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SPH Formalism

Created by Jaeden Bardati

Caltech

This homework will guide the student through the mathematical formalism of SPH particles. After this homework, you should have an adequate enough understanding of how to go from particle data from an SPH simulation to integrated continuous quantities that you might want to extract from it.

1 Relevant Background

Smoothed Particle Hydrodynamics (SPH) is a numerical technique that discretizes mass/volume in a way that is particularly useful in hydrodynamics codes (i.e. when solving the Navier-Stokes equations).

The premise is that we define a set of particles that have a location $\boldsymbol{r}_i$, a mass m_i, and are smeared over an effective "smoothing length" h_i according to some window function (also called kernel function) $W(|\boldsymbol{r}-\boldsymbol{r}_i|, h_i)$ where $\boldsymbol{r}$ is the distance to the particle. This window function can be virtually any continuous function, so long that it is normalized over whatever dimension of space used and that $W(|\boldsymbol{r}-\boldsymbol{r}_i|, h_i)$ and its derivatives $\to 0$ as $\boldsymbol{r} \to \infty$, but typically we use a Gaussian distribution (or something similar like a cubic spline). The particles can have other properties too, such as temperature T_i, velocity $\boldsymbol{v}_i$, internal energy ϵ_i, etc. I'll denote a general particle property with A_i.

An important quantity derived from the mass distribution of particles is the mass density. Since each particle contributes to the mass in a given location $\boldsymbol{r}$ weighted by the window function (which is in units of inverse volume, area or length depending on the dimension), the density can be given by the sum of the contributions of all the particles. For N particles indexed by j, the density is

$$\rho(\boldsymbol{r}) = \sum_j^N m_j W(|\boldsymbol{r} - \boldsymbol{r}_h|, h_j) \tag{1}$$

We can therefore compute the density at the location of a particle i with

$$\rho_i = \sum_j^N m_j W(|\boldsymbol{r}_j - \boldsymbol{r}_j|, h_j) \tag{2}$$

This is an important quantity since it allows us to weight by an effective volume for each particle m_j/ρ_j. Any quantity A at location $\boldsymbol{r}$ can therefore be computed with

$$A(\boldsymbol{r}) = \sum_j^N A_j \left(\frac{m_j}{\rho_j}\right) W(|\boldsymbol{r} - \boldsymbol{r}_j|, h_j) \tag{3}$$

We can find the derivatives or integrals of these quantities by simply applying them to the window function since the particle properties do not depend on $\boldsymbol{r}$ (only on $\boldsymbol{r}_j$).

$$\partial_r A(\boldsymbol{r}) = \sum_j^N A_j \left(\frac{m_j}{\rho_j}\right) \partial_r W(|\boldsymbol{r}-\boldsymbol{r}_j|, h_j) \tag{4}$$

$$\int A(\boldsymbol{r}) dr = \sum_j^N A_j \left(\frac{m_j}{\rho_j}\right) \int W(|\boldsymbol{r}-\boldsymbol{r}_j|, h_j) dr \tag{5}$$

If we are interested in finding the column density of hydrogen along the z direction, for example, we can simply use

$$n_H(x,y) \equiv \int_{-\infty}^{\infty} \frac{\rho(\boldsymbol{r})}{m_H} dz = \sum_j^N \frac{m_j}{m_H} \int_{-\infty}^{\infty} W(|\boldsymbol{r}-\boldsymbol{r}_j|, h_j) dz = \sum_j^N \frac{m_j}{m_H} W_{2\mathrm{D}}(|\boldsymbol{s}-\boldsymbol{s}_j|, h_j) \tag{6}$$

where $\boldsymbol{s}$ is a vector containing the 2D (x, y) coordinates. The last line exploits the fact that when integrating over a 3D Gaussian function, we obtain a 2D Gaussian. Unfornuately, it is not always this neat.

Alternatively, we could find the average of a quantity through a column, such as

$$\langle A \rangle_z = \frac{\int A(\boldsymbol{r}) dz}{\int dz} = \frac{\sum_j^N A_j \left(\frac{m_j}{\rho_j}\right) W_{2\mathrm{D}}(|\boldsymbol{s}-\boldsymbol{s}_j|, h_j)}{\sum_j^N \left(\frac{m_j}{\rho_j}\right) W_{2\mathrm{D}}(|\boldsymbol{s}-\boldsymbol{s}_j|, h_j)} \tag{7}$$

