Meshless Hydrodynamics

1 Partition of Unity

1.1 Introduction

The basic idea behind meshless hydrodynamics is to trace the fluid by particles and distribute the volume amongst the particles.

At every point $\mathbf{x}$ in space in the domain, we assign a volume partition $\psi_i(\mathbf{x})$ to each particle i such that

$$\sum_i \psi_i(\mathbf{x}) = 1 \qquad [1]$$

where i are all particles. For this reason, $\psi_i(\mathbf{x})$ is also called the "partition of unity".

In principle, ψ may be an arbitrary function. In practice, we want to constrain it and demand some properties such that we can make use of them in further computations.

We choose:

$$\psi_i(\mathbf{x}) \equiv \frac{1}{\omega(\mathbf{x})} W(\mathbf{x} - \mathbf{x}_i, h(\mathbf{x}))$$

where $h(\mathbf{x})$ is some "kernel size" and

$$\omega(\underline{x}) \equiv \sum_j W(\underline{x} - \underline{x}_j, h(\underline{x}))$$

is used to normalize the partition of unity so that definition [1] is satisfied.

Again, in principle W may be an arbitrary function at this point, but we demand:

1) $W(\underline{x} - \underline{x}_i, h(\underline{x}))$ is continuous

2) W must have compact support, i.e.
$W \to 0$ for $|\underline{x} - \underline{x}_i| >> h$

3) W is (spherically) symmetric:
$W = W(|\underline{x} - \underline{x}_i|, h(\underline{x}))$

These demands ensure second order accuracy, conservation of linear and angular momentum (demands 1 and 2), and locality of hydrodynamic operations (demand 3).

1.2 Particle Volume

1.2.1 Derivation

Suppose we have data defined on a set of interpolation points f_i, which in our case can correspond to function values at particle positions i. Then the interpolated value is given by

$$f(\underline{x}) = \sum_i f_i \, \psi_i(\underline{x}) \qquad [2]$$

and the gradient is given by

$$\underline{\nabla} f(\underline{x}) = \underline{\nabla}\Big(\sum_i f_i \, \psi_i(\underline{x})\Big) = \sum_i f_i \, \underline{\nabla} \psi_i(\underline{x})$$

[the f_i are treated as constant]

Using these definitions and the definition of the volume average of a function

$$V \langle f \rangle \equiv \int_V f(\underline{x}) \, dV$$

we get

$$V \langle f \rangle \equiv \int_V f(\underline{x}) \, dV = \int_V \sum_i f_i \, \psi_i(\underline{x}) \, dV =$$

$$= \sum_i f_i \int \psi_i(\underline{x}) \, dV = \sum_i f_i V_i$$

with

$$\boxed{V_i \equiv \int \Psi_i \, dV}$$

being the associated particle volume.

If we set $f(\underline{x}) = f_i = 1$, we obtain

$$V \langle f \rangle = V = \sum_i f_i V_i = \sum_i V_i$$

$$\Rightarrow V = \sum_i V_i$$

$\Rightarrow$ By construction, the total volume of particles is conserved in a closed system.

We can find an expression for the V_i in relation to the function $W(\underline{x} - \underline{x}_i, h(\underline{x}))$.

We assume that

- $W = W(|\underline{x} - \underline{x}_i|)$ is symmetric, and
- $\int W(\underline{x} - \underline{x}_i, h(\underline{x}))\, dV = 1$ is normed.

We also use:

$$(1) \quad f(\underline{x}) = \sum_i f(\underline{x}_i)\,\psi_i(\underline{x})$$

$$(2) \quad \psi_i(\underline{x}) = \frac{1}{\omega(\underline{x})}\, W(\underline{x}-\underline{x}_i) = \frac{W(\underline{x}-\underline{x}_i)}{\sum_j W(\underline{x}-\underline{x}_j)}$$

$$(3) \quad V_i = \int_V \psi_i(\underline{x})\, dV$$

Then:

$$V_i \overset{(1)}{=} \sum_j \psi_j(\underline{x}_i) V_j \overset{(3)}{=} \sum_j \psi_j(\underline{x}_i) \int_V \psi_j(\underline{x})\, dV$$

$$\overset{(2)}{=} \sum_j \frac{W(\underline{x}_i-\underline{x}_j)}{\sum_k W(\underline{x}_i-\underline{x}_k)} \int \psi_j(\underline{x})\, dV$$

$$= \frac{1}{\sum_k W(\underline{x}_i-\underline{x}_k)} \sum_j W(\underline{x}_i-\underline{x}_j) \int \psi_j(\underline{x})\, dV$$

$$= \frac{1}{\omega(\underline{x}_i)} \sum_j \int W(\underline{x}_i-\underline{x}_j)\, \psi_j(\underline{x})\, dV$$

$$\overset{(1)}{=} \frac{1}{\omega(\underline{x}_i)} \int W(\underline{x}_i-\underline{x})\, dV = \frac{1}{\omega(\underline{x}_i)} \int W(\underline{x}-\underline{x}_i)\, dV$$

$$= \frac{1}{\omega(\underline{x}_i)}$$

$$\Rightarrow \boxed{V_i = \frac{1}{\omega(\underline{x}_i)}} \qquad [3]$$

Expression [3] is only valid assuming that expression [2], i.e.

$$f(\underline{x}) = \sum_i f_i \, \psi_i(\underline{x})$$

and the volume integral of [2]:

$$\int_V f(\underline{x}) \, dV = \sum_i f(\underline{x}_i) V_i$$

are exact, which they are not in general.

As will be shown in the next section, the volume integral is $\mathcal{O}(h^2)$ accurate, giving us:

$$\boxed{V_i = \frac{1}{\omega(\underline{x}_i)} + \mathcal{O}(h^2)}$$

1.2.2 Taylor-Expansion of the Volume Integral

We compute now the accuracy of the volume integral of an arbitrary function $f(\underline{x})$ in the partition of unity formalism.

