Chapter 3

Smoothed Particle Hydrodynamics

As discussed in the previous chapter, hydrodynamic interactions must be included in any good ballistic stream model. In hydrodynamics, the stream is treated as a fluid with a force of interaction due to pressure gradients through the gas. The Euler equation is used to describe the acceleration due to the pressure gradients, also referred to as the hydrodynamic acceleration:

\[
\vec{a}_h = \frac{d\vec{v}_h}{dt} = -\frac{1}{\rho} \nabla P
\]  

(3.1)
where $\rho$ is the density and $P$ is the pressure, which can be related by the equation of state as described in Section 3.3.2. The hydrodynamic acceleration given in equation 3.1 is added to the ballistic acceleration found from the 3D-RTB problem in equations 2.1 - 2.3 to yield the hydrodynamic equation of motion that must be solved to determine the ballistic stream structure.

$$\ddot{a} = -\frac{1}{\rho} \nabla P + \ddot{a}_{ext}$$  \hspace{1cm} (3.2)

Unfortunately the hydrodynamic equation does not have an analytical solution and must be solved numerically.

There are many numerical strategies for solving hydrodynamic equations, each one with its own benefits and limitations. Computational simplicity and efficiency are often the determining factors in choosing a numerical strategy. For the polar accretion stream problem, the hydrodynamic equations are used for the ballistic stream portion, i.e. from the time gas enters the stream at L1 until it couples to a field line. This provides a definite “entry” boundary for the gas flow with known boundary conditions at the L1 plane. The gas “exits” the ballistic stream, and thus the hydrodynamic problem, when the coupling condition is satisfied. The coupling positions, however, are not
known a priori. The exit boundary is therefore indefinite and the entire region of the white dwarf’s Roche lobe should be included in the computational space. A grid method of solving the hydrodynamic equations would include a large amount of empty space wasting computational time. In addition, self gravitation within the gas stream can be neglected, simplifying the interactions necessary for a particle method of solving the problem. The magnetic field of the primary does not need to be included in the hydrodynamic calculations directly, but the coupling condition must be monitored continually to determine where the gas transitions and leaves the ballistic stream. By considering all of the above requirements, the method best suited to the polar accretion stream model is smoothed particle hydrodynamics (SPH).

### 3.1 What is SPH?

SPH is based on the concept that any field variable, such as density, can be approximated by a smoothed average according to the integral interpolant:

\[
    f(\vec{r}) \approx \langle f(\vec{r}) \rangle = \int f(\vec{r}) W(\vec{r} - \vec{r}'; h)d^3r'
\]  

(3.3)
where $f(\vec{r})$ is the field variable, $\langle f(\vec{r}) \rangle$ is the smoothed average of the field variable, and $W$ is the smoothing function or "kernel" which must satisfy:

$$
\int W(\vec{r}, h)d\vec{r} = 1 \quad \text{and} \quad \lim_{h \to 0} W(\vec{r}, h) = \delta(\vec{r})
$$

(3.4)

The parameter $h$ in the kernel function, often referred to as the smoothing length, represents the resolution of the smoothing, since features on the scale $\ll h$ will be smoothed over in the interpolation (Monaghan & Lattanzio 1985). A derivation of the integral interpolant approximation is given in Appendix C.1.

Numerically, integrals can be approximated by summations. In SPH, the approximation is made using a Monte Carlo summation, where $N$ points are randomly distributed in the volume of interest such that the probability of finding one of the points in a volume element $dV$ located at position $\vec{r}$ is proportional to $\rho(\vec{r})dV$ (Lucy 1977). The field variable is then approximated by:

$$
\langle f(\vec{r}) \rangle \approx \sum_{j=1}^{N} f_j W(\vec{r} - \vec{r}_j; h) \frac{m_j}{\rho_j}
$$

(3.5)

where $m_j$ is the mass of the $j^{th}$ point, $f_j$ and $\rho_j$ are the values of field variable
and density at the position of the $j^{th}$ point respectively. The Monte Carlo approximation converges for $N \to \infty$, see appendix C.1 for the derivation.

A distinct advantage of using the interpolant method is that spatial derivatives, such as gradients, of the field variable can be simplified using integration by parts, and the resulting expression is in terms of the gradient of the kernel:

$$
\langle \nabla f(\vec{r}) \rangle \approx \sum_{j=1}^{N} f_j \frac{m_j}{\rho_j} \nabla W(\vec{r} - \vec{r}_j; h) \quad (3.6)
$$

A full derivation of this equation is given in Appendix C.1.

In practical terms, the integration points can be thought of as “pseudo” particles which are small amounts of gas with a extended density distributions described by the smoothing kernel. These smoothed particles overlap and the superposition approximates the continuous distribution of the gas stream. The particles interact hydrodynamically through the pressure gradient between the particles.
3.1.1 SPH Equations

Using the general SPH equations 3.5 and 3.6, the hydrodynamic equations can be rewritten in a form suitable for numerical calculations.

