GIZMO Implementation Details

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1 Equations

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

$$\omega(\mathbf{x}) = \sum_j W(\mathbf{x} - \mathbf{x}_j, h(\mathbf{x})) \tag{2}$$

where $h(\mathbf{x})$ is some "kernel size" and $\omega(\mathbf{x})$ is used to normalise the volume partition at any point $\mathbf{x}$.

It can be shown that (assuming the kernel $W(\mathbf{x})$ is normalized such that $\int_V W(\mathbf{x}) \mathrm{d}V = 1$):

$$V_i = \int_V \psi_i(\mathbf{x}) \mathrm{d}V = \frac{1}{\omega(\mathbf{x}_i)} \tag{3}$$

$$V = \sum_i V_i \tag{4}$$

$$\int_V f(\mathbf{x}) \mathrm{d}V = \sum_i f(\mathbf{x}_i) V_i + \mathcal{O}(\Delta x^2) \tag{5}$$

Following Hopkins 2015, we arrive at the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}(V_i \mathbf{U}_{k,i}) + \sum_j \mathbf{F}_{k,ij} \cdot \mathbf{A}_{ij} = 0 \tag{6}$$

with

$$\mathbf{A}_{ij}^{\alpha} = V_i \tilde{\boldsymbol{\psi}}_j^{\alpha}(\mathbf{x}_i) - V_j \tilde{\boldsymbol{\psi}}_i^{\alpha}(\mathbf{x}_j) \tag{7}$$

for every component k of the Euler equations and every gradient component α

The $\tilde{\boldsymbol{\psi}}(\mathbf{x})$ come from the $\mathcal{O}(h^2)$ accurate discrete gradient expression from Lanson and Vila 2008:

$$\frac{\partial}{\partial x_\alpha} f(\mathbf{x}) \Big|_{\mathbf{x}_i} = \sum_j \left(f(\mathbf{x}_j) - f(\mathbf{x}_i) \right) \tilde{\boldsymbol{\psi}}_j^{\alpha}(\mathbf{x}_i) \tag{8}$$

$$\tilde{\boldsymbol{\psi}}_j^{\alpha}(\mathbf{x}_i) = \sum_{\beta=1}^{\beta=\nu} \mathbf{B}_i^{\alpha\beta} (\mathbf{x}_j - \mathbf{x}_i)^{\beta} \psi_j(\mathbf{x}_i) \tag{9}$$

$$\mathbf{B}_i = \mathbf{E_i}^{-1} \tag{10}$$

$$\mathbf{E}_i^{\alpha\beta} = \sum_j (\mathbf{x}_j - \mathbf{x}_i)^{\alpha} (\mathbf{x}_j - \mathbf{x}_i)^{\beta} \psi_j(\mathbf{x}_i) \tag{11}$$

where α and β again represent the coordinate components for ν dimensions.

2 Computations

2.1 Normalization

To compute the normalisations 2, we need to sum over all neighbouring particles and sum the kernels correctly. To evaluate the kernels, we use the `kernel_deval(xij, wij, wij_dx)` function in SWIFT.

If a kernel is defined as

$$W_i(\mathbf{x}) = W(\mathbf{x} - \mathbf{x}_i, h(\mathbf{x})) = \frac{1}{h(\mathbf{x})^{\nu}} w \left(\frac{|\mathbf{x} - \mathbf{x}_i|}{h(\mathbf{x})} \right)$$

then `kernel_deval` computes

$$\begin{aligned} \texttt{wij} &= w(\texttt{xij}) \\ \text{and} \quad \texttt{wij\_dx} &= \frac{\partial w(r)}{\partial r}\Big|_{r=\texttt{xij}} \\ \text{with} \quad \texttt{xij} &= \frac{|\mathbf{x}_i - \mathbf{x}_j|}{h(\mathbf{x}_i)} \end{aligned}$$

So for a specific particle i, we need to compute

$$\begin{aligned} \omega(\mathbf{x}_i) &= \sum_j W(\mathbf{x}_i - \mathbf{x}_j, h(\mathbf{x}_i)) \\ &= \sum_j \frac{1}{h(\mathbf{x}_i)^\nu} w\left(\frac{|\mathbf{x}_i - \mathbf{x}_j|}{h(\mathbf{x}_i)}\right) \\ &= \sum_j \frac{1}{h_i^\nu}\ \texttt{wij} \end{aligned}$$

with $h_i = h(\mathbf{x}_i)$.

2.2 Analytical gradients of $\psi(\mathbf{x})$

For the Ivanova et al. 2013 expression of the effective surfaces $\mathbf{A}_{ij}$, we need analytical gradients in Cartesian coordinates of $\psi_i(\mathbf{x}_j)$.