Reminder:

$$\sum_i \psi_i(\underline{x}) = 1$$

$$\psi_i(\underline{x}) = \psi(\underline{x} - \underline{x}_i) = \frac{1}{\omega(\underline{x}_i)} W(\underline{x} - \underline{x}_i)$$

(just notation)

For the volume integral of an arbitrary function $f(\underline{x})$, we write and Taylor-expand:

$$\int_V f(\underline{x})\, dV = \int f(\underline{x}) \underbrace{\sum_i \psi_i(\underline{x})}_{=1} dV = \sum_i \int f(\underline{x}) \psi_i(\underline{x})\, dV$$

$$= \sum_i \int \left[f(\underline{x}_i) + (\underline{x} - \underline{x}_i) \nabla f(\underline{x}_i) + \mathcal{O}((\underline{x} - \underline{x}_i)^2) \right] \psi_i(\underline{x})\, dV$$

$$= \sum_i f(\underline{x}_i) \int \psi_i(\underline{x})\, dV + \underbrace{\sum_i \int (\underline{x} - \underline{x}_i) \nabla f(\underline{x}_i) \psi_i(\underline{x})\, dV}_{=0;\ \text{will be shown later}} + \mathcal{O}((\underline{x} - \underline{x}_i)^2)$$

$$\boxed{= \sum_i f(\underline{x}_i) V_i + \mathcal{O}((\underline{x}_i - \underline{x}_i)^2)}$$

It remains to show that

$$\sum_i \int_V (\underline{x} - \underline{x}_i) \underline{\nabla} f(\underline{x}_i) \psi_i(\underline{x}) dV = 0$$

$$= \sum_i \underline{\nabla} f(\underline{x}_i) \int_V (\underline{x} - \underline{x}_i) \psi_i(\underline{x}) dV$$

It suffices to show that $\int_V (\underline{x} - \underline{x}_i) \psi_i(\underline{x}) dV = 0$.

For simplicity I demonstrate this only in 1D and set the boundaries to be $(-L, L)$, which may be infinite. (In case they aren't, we ignore for now what happens when a particle is close enough to the border such that the border is within compact support radius.)

Then we have:

$$\int_{-L}^{L} (x - x_i) \psi_i(x) dx = \int_{-L}^{L} (x - x_i) \psi(x - x_i, h(x)) dx$$

Let $s = x - x_i \Rightarrow ds = dx$

$$= \int_{-L+x_i}^{L+x_i} s \, \psi(s) ds$$

Now integrate by parts: $\int u' v \, ds = uv - \int u v' ds$

$u' = \psi(s) ds$ $\qquad v = s$

$u = \int_{-L+x_i}^{L+x_i} \psi(s) ds = \int_{-L}^{L} \psi_i(x) dx = V_i$ $\qquad v' = ds$

$$\Rightarrow \int_{-L+x_i}^{L+x_i} s\,\psi(s)\,ds = s V_i \Big|_{-L+x_i}^{L+x_i} - \int_{-L+x_i}^{L+x_i} V_i\,ds$$

$$= \Big[s V_i - s V_i \Big]_{-L+x_i}^{L+x_i} = 0 \qquad //$$

We have seen that the integral is $\mathcal{O}(\Delta x^2)$ accurate, where Δx is the mean interparticle distance. The mean interparticle distance is set by the compact support radius. (The radius is often chosen such that each particle has roughly the same user-defined number of neighbouring particles to interact with.)

A larger compact support radius leads to higher average interparticle distances, as particles with higher distances are included in the interactions.

This means that the mean interparticle distance is directly related, in fact proportional, to, the compact support radius, and we may as well refer to the integral as $O(h^2)$ accurate.

h also depends on the number of particles used for a specific problem. Assuming we keep the number of interacting neighbours fixed for some problem, using more particles to solve the exact same problem will decrease h and will thus lead to more accurate results.

2 Meshless Methods

2.1 Meshless Hydrodynamics à la Ivanova

We start off by writing the Euler equations: for every component k:

$$\frac{\partial \underline{u}_k}{\partial t} + \frac{\partial}{\partial x^\alpha} \underline{\underline{F}}_{k\alpha} = 0 \qquad [4]$$

where

$$\underline{u} = \begin{pmatrix} \rho \\ \rho \underline{v} \\ E \end{pmatrix}, \qquad \underline{\underline{F}} = \begin{pmatrix} \rho \underline{v} \\ \rho v_i v_j + P \, \underline{\underline{1}} \\ (E+P)\, \underline{v} \end{pmatrix}$$

we neglect external forces, source- and sink terms for now and apply the Einstein sum convention over Greek indices.

To obtain a weak solution to the Euler equations, we multiply them with an arbitrary, differentiable test function $\phi(\underline{x}, t)$ with compact support over the domain of interest, i.e for a domain $T \otimes V \in \mathbb{R}_0^+ \times \mathbb{R}^3$:

$$\phi(\underline{x}, t) = 0 \quad \text{if} \quad \underline{x} \notin V \text{ or } t \notin T$$

$$\text{or if} \quad \underline{x} \in \partial V \text{ or } t \in \partial T$$

on the boundaries (ϕ must be smooth to be differentiable)

Now integrate the product over the entire domain:

$$\iint_{T\,V} \Big[\underbrace{\frac{\partial U_k}{\partial t} + \frac{\partial}{\partial x_\alpha} F_{k\alpha}}_{=0} \Big] \phi(\underline{x}, t)\, dt\, dV = 0 \qquad [5]$$

Since ϕ has compact support, we can write

$$\int_T \frac{\partial}{\partial t}(U_k\, \phi)\, dt = \underbrace{U_k\, \phi}_{=0 \text{ on boundary edges}} \Big|_{t=0}^{T} = 0$$

$$\Rightarrow \int_T \frac{\partial}{\partial t}(U_k\, \phi) dt = \int \frac{\partial U_k}{\partial t} \phi\, dt + \int U_k \frac{\partial \phi}{\partial t}\, dt = 0$$

$$\Rightarrow \int \frac{\partial U_k}{\partial t} \phi\, dt = -\int U_k \frac{\partial \phi}{\partial t}\, dt \qquad [6]$$

For the divergence of the flux tensor, we use the Gauss theorem:

$$\int_V \frac{\partial}{\partial x_\alpha} f_\alpha\, dV = \oint_{\partial V} f_\alpha\, \hat{n}_\alpha\, d\partial V$$

where $\hat{n}_\alpha$ is the normal vector to the surface boundary ∂V.

