On a spatially-discrete formalism for mesh-less finite-volume methods

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1 Introduction

Numerical finite-volume methods are usually divided into Eulerian and Lagrangian schemes. In the former one, the discretization points are fixed in space, whereas in the latter the geometry they are moving with the fluid velocity, in which case it is convenient to think of them as physically associated with a fluid element. Usually, Eulerian scheme use a geometrical mesh, either structured (e.g. Cartesian) or unstructured, whereas Lagrangian methods are mostly considered to be related to particle methods. These two seemingly different approaches actually have a lot in common. It has recently been demonstrated that fully Lagrangian methods can be implemented on unstructured Voronoi meshes (Trease, 1988; Heß & Springel, 2010), while Eulerian scheme can be successfully formulated in entirely mesh-less form (Vila, 1999; Hietel et al., 2000; Junk, 2002; Lanson & Vila, 2008; Gaburov & Nitadori, 2011).

Here we present a generic formalism that leads to spatially discrete mesh-less finite-volume equations. The form of the these equations is the same as in the case of spatial discretization on a mesh. The geometrical quantities that are obtained from the mesh, such as volumes or areas, are translated into spatial integrals in the mesh-less schemes. Finally, we show that this generic formalism leads, via a few approximations, to standard SPH equations of motions. This explains why SPH, among other Lagrangian particle methods (Dilts, 1999, 2000; Abel, 2011), remains the most robust particle method in astrophysical computational fluid dynamics.

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1.1 Spatially discretized finite-volume equations

1.1.1 Mesh-based discretized equations

The conservative formulation of Euler equation of ideal hydrodynamics can be compactly written in the following integral form

$$\frac{d}{dt}\int_T q\,dV + \oint_{\partial T} \mathbf{F}\cdot d\mathbf{\Sigma} = \int_T S\,dV, \tag{1}$$

where T is volume of a fluid element, ∂T is its boundary with outward pointing normal, and q and $\mathbf{F}$ are defined as follows

$$q = \begin{pmatrix} \rho \\ \rho\mathbf{v} \\ e_{\rm tot} \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} \rho(\mathbf{v}-\mathbf{w}) \\ \rho\mathbf{v}\otimes(\mathbf{v}-\mathbf{w}) + P\hat{\mathbf{I}} \\ e_{\rm tot}(\mathbf{v}-\mathbf{w}) + P\mathbf{v} \end{pmatrix}. \tag{2}$$

Here, $\mathbf{w}$ is the mesh velocity, $\otimes$ is a tensor product, $\hat{\mathbf{I}}$ is a unit tensor, and the rest of the symbols carry their usual meaning. The source term S is identically zero for an isolated system with no external forces, i.e.:

$$S_{\rm isolated} = \begin{pmatrix} 0 \\ \mathbf{0} \\ 0 \end{pmatrix}. \tag{3}$$

In the presence of a gravitational potential ϕ then S would take the following form:

$$S_\phi = \begin{pmatrix} 0 \\ -\nabla\phi \\ -v\dot{\nabla}\phi \end{pmatrix}. \tag{4}$$

For a Eulerian scheme, the location of the mesh is time independent, thus $\mathbf{w} = 0$. In Lagrangian schemes the mesh moves with fluid velocity $\mathbf{w} = \mathbf{v}$, and so that volume integral of density over the fluid element, namely its mass, is exactly constant with time. The physical meaning of these equations is rather simple: the equations state that the volume integrated amount of a quantity q inside a given volume element is equal to the net negative flux of this quantity outside this volume.