Or weighted by mass instead with

$$\langle A \rangle_m = \frac{\int A(\boldsymbol{r}) dm}{\int dm} = \frac{\int A(\boldsymbol{r}) \rho(\boldsymbol{r}) dz}{\int \rho(\boldsymbol{r}) dz} = \frac{\sum_j^N A_j m_j W_{2\mathrm{D}}(|\boldsymbol{s}-\boldsymbol{s}_j|, h_j)}{\sum_j^N m_j W_{2\mathrm{D}}(|\boldsymbol{s}-\boldsymbol{s}_j|, h_j)} \tag{8}$$

With this framework, we can convert between the particle quantities to continuous functions. If we have an equation that governs the dynamics of the particles (e.g. Navier Stokes equations, Maxwell equations, etc.), we can use this framework to convert the continuous math equations to the approximate discretized solution that can be numerically integrated, and potentially back to other quantities or projections we are interested in.

2 Homework Problem

Problem 1. *(a)* Integrate the quantity $A(\boldsymbol{r})$ from some spherical radius $r = R$ to $r = 0$ at fixed θ and ϕ for a normalized Gaussian kernel to show that the result is like in equation 6 but there is some factor in the sum that depends on R and r_j due to the finite integral. You can write your answer using the special function

$$\mathrm{erf}(z) \equiv \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt \tag{9}$$

Now, change the bounds to a chord through the R sphere origin (i.e. from $r = -R$ to $r = R$). Show that as $R \to \infty$, the factor approaches unity.

(b) If we wanted to numerically find the average value of this quantity in a solid angle Ω (a cone shape with a spherical end), we can compute the quantity at a few special values of θ and ϕ within the given range and simply take their unweighted mean. How do we pick our grid of θ and ϕ such that we do not need to weight the mean?

Problem 2. *(a)* Show that for the line integral of a quantity $A(\boldsymbol{r})$ from $t_1 \to t_2$ along a general line defined by the vector equation $\boldsymbol{\ell}(t) = \boldsymbol{a} + t\hat{\boldsymbol{\ell}}$ is given by[1]

$$\int_{t_1}^{t_2} A(\boldsymbol{r}) d\ell = \sum_{j}^{N} \frac{A_j m_j}{\rho_j} I_j(\boldsymbol{\ell}) \tag{10}$$

for the integral

$$I_j(\boldsymbol{\ell}) = \text{sign}(\tilde{\ell}_1) \int_{\tilde{r}_{1,j}}^{b_j} \frac{\tilde{r}}{\sqrt{\tilde{r}^2 + b_j^2}} W(\tilde{r}, h_j) d\tilde{r} + \text{sign}(\tilde{\ell}_2) \int_{b_j}^{\tilde{r}_{2,j}} \frac{\tilde{r}}{\sqrt{\tilde{r}^2 + b_j^2}} W(\tilde{r}, h_j) d\tilde{r} \tag{11}$$

where $\tilde{r}_{n,j} \equiv \sqrt{b_j^2 + \tilde{\ell}_n^2}$, with $\tilde{\ell}_n \equiv t_n + \hat{\boldsymbol{\ell}} \cdot (\boldsymbol{a} - \boldsymbol{r}_j)$, and $b_j \equiv \left| (\boldsymbol{a} - \boldsymbol{r}_j) - \left[\hat{\boldsymbol{\ell}} \cdot (\boldsymbol{a} - \boldsymbol{r}_j) \right] \hat{\boldsymbol{\ell}} \right|$.

Hint: Consider the geometry, where b_j represents an impact parameter of the ray $\boldsymbol{\ell}(t)$ with the given particle at $\boldsymbol{r}_j$.

(b) If we integrate the above with a Gaussian window function $W(\tilde{r}, h_j) = Ae^{\tilde{r}^2/h_j^2}$ for some normalization factor A, show that

$$\int \frac{\tilde{r}}{\sqrt{\tilde{r}^2 + b_j^2}} W(\tilde{r}, h_j) d\tilde{r} = -\frac{hA}{2} \exp\left(-\frac{b_j^2}{h_j^2}\right) \Gamma\left(\frac{1}{2}, \frac{b_j^2 + \tilde{r}^2}{h_j^2}\right) + C \tag{12}$$

where $\Gamma(s, x) \equiv \int_x^\infty t^{s-1} e^{-t} dt$ is the incomplete gamma function. Also, make sure to normalize your Gaussian properly (i.e. find A). Then, show that when $\boldsymbol{a} = 0$ and $\hat{\boldsymbol{\ell}} = \hat{\boldsymbol{z}}$ from $t_1 = R$ to $t_2 = 0$ (i.e. radial integration to origin), you get the same thing that you found in problem 1a.

[1] Note that the line parameter t has dimensions of length, *not* e.g. time.