Schemes Based on Flux-conservative Form

By their very nature, the fluid equations (1)–(3) can be written in flux-conservative form. In 1-D, with no external forces,

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} \mathbf{F}(\mathbf{u}) = 0,$$

where

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho v \\ e \end{pmatrix} \quad \mathbf{F}(\mathbf{u}) = \begin{pmatrix} \rho v \\ \rho v^2 + p \\ (e + p)v \end{pmatrix}$$

(E.F.T.S.). Recall \( e \equiv \rho(\varepsilon + \frac{1}{2}v^2) = \) energy density.
When written in this form, it is clear that the techniques described before can be applied immediately (given an equation of state for $p$).

E.g., two-step Lax-Wendroff:

$$u_{j}^{n+1} = u_{j}^{n} - \frac{\Delta t}{\Delta x} \left( F^{n+1/2}_{j+1/2} - F^{n+1/2}_{j-1/2} \right),$$

where

$$F^{n+1/2}_{j\pm 1/2} = F(u^{n+1/2}_{j\pm 1/2}),$$

etc.

Note that all components of $u$ must be at same location on mesh $\Rightarrow$ staggered mesh not needed (compare with operator split method, below).

Scheme is stable provided $(|v| + c)\Delta t/\Delta x < 1$, where $c^2 = \gamma p/\rho$ ($c =$ sound speed).
Operator Split Schemes

- Simplest schemes, developed long ago by von Neumann, Richtmeyer, etc.

- The fluid equations (1)–(3) can be written as “sum” of two steps. In 1-D:

  \[ \begin{align*}
  & \text{A} \\
  & \frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial x} = 0 \\
  & \frac{\partial (\rho v)}{\partial t} + v \frac{\partial (\rho v)}{\partial x} = 0 \\
  & \frac{\partial e}{\partial t} + v \frac{\partial e}{\partial x} = 0 \\
  & \text{B} \\
  & \frac{\partial \rho}{\partial t} = 0 \\
  & \rho \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x} \\
  & \frac{\partial e}{\partial t} = -p \frac{\partial v}{\partial x}
  \end{align*} \]
Equations in A are all the form of scalar advection equations. Adopt high-order upwind schemes to solve $A \rightarrow \text{advection step}$ (transport).

Equations in B are all source terms in the equations that can be differenced directly $\rightarrow \text{source step}$.

Best to adopt staggered mesh with $v$ at cell edges, $p$, $ρ$, $e$ at cell centers.

(In multi-D, $v$ defined at cell faces—naturally describes flux of fluid into/out of cell.)
Leads to 2\textsuperscript{nd}-order accurate FDEs for the source terms. I.e.,

\[ v_{i-1/2}^{n+1} = v_{i-1/2}^n - \frac{\Delta t (p_i - p_{i-1})}{\frac{1}{2} (\rho_i + \rho_{i-1}) \Delta x}, \]

\[ e_i^{n+1} = e_i^n - \frac{\Delta t (v_{i+1/2} - v_{i-1/2}) p_i}{\Delta x}. \]

Operator split schemes are simple, easy to code, and easy to extend with more complex physics, e.g., MHD, radiation, etc.

But, they don’t treat regions with sharp \( p \) gradients as well as more modern schemes (e.g., Godunov).
Smoothed Particle Hydrodynamics

So far we have only considered methods that require dividing space into a grid. Can we represent the local fluid density without a grid?

- Advantage: not confined to a specific geometry, more adaptable.

- Represent fluid by large number ($\sim 10^{4-6}$) of “particles.”
- Each particle has a mass, Lagrangian position and velocity, internal energy, and possibly an initial density.
- Other quantities derived by smoothing over an “interpolating kernel” $W$ (units: 1/volume). In this way the statistical properties of the real fluid elements are treated in an average sense.
- Solve fluid equations in comoving frame with these smoothed quantities using any familiar method (leapfrog, RK, etc.)
The interpolating kernel

If \( f \) is some quantity (e.g., density), then its kernel estimate (per unit volume) \( \langle f \rangle \) is given by

\[
\langle f (\mathbf{r}) \rangle = \int f(\mathbf{r}') W(\mathbf{r} - \mathbf{r}'; h) \, d\mathbf{r}',
\]

where the integral is over all space,

\[
\int W(\mathbf{r} - \mathbf{r}'; h) \, d\mathbf{r}' = 1,
\]

and

\[
\lim_{h \to 0} W(\mathbf{r} - \mathbf{r}'; h) = \delta(\mathbf{r} - \mathbf{r}').
\]

(\( h \) is called the “smoothing length” and is typically chosen so that \( N \simeq 15 \) particles lie within \( h \) of any particle. The error for using this approximation goes as \( \sim O(h^2) \).)
For numerical work, split the fluid into small volume elements $\Delta \tau$ of mass $\rho \Delta \tau$, where $\rho$ is a representative density for the small fluid element. The integral can then be approximated by

$$\langle f(\mathbf{r}) \rangle = \sum_j m_j \frac{f(\mathbf{r}_j)}{\rho(\mathbf{r}_j)} W(\mathbf{r} - \mathbf{r}_j; h).$$

(Note $m_j / \rho_j$ takes the place of $\int d\mathbf{r}'$.)