Applying Gauss' theorem on the divergence of the flux tensor gives:

$$\int_V \frac{\partial}{\partial x_\alpha} (F_{k\alpha} \phi) \, dV = \oint_{\partial V} (F_{k\alpha} \underbrace{\phi) \cdot \hat{n}_\alpha}_{=0 \text{ along } \partial V} \, d\partial V = 0$$

$$= \int_V \frac{\partial}{\partial x_\alpha} F_{k\alpha} \phi \, dV + \int_V F_{k\alpha} \frac{\partial}{\partial x_\alpha} \phi \, dV$$

$$\Rightarrow \int \frac{\partial F_{k\alpha}}{\partial x_\alpha} \phi \, dV = - \int F_{k\alpha} \frac{\partial \phi}{\partial x_\alpha} \, dV \qquad [7]$$

Inserting [6] and [7] in [5] gives

$$\iint_{TV} \left[\frac{\partial U_k}{\partial t} \phi + \frac{\partial F_{k\alpha}}{\partial x_\alpha} \phi \right] dt \, dV = 0$$

$$= \iint \left[-\frac{\partial \phi}{\partial t} U_k - \frac{\partial \phi}{\partial x_\alpha} F_{k\alpha} \right] dt \, dV$$

$$= \iint \Big[\underbrace{\frac{\partial \phi}{\partial t} U_k}_{1} + \underbrace{\frac{\partial \phi}{\partial x_\alpha} F_{k\alpha}}_{2} \Big] dt \, dV = 0$$

We now insert our definition of the partition of unity to interpolate the values from discrete points:

$$f(x) = \sum_i f(x_i) \, \Psi_i(x)$$

$$\Rightarrow \left(\frac{\partial \phi}{\partial t} U_k \right) = \sum_i \left(\frac{\partial \phi(x_i)}{\partial t} U_k(x_i) \right) \Psi_i(x) \equiv \sum_i \frac{\partial \phi_i}{\partial t} U_{k,i} \, \Psi_i(x)$$

$$\Rightarrow \left(\frac{\partial \phi}{\partial x_\alpha} F_{k\alpha} \right) \equiv \sum_i \frac{\partial \phi_i}{\partial t} F_{k\alpha,i} \, \Psi_i(x)$$

For part ① of the integral we obtain

$$\iint_{TV} u_k \frac{\partial \phi}{\partial t} \, dV \, dt = \iint_{TV} \sum_i u_{k,i} \frac{\partial \phi_i}{\partial t} \psi_i(x) \, dV \, dt =$$

$$= \int_T \sum_i u_{k,i} \frac{\partial \phi_i}{\partial t} \int_V \psi_i(x) \, dV \, dt$$

$$= \int_T \sum_i u_{k,i} \frac{\partial \phi_i}{\partial t} V_i \, dt$$

Once again we make use of the compact support of the test function ϕ to rearrange the integral:

$$\int_T \sum_i \frac{\partial}{\partial t} \left(u_{k,i} V_i \phi_i \right) dt = \sum_i \underbrace{u_{k,i} V_i \phi_i \Big|_{t=0}^{T}}_{=0} = 0$$

$$= \int_T \sum_i \left[\frac{\partial}{\partial t} \left(u_{k,i} V_i \right) \phi_i + u_{k,i} V_i \frac{\partial \phi_i}{\partial t} \right] dt$$

$$\Rightarrow \int \sum_i \frac{\partial}{\partial t} \left(u_{k,i} V_i \right) \phi_i \, dt = - \int \sum_i u_{k,i} V_i \frac{\partial \phi_i}{\partial t} \, dt$$

giving us for ①:

$$\iint u_k \frac{\partial \phi}{\partial t} \, dV \, dt = \int_T \sum_i u_{k,i} \frac{\partial \phi_i}{\partial t} V_i \, dt = \boxed{- \int_T \sum_i \phi_i \frac{\partial}{\partial t} \left(u_{k,i} V_i \right) dt}$$

As for part ② of the integral:

$$② \iint_{TV} \frac{\partial \phi}{\partial x_\alpha} \cdot F_{k\alpha}\, dt\, dV = \iint_{TV} F_{k\alpha} \frac{\partial}{\partial x_\alpha}\left(\sum_i \phi_i \psi_i\right) dt\, dV$$

$$= \iint F_{k\alpha} \frac{\partial}{\partial x_\alpha}\left(\sum_i \phi_i \psi_i\right) \underbrace{\cdot 1}_{\text{add multiplication by } 1} \cdot dt\, dV$$

$$= \iint F_{k\alpha} \frac{\partial}{\partial x_\alpha}\left(\sum_i \phi_i \psi_i\right) \underbrace{\left(\sum_j \psi_j(x)\right)}_{=1} dt\, dV$$

remember $\phi_i = \phi(x_i) = \text{const}$

$$= \sum_{i,j} \iint \left[F_{k\alpha}\, \phi_i\, \psi_j(x) \frac{\partial \psi_i(x)}{\partial x_\alpha} \right] dt\, dV$$

$$= \sum_{i,j} \iint \left[F_{k\alpha}\, \phi_i\, \psi_j(x) \frac{\partial \psi_i(x)}{\partial x_\alpha} \underbrace{+ 0}_{\text{add zero}} \right] dt\, dV$$