The Euler equation (Eq. 1) has a simple formal spatial discretization on an arbitrary mesh

$$\frac{d}{dt}(\bar{q}_i V_i) + \sum_{j\in\partial T_i} (\mathbf{F}\cdot\mathbf{A})_{ij} = \bar{S}_i V_i. \tag{5}$$

Here, $\bar{q}_i$ and $\bar{S}_i$ are the mean values of q and S inside a mesh cell T_i which has volume V_i. The sum is carried out over each of the cell boundaries, and here we introduce a compact notation for the surface integral of a single face between mesh points i and j:

$$(\mathbf{F}\cdot\mathbf{A})_{ij} = \int_{\partial T_{i,j}} \mathbf{F}\cdot d\Sigma. \tag{6}$$

To achieve a second order approximation of this surface integral (Eq. 6) using the one-point quadrature rule, the flux of q between two particles, $\mathbf{F}_{ij}$ is evaluated at the face centroid. This equation states that for numerical purposes only a projection of the flux to the surface normal is required, which we write as $F^n_{ij}A_{ij} = \mathbf{F}_{ij}\cdot\mathbf{A}_{ij}$. It is simple to check that $F^n_{ij} = -F^n_{ji}$. Finally, the geometrical quantities (e.g. cell volumes and the areas of and normals to cell boundaries) can be directly computed from the mesh.

This discretized form can be straightforwardly applied to an equidistant three-dimensional Eulerian Cartesian grid. In this case, we have $V_i = V = l^3$, $A_{ij} = A = l^2$, where l is spacing between grid points along the coordinate axes. We note that in the case of a Eulerian scheme, $dq/dt = \partial q/\partial t$ becase $\mathbf{w} = 0$, thus we have:

$$\begin{aligned} V\frac{\partial \bar{q}_{i,j,k}}{\partial t} + A(F^x_{i+\frac{1}{2},j,k} - F^x_{i-\frac{1}{2},j,k}) - A(F^y_{i,j+\frac{1}{2},k} - F^y_{i,j-\frac{1}{2},k}) \\ +A(F^z_{i,j,k+\frac{1}{2}} - F^z_{i,j,k-\frac{1}{2}}) = \bar{S}_{i,j,k}V, \end{aligned} \tag{7}$$

where $\bar{q}_{i,j,k}$ is average value of q in a cell (i,j,k) and $F^x_{i+\frac{1}{2},j,k}, F^y_{i,j+\frac{1}{2},k}$, and $F^z_{i,j,k+\frac{1}{2}}$ are projections of fluxes of q between neighbouring cell onto $x-$, $y-$ and $z-$direction respectively. Now dividing both sides of this equation by V, we obtain a conventional form of second-order spatial discretization that is used on most Eulerian schemes on equidistant Cartesian grid

$$\frac{\partial \bar{q}_{i,j,k}}{\partial t} + \frac{F^x_{i+\frac{1}{2},j,k} - F^x_{i-\frac{1}{2},j,k}}{l} + \frac{F^y_{i,j+\frac{1}{2},k} - F^y_{i,j-\frac{1}{2},k}}{l} + \frac{F^z_{i,j,k+\frac{1}{2}} - F^z_{i,j,k-\frac{1}{2}}}{l} = \bar{S}_{i,j,k} \tag{8}$$

1.1.2 Mesh-less discretized equations

Any straightforward application of Eq. 5 to mesh-less scheme runs into a wall: a set of particles without underlying mesh lack a well defined definition of volume and areas. Therefore, the simple approach that works with mesh-based scheme fails in mesh-less case. Here, we seek a discrete formulation of mesh-less equations by starting from a weak form of conservation equations (e.g. Vila 1999)

$$\int (\dot{\varphi}q + \nabla\varphi\cdot\mathbf{F} + \varphi S)\, dV\, dt = 0, \tag{9}$$

where the volume integral is taken over all the space-time domain, φ is a differentiable function, and $\dot{\varphi} = \partial\varphi/\partial t + \mathbf{w}\cdot\nabla\varphi$ is an advective derivative in the particle velocity field $\mathbf{w}$. As with the mesh-based scheme, when $\mathbf{w} = 0$ and $\mathbf{w} = \mathbf{v}$ the final equations will describe Eulerian and Lagrangian scheme respectively. One of the reasons to use this integral form of conservative equations instead of Eq. 1 is lack of explicit references to surface integrals, which proves to be important in the subsequent derivation.