From eq. 1 we have that

$$\psi_j(\mathbf{x}_i) = \frac{W(\mathbf{x}_i - \mathbf{x}_j, h(\mathbf{x}_i))}{\omega(\mathbf{x}_i)}$$

Let $r_{ij} \equiv |\mathbf{x}_i - \mathbf{x}_j|$ and $q_{ij} \equiv \frac{r_{ij}}{h_i}$. Then

$$\frac{\partial}{\partial x}\psi_j(\mathbf{x}_i) = \frac{\partial}{\partial x}\frac{W(\mathbf{x}_i - \mathbf{x}_j, h(\mathbf{x}_i))}{\omega(\mathbf{x}_i)} = \frac{\partial}{\partial x}\frac{W(r_{ij}, h_i)}{\omega(\mathbf{x}_i)}$$

$$
\begin{aligned}
&= \frac{\frac{\partial W}{\partial x}(r_{ij}, h_i)\ \omega(\mathbf{x}_i) - W(r_{ij}, h_i)\frac{\partial \omega}{\partial x}(\mathbf{x}_i)}{\omega(\mathbf{x}_i)^2} \\
&= \frac{1}{\omega(\mathbf{x}_i)}\frac{\partial W}{\partial x}(r_{ij}, h_i) - \frac{1}{\omega(\mathbf{x}_i)^2} W(r_{ij}, h_i) \frac{\partial}{\partial x}\sum_k W(r_{ik}, h_i) \\
&= \frac{1}{\omega(\mathbf{x}_i)}\frac{\partial W}{\partial x}(r_{ij}, h_i) - \frac{1}{\omega(\mathbf{x}_i)^2} W(r_{ij}, h_i) \sum_k \frac{\partial W}{\partial x}(r_{ik}, h_i) \qquad (12)
\end{aligned}
$$

If a kernel[1] is defined as

$$W_j(\mathbf{x}_i) = W(\mathbf{x}_i - \mathbf{x}_j, h_i)) = \frac{1}{h_i^\nu} w\left(\frac{|\mathbf{x}_i - \mathbf{x}_j|}{h_i}\right) = \frac{1}{h_i^\nu} w(q_{ij})$$

and we assume that the smoothing length h_i is treated as constant at this point, then the gradient of the kernel is given by

$$
\begin{aligned}
\frac{\partial}{\partial x} W_j(\mathbf{x}_i) &= \frac{\partial}{\partial x}\left(\frac{1}{h_i^\nu} w(q_{ij})\right) \\
&= \frac{1}{h_i^\nu}\frac{\partial w(q_{ij})}{\partial q_{ij}} \frac{\partial q_{ij}(r_{ij})}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial x} \qquad (13)
\end{aligned}
$$

We now use

$$
\begin{aligned}
\frac{\partial q_{ij}(r_{ij})}{\partial r_{ij}} &= \frac{\partial}{\partial r_{ij}} \frac{r_{ij}}{h_i} = \frac{1}{h_i} \qquad (14) \\
\frac{\partial r_{ij}}{\partial x} &= \frac{\partial}{\partial x}\sqrt{(\mathbf{x}_i - \mathbf{x}_j)^2} = \frac{1}{2}\frac{1}{\sqrt{(\mathbf{x}_i - \mathbf{x}_j)^2}} \cdot 2(\mathbf{x}_i - \mathbf{x}_j) \\
&= \frac{\mathbf{x}_i - \mathbf{x}_j}{r_{ij}} \qquad (15)
\end{aligned}
$$

To be perfectly clear, we should in fact write

$$r_j(\mathbf{x}) \equiv |\mathbf{x} - \mathbf{x}_j|$$

[1] Helpful way to think of the indices: $W_j(\mathbf{x}_i) = W(|\mathbf{x}_j - \mathbf{x}_i|, h_i)$ is the kernel value of particle i at position $\mathbf{x}_i$ evaluated at the position $\mathbf{x}_j$. Personally I would've used the indices the other way around for simplified thinking, but I'm going to stick to this notation because Hopkins also uses it.

which again leads to

$$
\begin{aligned}
\frac{\partial r_{ij}}{\partial x} &= \frac{\partial r_j(\mathbf{x}_i)}{\partial x} = \frac{\partial r_j(\mathbf{x})}{\partial x}\bigg|_{\mathbf{x}=\mathbf{x}_i} \\
&= \frac{\partial}{\partial x}\sqrt{(\mathbf{x}-\mathbf{x}_j)^2}\Big|_{\mathbf{x}=\mathbf{x}_i} = \frac{1}{2}\frac{1}{\sqrt{(\mathbf{x}-\mathbf{x}_j)^2}} \cdot 2(\mathbf{x}-\mathbf{x}_j)\Big|_{\mathbf{x}=\mathbf{x}_i} \\
&= \frac{\mathbf{x}-\mathbf{x}_j}{r_j(\mathbf{x})}\bigg|_{\mathbf{x}=\mathbf{x}_i} = \frac{\mathbf{x}_i-\mathbf{x}_j}{r_{ij}}
\end{aligned}
$$