$$= \sum_{i,j} \iint \left[F_{k\alpha}\, \phi_i\, \psi_j \frac{\partial \psi_i}{\partial x_\alpha} \underbrace{- F_{k\alpha}\, \phi_i \frac{\partial \psi_j}{\partial x_\alpha} \psi_i}_{=0,\ \text{shown later}} \right] dV\, dt$$

$$= \sum_{i,j} \iint F_{k\alpha}\, \phi_i \left[\psi_j \frac{\partial \psi_i}{\partial x_\alpha} - \psi_i \frac{\partial \psi_j}{\partial x_\alpha} \right] dV\, dt$$

$$= \sum_{i,j} \int_T \phi_i \int_V F_{k\alpha} \cdot d\Sigma_{ji,\alpha}$$

where I introduced

$$d\Sigma_{ji,\alpha} = \left[\psi_j \frac{\partial \psi_i}{\partial x_\alpha} - \psi_i \frac{\partial \psi_j}{\partial x_\alpha} \right] dV$$

We can approximate the volume integral by a single point quadrature:

$$\int_V F_{k\alpha} \cdot d\Sigma_{ji,\alpha} \approx F_{ij,k\alpha} A_{ji,\alpha}$$

where $A_{ji,\alpha}$ is given by

$$A_{ji,\alpha} \equiv \int d\Sigma_{ji,\alpha} = \int_V \left[\psi_j \frac{\partial \psi_i}{\partial x_\alpha} - \psi_i \frac{\partial \psi_j}{\partial x_\alpha} \right] dV$$

$F_{ij,k}$ is the component of the flux tensor through the abstract interface ("effective surface") A_{ij} between particle i and j, similar to the flux through the face of a cell in a finite volume method.

The discretization of the volume integral of A_{ij} will be discussed later. First it needs to be shown that the zero we added during the derivation is really a zero:

$$\sum_{i,j} F_{k\alpha} \psi_i \phi_i \frac{\partial \psi_j}{\partial x_\alpha} = \sum_i F_{k\alpha} \psi_i \phi_i \underbrace{\frac{\partial}{\partial x_\alpha} \Big(\underbrace{\sum_j \psi_j (x)}_{=1} \Big)}_{=0} = 0 \quad //$$

This part was added so that the expression is antisymmetric between particle i and j, i.e. it results in $A_{ij} = -A_{ji}$.

Finally, combining our results for ① and ②, we get

$$\iint_{TV} \left[\frac{\partial U_k}{\partial t} + \frac{\partial F_{k\alpha}}{\partial x_\alpha} \right] \phi \, dt \, dV = \iint_{TV} \left[\frac{\partial \phi}{\partial t} U_k + \frac{\partial \phi}{\partial x_\alpha} F_{k\alpha} \right] dt \, dV = 0$$

$$= \int_T \left[- \sum_i \frac{\partial}{\partial t} (U_{k,i} \, V_i) \phi_i + \sum_{ij} \phi_i F_{ij,k\alpha} \, A_{ji,\alpha} \right] dt =$$

$$= \int_T \sum_i \phi_i \left[\frac{\partial}{\partial t} (U_{k,i} \, V_i) + \sum_j F_{ij,k\alpha} \, A_{ij,\alpha} \right] dt = 0$$

Note that i and j were switched in A_{ij} to get rid of the minus sign that entered through the state vector part ① of the integral. Also note that A_{ij} is defined with switched indices i and j compared to the definition in Ivanova et al. 2013. This is so that comparisons with the Hopkins 2015 expression are easier to do.

The obtained expression must be valid for all ϕ_i and times t, giving us

$$\boxed{\frac{\partial}{\partial t} (U_{k,i} \, V_i) + \sum_j F_{ij,k\alpha} \, A_{ij,\alpha} = 0}$$

with

$$\boxed{A_{ij,\alpha} = \int_V \left[\psi_i \frac{\partial \psi_j}{\partial x_\alpha} - \psi_j \frac{\partial \psi_i}{\partial x_\alpha} \right] dV}$$

Finally, we need to find a discrete approximation for the volume integral

$$A_{ij,\alpha} = \int_V \left[\psi_i \frac{\partial \psi_j}{\partial x_\alpha} - \psi_j \frac{\partial \psi_i}{\partial x_\alpha} \right] dV$$

First consider only the part $\int_V \psi_i(x) \frac{\partial \psi_j(x)}{\partial x_\alpha} dV$.

By Taylor-expanding $\frac{\partial \psi_j(x)}{\partial x_\alpha}$ around $x = x_i$, we get

$$\int_V \psi_i(x) \left[\frac{\partial \psi_j(x_i)}{\partial x_\alpha} + (x - x_i) \frac{\partial^2 \psi_j(x_i)}{\partial x_\alpha^2} + \mathcal{O}((x-x_i)^2) \right] dV =$$

$$= \frac{\partial \psi_j(x_i)}{\partial x_\alpha} \int_V \psi_i(x) dV + \frac{\partial^2 \psi_j(x_i)}{\partial x_\alpha^2} \underbrace{\int \psi_i(x)(x-x_i) dV}_{=0} + \mathcal{O}((x-x_i)^2)$$

$$= \frac{\partial \psi_j(x_i)}{\partial x_\alpha} V_i + \mathcal{O}(h^2)$$

by following the same arguments as is done in the volume integral Taylor expansion in section 1.2.2. The same process can analogously be applied to the second part of the integral giving us

$$\boxed{A_{ij,\alpha} = V_i \frac{\partial \psi_j(x_i)}{\partial x_\alpha} - V_j \frac{\partial \psi_i(x_j)}{\partial x_\alpha} + \mathcal{O}(h^2)}$$

2.2 Meshless Hydrodynamics à la Hopkins

We start from the Euler equations:

$$\frac{\partial \underline{U}}{\partial t} + \frac{\partial}{\partial x_\alpha} \underline{\underline{F}}_\alpha = 0$$

with $\underline{U} = \begin{pmatrix} \rho \\ \rho \underline{v} \\ E \end{pmatrix}$, $\underline{\underline{F}} = \begin{pmatrix} \rho \underline{v} \\ \rho v_i v_j + P \mathbb{1} \\ (E+P) \underline{v} \end{pmatrix}$

The Euler equations are Galilei-invariant, i.e. keep their form in any inertial system, provided you transform all the physical quantities and derivatives properly. (Partial derivatives are not invariant!)