In order to spatially discretize Eq. 9, we introduce a partition of unity $\psi_i(\mathbf{x})$, which is a function defined such that $\sum_i \psi(\mathbf{x}) = 1$. Here, index "$i$" refers to the i-th particle, and the sum is carried out over all particles. If data is defined on a set of interpolation points, q_i, the interpolated value at an arbitrary location $\mathbf{x}$ is $q(\mathbf{x}) = \sum_i q_i \psi_i(\mathbf{x})$, and its gradient is $\nabla q(\mathbf{x}) = \sum_i q_i \nabla \psi_i(\mathbf{x})$. Using these definitions we obtain

$$V\bar{f} = \int f(\mathbf{x})\, dV = \int \sum_i f_i \psi_i(\mathbf{x})\, dV = \sum_i f_i \int \psi_i(\mathbf{x})\, dV = \sum_i f_i V_i, \tag{10}$$

where the integral is taken over all the computational volume. A corollary to this is the definition of the volume. Substituting $f(\mathbf{x}) = 1$ into above integral we find

$$V = \sum_i V_i, \qquad \text{where} \qquad V_i = \int \psi_i(\mathbf{x})\, dV, \tag{11}$$

where V_i is the effective volume of particle i. By construction, the total volume of particles is conserved in a closed system.

In the next step, we apply similar procedure to the second term of the integral in Eq. 9. Leaving the time integral temporarily out of the derivation and focusing on spatial discretization, we write

$$\begin{aligned} \int \nabla\varphi \cdot \mathbf{F}(\mathbf{x})\, dV &= \int \sum_{i,j} \psi_i(\mathbf{x}) \varphi_j \nabla\psi_j(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x})\, dV \\ &= \int \sum_{i,j} \psi_i(\mathbf{x}) (\varphi_j - \varphi_i) \nabla\psi_j(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x})\, dV, \end{aligned} \tag{12}$$

here, we insert $1 = \sum_i \psi_i(\mathbf{x})$ into the integrand and the definition of a gradient inside the integrand. In the last term we also made use of the following:

$$\begin{aligned} & \sum_{i,j} \psi_i(\mathbf{x})(-\varphi_i) \nabla\psi_j(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x}) \\ = & \sum_i \psi_i(\mathbf{x})(-\varphi_i) \mathbf{F}(\mathbf{x}) \cdot \nabla \sum_j \psi_j(\mathbf{x}) \\ = & \sum_i \psi_i(\mathbf{x})(-\varphi_i) \mathbf{F}(\mathbf{x}) \cdot \nabla 1 \\ \equiv & \; 0 \end{aligned} \tag{13}$$

in order to add $\sum_{i,j} \psi_i(\mathbf{x})(-\varphi_i) \nabla\psi_j(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x}) \equiv 0$, which might appear to be introducing an unnessecary complication. However later – in §1.2 – it will become clear that the form of that last term, which seems unnecessary in the current formulation, is crucial for the preservation of certain vital conservative properties when particular approximations are invoked. We use this identity to add $\sum_{i,j} = 0$ into Eq. 13. It may appear to be an

unnecessary complication, but as can be seen in the next step, it allows us to rewrite the Eq. 13 in a manifestly symmetric form, from which the local conservation follows. This is a crucial step that provide us with the leeway to approximate spatial integrals with some form of a numerical quadrature without being worried that this fundamental symmetry is broken. An example of this approximation is shown in §1.2.