Inserting expressions 14 and 15 in 13, we obtain

$$
\frac{\partial}{\partial x}W_j(\mathbf{x}_i) = \frac{1}{h_i^{\nu+1}}\frac{\partial w(q_{ij})}{\partial q_{ij}}\frac{\mathbf{x}_i-\mathbf{x}_j}{r_{ij}} \tag{16}
$$

$\frac{\partial w(q_{ij})}{\partial q_{ij}}$ is given by `wij_dx` of `kernel_deval`.

Finally, inserting 16 in 12 we get

$$
\frac{\partial}{\partial x}\psi_j(\mathbf{x}_i) = \frac{1}{\omega(\mathbf{x}_i)}\frac{1}{h_i^{\nu+1}}\texttt{wij\_dx}\frac{\mathbf{x}_i-\mathbf{x}_j}{r_{ij}} - \frac{1}{\omega(\mathbf{x}_i)^2}W(r_{ij},h_i)\sum_k\frac{1}{h_i^{\nu+1}}\texttt{wik\_dx}\frac{\mathbf{x}_i-\mathbf{x}_k}{r_{ik}} \tag{17}
$$

The definition of r_{ij} requires a bit more discussion. Since kernels used in hydrodynamics (at least in those methods currently implemented in SWIFT) are usually taken to be spherically symmetric, we might as well have defined

$$
r'_{ij} = |\mathbf{x}_j - \mathbf{x}_i|
$$

which would leave the evaluation of the kernels invariant $[r'_{ij} = r_{ij}]$, but the gradients would have the opposite direction:

$$
\frac{\partial r'_{ij}}{\partial x} = \frac{\mathbf{x}_j-\mathbf{x}_i}{r'_{ij}} = -\frac{\mathbf{x}_i-\mathbf{x}_j}{r_{ij}} = -\frac{\partial r_{ij}}{\partial x}
$$

So which definition should we take?

Consider a one-dimensional case where we choose two particles i and j such that $x_j > x_i$ and $q_{ij} = |x_j - x_i|/h_i < H$, where H is the compact support radius of the kernel of choice. Because we're considering a one-dimensional case with $x_j > x_i$, we can now perform a simple translation such that particle i is at the origin, i.e. $x'_i = 0$ and $x'_j = x_j - x_i = |x_j - x_i| = r_{ij}$. In this scenario, the gradient in Cartesian coordinates and in spherical coordinates must be the same:

$$\begin{aligned} \frac{\partial}{\partial x'} W(|x'_i - x'|, h_i)\Big|_{x'=x'_j} &= \frac{\partial}{\partial r_{ij}} W(r_{ij}, h_i) \\ \Rightarrow \quad \frac{1}{h_i^\nu} \frac{\partial w(q'_{ij})}{\partial q'_{ij}} \frac{\partial q'_{ij}(r'_{ij})}{\partial r'_{ij}} \frac{\partial r'_i(x')}{\partial x'}\Big|_{x'=x'_j} &= \frac{1}{h_i^\nu} \frac{\partial w(q_{ij})}{\partial q_{ij}} \frac{\partial q_{ij}(r_{ij})}{\partial r_{ij}} \end{aligned} \tag{18}$$

We have the trivial case where

$$\begin{aligned} r'_{ij} &= |x'_i - x'_j| = |x_i - x_j| = r_{ij} \\ q'_{ij} &= r'_{ij}/h_i = q_{ij} \\ \Rightarrow \quad \frac{\partial w(q'_{ij})}{\partial q'_{ij}} &= \frac{\partial w(q_{ij})}{\partial q_{ij}}, \quad \frac{\partial q'_{ij}(r'_{ij})}{\partial r'_{ij}} = \frac{\partial q_{ij}(r_{ij})}{\partial r_{ij}} \end{aligned}$$

giving us the condition from 18:

$$\frac{\partial r'_i(x')}{\partial x'}\Big|_{x'=x'_j} = 1 = \frac{\partial r_i(x)}{\partial x} \tag{19}$$

this is satisfied for

$$\begin{aligned} & r_j(\mathbf{x}) = |\mathbf{x} - \mathbf{x}_j| \\ & \Rightarrow r_{ij} = |\mathbf{x}_i - \mathbf{x}_j|, \quad \text{not} \quad r_{ij} = |\mathbf{x}_j - \mathbf{x}_i| \end{aligned}$$

References

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