Suppose now we have a fluid moving in a frame of reference with velocity $\underline{v}^F$.

With respect to the rest frame, the Euler equations are

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_\alpha} \left(F_{i\alpha} - v^F_\alpha U_i \right) = 0$$

for every component i.

Note that the fluid quantities U_i, F_{ij} are as seen in the moving frame, but the derivatives are taken with respect to the rest frame.

To obtain a weak solution for the equation, we again multiply the conservation law by a test function $\phi = \phi(\underline{x}, t)$ with compact support and require that ϕ is also differentiable. We then have, when integrating over the entire domain:

$$\int_V \left[\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_\alpha}\left(F_{i\alpha} - v_\alpha{}^F U_i \right) \right] \phi \, dV = 0$$

$$= \int_V \left[\frac{\partial U_i}{\partial t} - v_\alpha{}^F \frac{\partial U_i}{\partial x_\alpha} + \frac{\partial}{\partial x_\alpha} F_{i\alpha} \right] \phi \, dV = 0$$

Let us now transform the derivatives properly into the moving frame. Let $\frac{df}{dt}$ denote the partial derivative w.r.t. time and

$\frac{df}{dx_i}$ the derivative w.r.t. spatial coordinate x_i.

i.e. in the moving frame x', we have

$$\frac{df}{dx'}(x') = \frac{\partial f}{\partial x}(x) \qquad \text{for } x = (t, x_i)$$

with $\quad x_i' = x_i'(t) = x_i - v_i^F t$

By definition, we have

$$\frac{\partial f}{\partial t} = \lim_{\Delta t \to 0} \frac{f(x, t+\Delta t) - f(x,t)}{\Delta t}$$

$$\frac{\partial f}{\partial x} = \lim_{\Delta t \to 0} \frac{f(x+\Delta x, t) - f(x,t)}{\Delta x}$$

Then we have

$$\frac{df}{dt}(x', t) = \lim_{\Delta t \to 0} \frac{f(x', t+\Delta t) - f(x', t)}{\Delta t} =$$

$$= \lim_{\Delta t \to 0} \frac{f(x - v(t+\Delta t), t+\Delta t) - f(x-vt, t)}{\Delta t}$$

$$\approx \frac{f(x-vt, t) + \left.\frac{\partial f}{\partial x}\right|_{(x-vt,t)} \cdot v\Delta t + \left.\frac{\partial f}{\partial t}\right|_{(x-vt,t)} \Delta t - f(x-vt, t)}{\Delta t}$$

$$= \frac{\partial f}{\partial t} - v\frac{\partial f}{\partial x}$$

And

$$\frac{df}{dx'}(x',t) = \lim_{\Delta x \to 0} \frac{f(x'+\Delta x, t) - f(x', t)}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{f(x-vt+\Delta x, t) - f(x-vt, t)}{\Delta x}$$

$$\approx \lim_{\Delta x \to 0} \frac{f(x-vt,t) + \left.\frac{\partial f}{\partial x}\right|_{(x-vt,t)} \Delta x \quad - f(x-vt,t)}{\Delta x}$$

$$= \left.\frac{\partial f}{\partial x}\right|_{(x-vt,t)}$$

Then we can write in the moving frame:

$$\int_V \left[\frac{\partial U_i}{\partial t} - v_\alpha^F \frac{\partial U_i}{\partial x_\alpha} + \frac{\partial}{\partial x_\alpha} F_{i\alpha} \right] \phi \, dV =$$

$$= \int_V \left[\frac{dU_i}{dt} - \frac{d}{dx_\alpha} F_{i\alpha} \right] \phi \, dV$$

$$= \int_V \left[\frac{dU_i}{dt} \phi - \frac{dF_{i\alpha}}{dx_\alpha} \phi \right] dV$$

We can rewrite both terms:

1) Provided ϕ is a Lagrangian function, i.e. $\frac{d\phi}{dt} = 0$, we have

$$\int_V \frac{dU_i}{dt}\phi \, dV = \int \left(\frac{dU_i}{dt}\phi + U_i \underbrace{\frac{d\phi}{dt}}_{=0} \right) dV = \int \frac{d}{dt}(U_i \phi)\, dV$$

$$= \frac{d}{dt}\int_V U_i \phi \, dV$$

2) $$\int_V \frac{d}{dx_\alpha}(F_{i\alpha})\,\phi\, dV = \int \left(\frac{d}{dx_\alpha}(F_{i\alpha}\phi) - F_{i\alpha}\frac{d\phi}{dx_\alpha} \right) dV$$

$$= -\int F_{i\alpha}\frac{d\phi}{dx_\alpha}\, dV + \underbrace{\oint_{\partial V} F_{i\alpha}\phi\, \hat{n}_\alpha \, d\partial V}_{=0 \text{ because compact support}}$$

$$= -\int F_{i\alpha}\frac{d\phi}{dx_\alpha}\, dV$$

giving us:

$$\boxed{\frac{d}{dt}\int_V U_i \phi\, dV - \int F_{i\alpha}\frac{d\phi}{dx_\alpha}\, dV = 0}$$