To proceed further, we rewrite the double sum in the following form

$$\sum_{i,j} \psi_i(\mathbf{x})(\varphi_j - \varphi_i)\nabla\psi_j(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x}) = \sum_{i,j} \varphi_i(\psi_j(\mathbf{x})\nabla\psi_i(\mathbf{x}) - \psi_i(\mathbf{x})\nabla\psi_j(\mathbf{x})) \cdot \mathbf{F}(\mathbf{x}), \quad (14)$$

where to obtain this expression the indices i and j have exchanged places. Substituting this expression into the integral above, we obtain

$$\begin{aligned} \int \nabla\varphi \cdot \mathbf{F}(\mathbf{x})\, dV &= \int \sum_{i,j} \varphi_i \left[\psi_j(\mathbf{x})\nabla\psi_i(\mathbf{x}) - \psi_i(\mathbf{x})\nabla\psi_j(\mathbf{x})\right] \cdot \mathbf{F}(\mathbf{x})\, dV \\ &= \sum_{i,j} \varphi_i \int \mathbf{F}(\mathbf{x}) \cdot d\mathbf{\Sigma}_{ij}. \end{aligned} \quad (15)$$

The integral on the right-hand side can be interpreted as a surface integral over a virtual boundary between particle i and j. As a result, we can define an effective inter-particle surface as:

$$\mathbf{A}_{ij} = \int d\mathbf{\Sigma}_{ij} = \int \left[\psi_j(\mathbf{x})\nabla\psi_i(\mathbf{x}) - \psi_i(\mathbf{x})\nabla\psi_j(\mathbf{x})\right]\, dV. \quad (16)$$

Therefore, by analogy with Eq. 1 and Eq. 5 we write

$$\int \nabla\varphi \cdot \mathbf{F}(\mathbf{x})\, dV = \sum_{i,j} \varphi_i \int \mathbf{F}(\mathbf{x}) \cdot d\mathbf{\Sigma}_{ij} = \sum_{i,j} \varphi_i \left(\mathbf{F} \cdot \mathbf{A}\right)_{ij}. \quad (17)$$

Here, we can also use a second-order approximation to the last integral by writing $(\mathbf{F} \cdot \mathbf{A})_{ij} \approx \mathbf{F}_{ij} \cdot \mathbf{A}_{ij} = F^n_{ij} A_{ij}$, where F^n_{ij} is a projection of flux onto surface normal evaluated at the centroid of the overlapping regions. For Lagrangian fluid dynamics, this step is usually not used because we can compute fluxes directly at each of the particle's location. However, when a mesh-less method is used in context of a Godunov scheme, the available information is usually an inter-particle (or inter-cell) flux projected onto the face normal. This flux is the evaluated at the centroid of the overlapping region and then multiplied by the effective area of two particles to achieve second order accuracy (e.g. Vila (1999); Gaburov & Nitadori (2011)).

To complete the derivation, we apply spatial discretization to the first term inside integral in Eq. 9. Here, we insert $1 = \sum_i \psi_i(\mathbf{x})$ inside the integrand to obtain

$$\begin{aligned} \int \left(\dot{\varphi} q\, dV\right)\, dt &= \int \left(\int \dot{\varphi} q \sum_i \psi_i(\mathbf{x})\, dV\right)\, dt \approx \int \left(\sum_i \dot{\varphi}_i q_i \left[\int \psi_i(\mathbf{x})\, dV\right]\right)\, dt \\ &= \int \left(\sum_i \dot{\varphi}_i q_i V_i\right)\, dt, \end{aligned} \quad (18)$$

where in the approximation step we applied one-point quadrature to the spatial integral, with q_i and φ_i located at the particle's location. Next, we apply integration by parts to the right hand side to obtain

$$\int \left(\sum_i \frac{d\varphi_i}{dt} \, q_i \, V_i \right) \, dt = \sum_i \int \left(\frac{d}{dt} (\varphi_i \, q_i \, V_i) \right) \, dt - \int \left(\sum_i \frac{d}{dt} (q_i V_i) \varphi_i \right) \, dt \tag{19}$$

The first term is an integral that depends only on the time-domain boundaries, which we set equal to zero. Therefore we are left with only the second term. Combining this together with Eq. 17, we obtain the following spatially discrete form of Eq. 9

$$\int \, dt \, \sum_i \varphi_i \left(-\frac{d}{dt} (q_i V_i) - \sum_j (\mathbf{F} \cdot \mathbf{A})_{ij} + S_i V_i \right) = 0. \tag{20}$$

This integral must be zero for any arbitrary set of φ_i and all times. Hence the term inside the brackets must also always be equal to zero. This leads to a spatially discrete form of finite-volume equations on a set of particles

$$\frac{d}{dt} (q_i V_i) + \sum_j (\mathbf{F} \cdot \mathbf{A})_{ij} = S_i V_i, \tag{21}$$

This equation has the same form as Eq. 2, except that here a surface element between two particles is defined as a volume integral on the overlapping regions of the corresponding partition of unity.