The interpolating kernel can be any analytically differentiable function that satisfies the normalization and limiting properties above. E.g.,

3-D Gaussian kernel:

$$W(\mathbf{r}; h) = \frac{1}{(\pi h^2)^{3/2}} e^{-r^2/h^2}.$$
3-D spline kernel:

\[ W(r; h) = \frac{1}{\pi h^3} \begin{cases} 
1 - \frac{3}{2} s^2 + \frac{3}{4} s^3 , & 0 \leq s < 1 \\
\frac{1}{4} (2 - s)^3 , & 1 \leq s < 2 \\
0 , & s \geq 2 
\end{cases} \]

where \( s \equiv r/h \).

In practice, choose \( W \) so that it falls off rapidly for \( |r - r_j| \geq h \), hence only need to sum over nearest neighbours.
Note the kernel estimate of the gradient of \( f(r) \) is just

\[
\langle \nabla f(r) \rangle = \sum_j m_j \frac{f(r_j)}{\rho(r_j)} \nabla W(r - r_j; h)
\]

(since the \( \nabla \) operator is taken with respect to the space coordinates \( r \) and \( W \) is the only quantity that depends on \( r \)). However, it is often better to use the identity \( \rho \nabla f = \nabla (\rho f) - f \nabla \rho \) to give

\[
\langle \rho_i \nabla f_i \rangle = \sum_j m_j (f_j - f_i) \nabla_i W_{ij},
\]

where \( \nabla_i W_{ij} \) is the gradient of \( W(r_i - r_j; h) \) w.r.t. the coordinates of particle \( i \).

\(^a\)Because \( \langle \nabla_i (\rho_i f_i) \rangle = \sum_j m_j f_j \nabla_i W_{ij} \) and \( f_i \langle \nabla_i \rho_i \rangle = \sum_j m_j f_i \nabla_i W_{ij} \).
The equations of fluid dynamics, SPH version

Recall the continuity equation

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}$$

where the derivative is taken in the fluid frame.

The SPH equivalent would be

$$\frac{D\rho_i}{Dt} = \sum_j m_j \mathbf{v}_{ij} \cdot \nabla W_{ij},$$

where $\mathbf{v}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$ (we used that vector identity again, replacing the gradient with the divergence).
But we could estimate the density everywhere directly by

$$\langle \rho(r) \rangle = \sum_j m_j W(r - r_j; h).$$

This means we don’t really need to solve the continuity equation (except in practice it turns out it is better to solve the equation for technical reasons; see Monaghan 1992).

The momentum equation without external forces

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p$$

becomes

$$\frac{Dv_i}{Dt} = -\sum_j m_j \left( \frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla_i W_{ij},$$
where the pressure gradient has been symmetrized by

\[
\frac{\nabla p}{\rho} = \nabla \left( \frac{p}{\rho} \right) + \frac{p}{\rho^2} \nabla \rho
\]

in order to ensure conservation of linear and angular momentum (the momentum equation becomes a central force law between particles \(i\) and \(j\), assuming \(W\) is Gaussian).
Finally, the energy equation

\[
\frac{D\varepsilon}{Dt} = -\frac{p}{\rho} (\nabla \cdot \mathbf{v})
\]

becomes

\[
\frac{D\varepsilon}{dt} = \frac{1}{2} \sum_{j} m_j \left( \frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \mathbf{v}_{ij} \cdot \nabla_i W_{ij},
\]

where the factor of \(1/2\) comes from symmetrization (it is a characteristic of SPH that gradient terms can be written in many different ways, just as there are a variety of FDE representations).
Particles are moved using

\[
\frac{D\mathbf{r}_i}{Dt} = \mathbf{v}_i,
\]

or, to ensure particles move with a velocity similar to the average velocity in their neighbourhood,

\[
\frac{D\mathbf{r}_i}{Dt} = \mathbf{v}_i + \epsilon \sum_j m_j \left( \frac{\mathbf{v}_{ji}}{\bar{\rho}_{ij}} \right) W_{ij},
\]

where \( \bar{\rho}_{ij} \equiv (\rho_i + \rho_j)/2 \) and \( 0 \leq \epsilon \leq 1 \) is a constant (the “X” factor).

As usual, also need an equation of state.

Can add other forces, i.e., viscosity, magnetic fields, etc.

Can implement adaptive smoothing lengths.
Summary

- SPH is based on microscopic picture of real fluid. But real fluid has many more particles than can be followed on a computer, so “smoothing” is used.

- Advantage of scheme is that it is adaptive—particles go where density is high. Good for following dynamics where gravity dominates because of its $N$-body-like foundation.

- Disadvantage of scheme is that it does not resolve low-density regions well, it does not handle regions with strong $p$ gradients well (shocks), and it is expensive (need a way to find nearest neighbours $\Rightarrow$ tree code!).

- Finite differencing methods are attractive because mathematical properties of FDEs well studied, and can prove/analyze stability, convergence rate, etc. of various schemes.