Now insert the definition of the partition of unity:

$$f(x) = \sum_i f(x_i)\, \Psi_i(x)$$

$$\int_V f(x)\, dV = \int \sum_i f(x_i)\, \Psi_i(x)\, dV$$

$$= \sum_i f_i \int \Psi_i(x)\, dV = \sum_i f_i V_i$$

Inserting these definitions we get

$$\frac{d}{dt} \int U_k \phi\, dV - \int F_{k\alpha} \frac{d\phi}{dx_\alpha}\, dV = 0$$

$$= \frac{d}{dt} \int \sum_i U_{k,i}\, \phi_i\, \Psi_i\, dV - \int \sum_i \left(F_{k\alpha,i} \left.\frac{d\phi}{dx_\alpha}\right|_{x=x_i} \right) \Psi_i(x)\, dV$$

$$= \frac{d}{dt} \left[\sum_i U_{k,i}\, \phi_i \int \Psi_i(x)\, dV \right] - \sum_i F_{k\alpha,i} \left.\frac{d\phi}{dx_\alpha}\right|_{x=x_i} \int \Psi_i(x)\, dV$$

$$= \frac{d}{dt} \sum_i U_{k,i}\, \phi_i\, V_i - \sum_i F_{k\alpha,i} \left.\frac{d\phi}{dx_\alpha}\right|_{x=x_i} V_i$$

Again using the assumption that $\frac{d\phi}{dt} = 0$:

$$\sum_i \left[\phi_i \frac{d}{dt}(U_{k,i} V_i) - V_i F_{k\alpha,i} \left.\frac{d\phi}{dx_\alpha}\right|_{x=x_i} \right] = 0$$

Now insert the expression for the gradient:

$$\left.\frac{df}{dx_\alpha}\right|_{x=x_i} = \sum_j \left(f(x_j) - f(x_i)\right) \tilde{\hat{\psi}}_j^\alpha(\underline{x}_i)$$

On the flux part, we get:

$$\sum_i V_i F_{k\alpha,i} \left.\frac{d\phi}{dx_\alpha}\right|_{x=x_i} = \sum_i V_i F_{k\alpha,i} \sum_j (\phi_j - \phi_i) \tilde{\hat{\psi}}_j^\alpha(x_i) =$$

$$= \underbrace{\sum_{i,j} V_i F_{k\alpha,i}\, \phi_j \tilde{\hat{\psi}}_j^\alpha(x_i)}_{i \Leftrightarrow j} - \sum_{i,j} V_i F_{k\alpha,i}\, \phi_i \tilde{\hat{\psi}}_j^\alpha(x_i)$$

$$= \sum_{i,j} V_j F_{k\alpha,j}\, \phi_i \tilde{\hat{\psi}}_i^\alpha(x_j) - \sum_{i,j} V_i F_{k\alpha,i}\, \phi_i \tilde{\hat{\psi}}_j^\alpha(x_i)$$

$$= -\sum_{i,j} \phi_i \left[V_i F_{k\alpha,i} \tilde{\hat{\psi}}_j^\alpha(x_i) - V_j F_{k\alpha,j} \tilde{\hat{\psi}}_i^\alpha(x_j) \right]$$

We obtain:

$$\sum_i \left[\phi_i \frac{d}{dt}(U_{k,i} V_i) + \phi_i \sum_j \left[V_i F_{k\alpha,i} \tilde{\hat{\psi}}_j^\alpha(\underline{x}_i) - V_j F_{k\alpha,j} \tilde{\hat{\psi}}_i^\alpha(x_j) \right] \right.$$

$$= \sum_i \phi_i \left[\frac{d}{dt}(U_{k,i} V_i) + \sum_j \left(V_i F_{k\alpha,i} \tilde{\hat{\psi}}_j^\alpha(x_i) - V_j F_{k\alpha,j} \tilde{\hat{\psi}}_i^\alpha(x_j) \right) \right] = 0$$

This must hold for an arbitrary Φ_i and for all i; therefore the expression between brackets must vanish:

$$\frac{d}{dt}(U_{k,i} V_i) + \sum_j \left[V_i F_{k\alpha,i} \tilde{\Psi}_j^\alpha - V_j F_{k\alpha,j} \tilde{\Psi}_i \right] = 0$$

We replace the $F_{k\alpha,i/j}$ with a solution of a (time-centered) Riemann problem between the particles i and j with states $\underline{U}_i$ and $\underline{U}_j$. We denote this flux as $\underline{\tilde{F}}_{ij}$.

Finally, we define

$$A_{ij}^\alpha \equiv V_i \tilde{\Psi}_j^\alpha(\underline{x}_i) - V_j \tilde{\Psi}_i^\alpha(\underline{x}_j)$$

and obtain

$$\boxed{\frac{d}{dt}(V_i U_{i,k}) + \sum_j F_{k\alpha,ij} A_{ij}^\alpha = 0}$$

2.3 Conservation Properties

When solving finite-volume equations, certain properties ought to be satisfied exactly by the underlying numerical scheme as a necessary condition for obtaining the correct solution.

We can look at three conservation properties:

1) Local conservation

A quantity q that leaves a particle (mesh cell) i in a particular direction (or through a given surface) will be received by the relevant neighbour particle (mesh-cell) j.

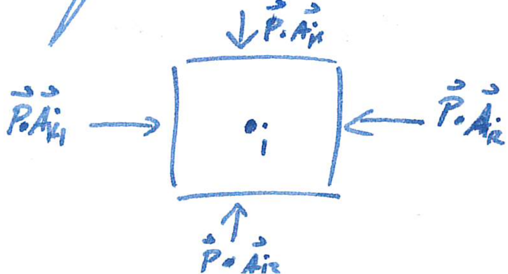
In practice, this means $A_{ij} = -A_{ji}$

2) Closure condition

The vector sum of cell boundary areas (or that of the effective areas between all neighbours in the case of a mesh-less scheme) is identically zero, i.e.

$$\sum_j A_{ij} = 0$$

The closure condition guarantees that the time derivatives of the relevant local quantities are always consistent with the corresponding fluxes between the cells. For example, if the pressure is constant for each particle or mesh cell, the net force (∇ Pressure) on each particle or mesh cell is zero for any mesh or particle distribution.



$$\vec{F}_{tot} = \sum_j P_j A_{ij}$$

$$= P \sum_j A_{ij} = 0$$

as it should be for $P = \text{const}$

if $\sum_j A_{ij} = 0$

Bert/Ivanova formulation

We have

$$A_{ij} = \int_V \left[\psi_j \nabla \psi_i - \psi_i \nabla \psi_j \right] dV$$

1) Local conservation

It is trivial to verify that $A_{ij} = -A_{ji}$ here.