The density at particle $i$ is described by:

$$
\rho_i = \sum_{j=1}^{N} m_j W_{ij} \tag{3.7}
$$

where $W_{ij} = W(\vec{r}_i - \vec{r}_j; h)$

The acceleration at particle $i$ is given by:

$$
\frac{d\vec{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla W_{ij} + \vec{a}_{ext} \tag{3.8}
$$

This uses a symmetric version of the gradient equation as recommended by many authors (Benz 1990; Monaghan & Lattanzio 1985) to insure that the forces between particle pairs are symmetric.

If an adiabatic equation of state is being used, refer to Section 3.3.2, then the conservation of thermal energy equation is also needed:

$$
\frac{du}{dt} = -\frac{P}{\rho} \nabla \cdot \vec{v} \tag{3.9}
$$
where $u$ is the thermal energy. This translates into the SPH equation for the change in thermal energy for particle $i$:

$$\frac{du_i}{dt} = \frac{P_i}{\rho_i^2} \sum_{j=1}^{N} m_j (\vec{v}_i - \vec{v}_j) \cdot \nabla W_{ij}$$  \hspace{1cm} (3.10)

A full derivation of the SPH equations for density, acceleration, and change in thermal energy is given in Appendix C.2.

### 3.2 Choices of SPH parameters

#### 3.2.1 Kernel

The choice of a smoothing kernel has many considerations. First the kernel must satisfy the conditions in equations 3.4 for the integral interpolation to be valid. In addition to these conditions, the first derivative of the kernel should be continuous for computations of the pressure gradient. The kernel should be centrally condensed, as highly peaked functions give smaller errors. The most computationally efficient kernels use “compact support” meaning that the kernel drops to zero after a limited range instead of extending to infinity.
Considering all of these factors, there are still many possible kernel functions that would be satisfactory for any given problem. However, there is one kernel function, the spline kernel, which has been extensively tested for use with SPH and recommended by many authors (Monaghan 1992; Benz 1990). The spline kernel has been adopted in this dissertation and is described by:

$$W(\vec{r}, h) = \frac{1}{\pi h^3} \begin{cases} 
1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & \text{for } 0 \leq q < 1 \\
\frac{1}{4}(2 - q)^3 & \text{for } 1 \leq q < 2 \\
0 & \text{for } q > 2 
\end{cases}$$

(3.11)

where $$q = \frac{|\vec{r}|}{h}$$

(3.12)

### 3.2.2 Smoothing Length and Number of Particles

Two approximations are used in the derivation of the SPH equations, the integral interpolant and the Monte Carlo Summation. The numerical parameters introduced in these approximations, the smoothing length h and the number of particles N, must be chosen appropriately to obtain the accuracy and resolution desired. The two parameters are correlated since smaller smoothing lengths require a larger number of particles for accurate results.
The values computed for physical quantities are really an average over the nearest neighboring particles. If there are an insufficient number of particles within the smoothing distance, the results will be dominated by errors due to the random placement of the particles. The minimum number of neighbors needed for reasonable results is approximately 20 (Steinmetz & Müller 1993). If a particle has more than 150 neighboring particles, the computational efficiency is reduced due to excessive calculations.

The best results are found using the smallest smoothing lengths and the greatest number of particles. However, the computational time required increases dramatically with the number of particles in a model, placing a limitation on this parameter. In turn, the limit on the number of particles determines the minimum smoothing length that can be achieved for that model. Determining the best values for the smoothing length and particle number requires some experimentation. The initial number of particles and the smoothing lengths are estimated and a test run of the model is started. The parameters are then adjusted as necessary to yield results with sufficient numbers of neighboring particles at the desired resolution with a reasonable computational time.

In addition, SPH can be implemented with either fixed or variable smooth-
ing lengths. In fixed smoothing length implementations, the value of $h$ is a constant in time and the same for every particle. Fixed smoothing lengths are the most straightforward and simplest to program, and the resulting model has a constant spatial resolution. Particles which are in high density regions end up with a large number of neighboring particles, leading to some degree of computational inefficiency. Particles in low density regions, however, have much fewer neighboring particles which can lead to inaccuracies if the density drops too much.

The variable smoothing length implementation of SPH allows each particle to have a different value for $h$, which can change with time. High density regions will have smaller smoothing lengths and thus higher resolution. The low density regions must have larger smoothing lengths and thus lower resolution, but will not have inaccuracies due to insufficient neighbors. The result is a more computationally efficient model with variable spatial resolution and much more complex programming.

The smoothing length of each particle, in the variable smoothing length method, is related to its density by the relation:

$$h_i = k \left( \frac{\rho_i}{m_i} \right)^{-\frac{1}{3}}$$

(3.13)
where $k$ is a constant of order unity (Steinmetz & Müller 1993). The value for $k$ is set based on test runs to determine that the model has sufficient neighboring particles. The SPH equations must be adjusted such that the kernel function becomes:

$$W_{ij} = W(W(\vec{r}_i - \vec{r}_j; \frac{h_i + h_j}{2})$$

(3.14)

The smoothing length is then adjusted over time by using the density estimate from the previous time step.

