrophysical regimes. Our first goal was to create a non-classified and readily available code capable of simulating experiments, including future experiments containing magnetic fields, from the newly emerging field of laboratory astrophysics. Whereas previously AstroBEAR could only handle ideal gasses and had no capability to accurately handle the laboratory environment, we added a non-ideal EOS framework to allow AstroBEAR to simulate laboratory experiments. We then used this new framework along with the SESAME tables to simulate shocks and jets from specific laboratory experiments carried out on the OMEGA Laser in Rochester, NY. Comparisons between ideal simulations, the new non-ideal simulations, and experimental data show AstroBEAR’s enhanced ability to simulate multiple non-ideal materials found in the laboratory environment. This achievement is a major step towards a non-classified MHD code capable of handling both the laboratory and astrophysical regimes.

The second main goal was to improve AstroBEAR’s ability to handle the radiative cooling zones found in the post-shock regions of astrophysical jets and thus more accurately produce synthetic emission maps for comparison with astronomical data.
After improving the code's radiative cooling routines, we compared 1D radiative shocks with analogous shocks generated by the Raymond code, generally accepted as an accurate 1D non-LTE astrophysical shock code. These comparisons show for the first time that an MHD code is handling post-shock radiative cooling correctly limited mainly by the resolution of the simulations and the types of microphysics included in the code. This validation represents another major step towards a code capable of linking laboratory and astronomical data.

With the newly improved radiative cooling routines we simulated an astrophysical object with a unique morphology, HH 110, so as to further our general understanding of the origins of HH jets and learn more about HH 110 specifically. The simulations show that HH 110 must be generated by a jet that is both pulsing and precessing in nature. This conclusion also requires that future stellar jet formation and collimation models must provide mechanisms to create variable jet outflows and further supports the dynamic outflow models over static models for jet formation.

5.1 Future Work

AstroBEAR's current non-ideal EOS capability marks only the beginning of its potential ability to simulate complex laboratory experiments and AstroBEAR is now unique in its ability to handle magnetic fields and laboratory simulations. Thus, AstroBEAR represents a new non-classified tool that will allow more researchers and graduate students to contribute to future magnetized laboratory jet experiments using MHD simulations. The resolution of our laboratory simulations is currently limited by the computationally expensive manner in which the code handles the inversion of the SESAME tables. The next step in this research will be to rework this section of
the code and greatly enhance our ability to do high resolution and 3D simulations. From a microphysics standpoint, there are other capabilities that can be added to better simulate the laboratory environment now that the code can handle multiple non-ideal materials. To get more accurate laboratory simulations the code needs to simulate the actual laser deposition present in the laboratory experiments. Adding laser deposition to the code will require the addition of new physics to the code, e.g. radiation diffusion, and represents another important avenue for future research. Finally more can be done to improve upon the treatment of computational cells containing materials with different phases. This mixed-cell problem itself represents an entire field of research in the computational physics community and provides another avenue for further work to improve AstroBEAR.

The radiative cooling capability of the code can be improved even further to handle gas below 8000 K. While the cooling below this temperature may have a negligible effect on the hydrodynamics of a jet simulation, it can affect the line emission in this temperature range. Extending the cooling below 8000 K is the next step in improving AstroBEAR to generate the most accurate synthetic data for comparison with observational data. As with the laboratory simulations, the code's lack of ability to handle radiation transport limits the velocity of shocks that it can accurately simulate. Adding radiation transport to the code is another area of future research that would enhance the code's ability to handle shocks in astrophysical as well as laboratory environments.
Bibliography


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S05 #2

S05 #3

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S05 #5

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