2) Closure condition

$$\sum_j A_{ij} = \sum_j \int \left[\psi_j \nabla \psi_i - \psi_i \nabla \psi_j \right] dV$$

using $\nabla(\psi_j \psi_i) = \nabla \psi_j \, \psi_i + \psi_j \nabla \psi_i$

$$= \sum_j \int \left[\nabla(\psi_j \psi_i) - \psi_i \nabla \psi_j - \psi_i \nabla \psi_j \right] dV$$

$$= \sum_j \int \left[\nabla(\psi_j \psi_i) - 2 \psi_i \nabla \psi_j \right] dV$$

For the first part of the integral, we have

$$\int_V \nabla(\psi_i \psi_j)\, dV = \int_{\partial V} \psi_i \psi_j \hat{n}\, d\partial V = 0$$

because we demand that $\forall i \ \psi_i(x \in \partial V) = 0$ with ∂V being the boundary of our domain.

For the second part, we have:

$$\sum_j \int_V \psi_i \nabla \psi_j(x)\, dV = \underbrace{\int_V \psi_i \nabla(\underbrace{\sum_j \psi_j(x)}_{=1})\, dV}_{=0} = 0$$

Which indeed, put together, gives us

$$\sum_j A_{ij} = \sum_j \int_V [\nabla(\psi_i \psi_j) - 2\psi_i \nabla \psi_j]\, dV = 0$$

satisfying the closure condition.

Hopkins formulation

We have

$$A_{ij} = V_i \hat{\psi}_j(\underline{x}_i) - V_j \hat{\psi}_i(\underline{x}_j)$$

1) Local Conservation

Again it is trivial to show that $A_{ij} = -A_{ij}$ in this case as well.

2) Closure condition

The proof that Hopkins' version of the meshless hydrodynamics satisfies the closure condition is not present in literature, not trivial to do (I'm not even sure it can be done, at least I can't.)

2.5 Case Study: Uniform Box

Consider the special case of a (periodic) uniform box, where all particles have the same smoothing length as they are uniformly distributed.

With the same amount of neighbours and smoothing lengths everywhere, all the partitions of unity will give the same value at a different particle's position compared to that particle's value of ψ at the position of the first particle, i.e.

$$\psi_j(\underline{x}_i) = \psi_i(\underline{x}_j)$$

$$\frac{W(|\underline{x}_i - \underline{x}_j|, h)}{\sum_k W(|\underline{x}_i - \underline{x}_k|, h)} = \frac{W(|\underline{x}_j - \underline{x}_i|, h)}{\sum_k W(|\underline{x}_j - \underline{x}_k|, h)}$$

Since the distribution is the same everywhere and the particles have the same smoothing lengths, the normalizations will be equal.

We have our expressions for the effective surfaces:

$$A_{ij}^{\alpha} = V_i \tilde{\psi}_j^{\alpha}(\underline{x}_i) - V_j \tilde{\psi}_i^{\alpha}(\underline{x}_j) \quad \text{[Hopkins]}$$

and

$$A_{ij}^{\alpha} = V_j (\nabla \psi_i(\underline{x}_j))^{\alpha} - V_i (\nabla \psi_j(\underline{x}_j))^{\alpha}$$

So how come the effective surfaces in this scenario aren't zero?

Hopkins' Version

Starting from scratch, we have

$$\psi_j(\underline{x}_i) = \psi_i(\underline{x}_j)$$

$$\underline{\underline{E}}_i^{\alpha\beta} \equiv \sum_j (\underline{x}_j - \underline{x}_i)^\alpha (\underline{x}_j - \underline{x}_i)^\beta \psi_j(\underline{x}_i)$$

for the uniform periodic box,

$$\sum_j (\underline{x}_j - \underline{x}_i)^\alpha (\underline{x}_j - \underline{x}_i)^\beta$$

will be the same for all particles i.

With $\psi_j(\underline{x}_i) = \psi_i(\underline{x}_j)$:

$$\Rightarrow \underline{\underline{E}}_i^{\alpha\beta} = \underline{\underline{E}}_j^{\alpha\beta}$$

$$\Rightarrow \underline{\underline{B}}_i \equiv \underline{\underline{E}}_i^{-1} = \underline{\underline{E}}_j^{-1} \equiv \underline{\underline{B}}_j$$

Since the normalizations will also be equal, we have that

$$V_i = \frac{1}{\omega(\underline{x}_i)} = \frac{1}{\sum_k W(|\underline{x}_i - \underline{x}_k|, h)} = V_j$$

Now inserting

$$\tilde{\psi}_j^\alpha(\underline{x}_i) = \underline{\underline{B}}_i^{\alpha\beta}(\underline{x}_j - \underline{x}_i)^\beta \psi_j(\underline{x}_i)$$

into the expression for the effective surface:

$$A_{ij}^\alpha = V_i \tilde{\psi}_j^\alpha(\underline{x}_i) - V_j \tilde{\psi}_i^\alpha(\underline{x}_j)$$

$$= V_i \underline{\underline{B}}_i^{\alpha\beta}(\underline{x}_j - \underline{x}_i)^\beta \psi_j(\underline{x}_i) -$$

$$- V_j \underline{\underline{B}}_j^{\alpha\beta}(\underline{x}_i - \underline{x}_j)^\beta \psi_i(\underline{x}_j)$$