### 3.3 Other Numerical Topics

#### 3.3.1 Time Integration

The position and velocity of the particles are advanced in time according to the leapfrog algorithm (Hernquist & Katz 1989). Once the initial positions and velocities of each SPH particle are set, the accelerations are computed by the SPH equations. The velocities are then advanced by a half time step.
according to:

\[ \vec{v}(t_0 + \frac{\Delta t}{2}) = \vec{v}(t_0) + \frac{\Delta t}{2} D\vec{v}(t_0) \]  

(3.15)

where \( t_0 \) is the initial time, \( \Delta t \) is the time step, and \( D \) represents the time derivative \( d/dt \). Then the position and velocity are advanced to the next full time step by:

\[ \vec{r}(t + \Delta t) = \vec{r}(t) + \Delta t \vec{v}(t + \frac{\Delta t}{2}) \]  

(3.16)

\[ \vec{v}(t + \Delta t) = \vec{v}(t + \frac{\Delta t}{2}) + \frac{\Delta t}{2} D\vec{v}(t) \]  

(3.17)

Subsequent half time steps for the velocity are computed by:

\[ \vec{v}(t + \frac{\Delta t}{2}) = \vec{v}(t - \frac{\Delta t}{2}) + \Delta t D\vec{v}(t) \]  

(3.18)

If the thermal energy is also being computed from the SPH equations, it
is advanced in time analogous to the velocity equations:

\[
\begin{align*}
    u(t_0 + \frac{\Delta t}{2}) &= u(t_0) + \frac{\Delta t}{2} Du(t_0) \\
    u(t + \Delta t) &= u(t + \frac{\Delta t}{2}) + \frac{\Delta t}{2} Du(t) \\
    u(t + \frac{\Delta t}{2}) &= u(t - \frac{\Delta t}{2}) + \Delta t Du(t)
\end{align*}
\] (3.19) (3.20) (3.21)

3.3.2 Thermodynamic Equation of State

As mentioned in the opening of this chapter, the thermal pressure of the gas is needed to solve the hydrodynamic equation. The pressure of each SPH particle is calculated using the equation of state assumed for the gas. There are, however, several possibilities for the equation of state.

In general the gas is assumed to be an ideal gas. Therefore, the pressure is related to the density and temperature of the gas by:

\[
P_i = \rho_i \frac{kT_i}{m_H}
\] (3.22)

where \( P_i \), \( \rho_i \), and \( T_i \) are the thermal pressure, density, and temperature of the \( i^{th} \) particle, and \( m_H \) is the mass of hydrogen. The gas is assumed to be hydrogen with only negligible amounts of other elements. The density
is computed from the SPH equations, but the temperature depends on the assumed thermal behavior of the gas.

An isothermal gas is the most commonly assumed condition. For this case the constant temperature yields the isothermal speed of sound for the gas:

\[ c_{iso} = \sqrt{\frac{kT}{m_H}} \]  

(3.23)

The equation of state then simplifies to:

\[ P_i = \rho_i c_{iso}^2 \]  

(3.24)

The thermal energy of the SPH gas particles does not need to be calculated for an isothermal gas, simplifying the overall computations necessary.

Another possibility is to treat the gas as adiabatic, where the gas pressure can be easily related to the density and thermal energy of each particle:

\[ P_i = (\gamma - 1)\rho_i u_i \]  

(3.25)

where \( \gamma \) is the ratio of specific heats of the gas, 5/3 for atomic hydrogen.
The density and thermal energy are calculated from the SPH equations. The
temperature and speed of sound can also be derived from the thermal energy
according to:

\[
T_i = \frac{(\gamma - 1)m_H u_i}{k} \quad \text{(3.26)}
\]
\[
c_i = \sqrt{(\gamma - 1)u_i} \quad \text{(3.27)}
\]

Other possibilities for the thermal behavior can be developed using posi-
tion dependent temperatures or heating terms in the thermal energy equa-
tions. These kinds of models are developed to approximate the effects of
radiation from the accretion region.

### 3.3.3 Boundaries

In the derivation of the general SPH equations (see Appendix C), it was
assumed that the volume of integration was sufficiently large such that the
density drops to zero at the surface of the volume. If this is not true for
a particular problem, the boundary must be carefully treated to yield the
correct results.

For the polar accretion stream models, the L1 boundary does not have
zero density. For any particle within 2h of the boundary, the contribution to the density and pressure gradient from behind the L1 boundary must be accounted for some how. Fortunately the density profile behind the L1 point can be described analytically with a few basic assumptions. Therefore, the SPH contributions from other particles are calculated normally and the analytical contributions are added in.

3.3.4 Viscosity

So far the derivations of the SPH equations have all assumed an inviscid fluid. The effects of viscosity are important in some astrophysical applications, and viscosity can be included in the SPH formalism. In particular, shocks require the inclusion of artificial viscosity for SPH to handle them adequately (Benz 1990). Fortunately, the ballistic portion of the polar accretion stream does not contain any shocks and can be adequately modeled as an inviscid fluid.