Using $V_i = V_j$, $\underline{\underline{B}}_i = \underline{\underline{B}}_j$, $\psi_j(\underline{x}_i) = \psi_i(\underline{x}_j)$:

$$A_{ij}^\alpha = V_i \underline{\underline{B}}_i^{\alpha\beta} \psi_j(\underline{x}_i)\left[(\underline{x}_j - \underline{x}_i) - (\underline{x}_i - \underline{x}_j)\right]^\beta$$

$$= \underline{2 V_i \underline{\underline{B}}_i^{\alpha\beta}(\underline{x}_j - \underline{x}_i)^\beta \psi_j(\underline{x}_i)}$$

$\Rightarrow$ It is the $(\underline{x}_j - \underline{x}_i)$ term's anti-symmetry that makes $A_{ij} \neq 0$

Ivanova Version

We again start off with

$$\Psi_j(\underline{x}_i) = \Psi_i(\underline{x}_j)$$

and use the analytical expression for

$\nabla \Psi_j(\underline{x})$:

$$\nabla \Psi_j(\underline{x}) = \frac{\partial}{\partial x} \Psi_j(\underline{x}_i) = \frac{\partial}{\partial x} \frac{W(|\underline{x}_i - \underline{x}_j|, h)}{\sum_k W(|\underline{x} - \underline{x}_k|, h)}$$

let $r_j \equiv |\underline{x} - \underline{x}_j|$, $\sum_k W(|\underline{x} - \underline{x}_k|, h) \equiv \omega(\underline{x})$

$$= \frac{\partial}{\partial x} \frac{W(r_j, h)}{\omega(\underline{x})}$$

$$= \frac{\frac{\partial W(r_j)}{\partial x} \omega(\underline{x}) - W(r) \frac{\partial \omega(\underline{x})}{\partial x}}{\omega(\underline{x})^2}$$

$$= \frac{1}{\omega(\underline{x})} \frac{\partial W(r_j)}{\partial x} - \frac{W(r_j) \frac{\partial}{\partial x} \sum_k W(r_k, h)}{\omega(\underline{x})^2}$$

$$= \frac{1}{\omega(\underline{x})} \frac{\partial W(r_j)}{\partial r_j} \frac{\partial r_j}{\partial x} - \frac{W(r_j)}{\omega(\underline{x})^2} \sum_k \frac{\partial W(r_k)}{\partial r_k} \frac{\partial r_k}{\partial x}$$

With $r_j = |\underline{x} - \underline{x}_j| = \sqrt{(\underline{x} - \underline{x}_j)^2}$

$$\rightarrow \frac{\partial r_j}{\partial x} = \frac{\partial}{\partial x} \sqrt{(x - x_j)^2}$$

$$= \frac{1}{2} \frac{1}{\sqrt{(x - x_j)^2}} \cdot 2 (x - x_j) \cdot 1$$

$$= \frac{x - x_j}{|x - x_j|} = \frac{x - x_j}{r}$$

This gives us

$$\nabla \psi_j(\underline{x}) = \frac{1}{\omega(\underline{x})} \frac{\partial W}{\partial r}(r_j) \frac{x - x_j}{r_j} -$$

$$- \frac{W(r_j)}{\omega(\underline{x})^2} \sum_k \frac{\partial W}{\partial x}(r_k) \frac{x - x_k}{r_k}$$

For identical smoothing lengths and neighbour positions of particles i and j, we have again

$$W(|\underline{x}_i - \underline{x}_j|, h) = W(|\underline{x}_j - \underline{x}_i|, h)$$

$$\psi_j(\underline{x}_i) = \psi_i(\underline{x}_j)$$

$$V_i = \frac{1}{\omega(\underline{x}_i)} = \frac{1}{\omega(\underline{x}_j)} = V_j$$

Then

$$A_{ij} = V_j \nabla \Psi_i (\underline{x}_j) - V_i \nabla \Psi_j (\underline{x}_i)$$

$$= V_i \left(\nabla \Psi_i (\underline{x}_j) - \nabla \Psi_j (\underline{x}_i) \right)$$

$$= V_i \Bigg[\Bigg(\frac{1}{\omega(\underline{x}_j)} \frac{\partial W(|x_j - x_i|)}{\partial r} \frac{x_j - x_i}{r} -$$

$$- \frac{W(|x_j - x_i|)}{\omega(\underline{x}_j)^2} \sum_k \frac{\partial W(|x_j - x_k|)}{\partial x} \frac{x_j - x_k}{r_k} \Bigg) -$$

$$- \Bigg(\frac{1}{\omega(\underline{x}_i)} \frac{\partial W(|x_i - x_j|)}{\partial r} \frac{x_i - x_j}{r} -$$

$$- \frac{W(|x_i - x_j|)}{\omega(\underline{x}_i)^2} \sum_k \frac{\partial W(|x_i - x_k|)}{\partial x} \frac{x_i - x_k}{r_k} \Bigg) \Bigg]$$

The sums $\sum_k$ over all neighbours will be the same and therefore drop out

$$= V_i \Bigg[\frac{1}{\omega(\underline{x}_j)} \frac{\partial W(|\underline{x}_j - \underline{x}_i|)}{\partial r} \frac{x_j - x_i}{r} -$$

$$- \frac{1}{\omega(\underline{x}_i)} \frac{\partial W(|x_i - x_j|)}{\partial r} \frac{x_i - x_j}{r} \Bigg]$$

$$= \frac{V_i}{\omega(\underline{x}_i)} \frac{\partial W(|x_i - x_j|)}{\partial r} \cdot 2 \frac{x_j - x_i}{r}$$

$$= 2V_i^2 \frac{\partial W}{\partial r} \frac{x_j - x_i}{r}$$

$\Rightarrow$ Again the surfaces are non-zero because of the gradient: The partial derivative w.r.t. Cartesian coordinates introduces the directionality $\underline{x}_j - \underline{x}_i$, which is trivially antisymmetric.