1.1.3 Derivation of SPH equations of motion

As an example of this new formalism, we use it to derive equations of Lagrangian fluid dynamics which have the same form as the SPH equations of motion. In SPH, the partition of unity is defined by the following expression

$$\psi_i(\mathbf{x}) = \frac{m_i}{\rho(\mathbf{x})} W(\mathbf{x} - \mathbf{x}_i, h(\mathbf{x})), \tag{22}$$

It is a simple task to check that this leads to the SPH summation identity,

$$\rho(\mathbf{x}) = \sum_i m_i W(\mathbf{x} - \mathbf{x}_i, h(\mathbf{x})).$$

In the next step we evaluate effective volume of the particle using Eq. 11

$$V_i = \int \psi_i(\mathbf{x}) \, dV = \int \frac{m_i}{\rho(\mathbf{x})} W(\mathbf{x} - \mathbf{x}_i, h(\mathbf{x})) \, dV \tag{23}$$

where $W(\mathbf{x} - \mathbf{x}_i, h(\mathbf{x}))$ is an SPH kernel, and $h(\mathbf{x})$ is each SPH particle's smoothing length. In order to obtain this integral in a closed form, we approximate the kernel inside

this integrand as a delta function, namely $W(\mathbf{x}-\mathbf{x}_i, h(\mathbf{x})) \approx \delta(\mathbf{x}-\mathbf{x}_i)$. This permits analytical evaluation of an SPH particle volume $V_i \approx m_i/\rho_i$, which is consistent with the usual definition of the SPH particle number density $n_i = 1/V_i = \rho_i/m_i$.

To compute SPH forces, we apply a similar approximation to compute $(\mathbf{F}\cdot\mathbf{A})_{ij}$, in order to evaluate the flux of momentum. Because SPH is a Lagrangian method, the flux of the momentum is a diagonal tensor $\mathbf{F} = P\hat{\mathbf{I}}$. Hence we can write

$$
\begin{aligned}
(\mathbf{F}\cdot\mathbf{A})_{ij} &= \int \mathbf{F}(\mathbf{x})\cdot d\mathbf{\Sigma}_{ij} \qquad (24)\\
&= \int \left[\psi_i(\mathbf{x})\left(\mathbf{F}(\mathbf{x}) : \nabla\psi_j(\mathbf{x})\right) - \psi_j(\mathbf{x})\left(\mathbf{F}(\mathbf{x}) : \nabla\psi_i(\mathbf{x})\right)\right] dV\\
&= \int \left(\frac{m_i}{\rho(\mathbf{x})} W(\mathbf{x}-\mathbf{x}_i, h(\mathbf{x})) P(\mathbf{x}) \nabla\psi_j(\mathbf{x}) - \frac{m_j}{\rho(\mathbf{x})} W(\mathbf{x}-\mathbf{x}_j, h(\mathbf{x})) P(\mathbf{x}) \nabla\psi_i(\mathbf{x})\right) dV,
\end{aligned}
$$

where the ":" symbol denotes contraction of a tensor with a vector to produce another vector. In order to be able to analytically evaluate this integral, we approximate the kernel (but not its gradient) using Dirac's delta function $W(\mathbf{x}-\mathbf{x}_i, h(\mathbf{x}))\nabla\psi_j(\mathbf{x}) \approx \delta(\mathbf{x}-\mathbf{x}_i)\nabla\psi_j(\mathbf{x})$. Ignoring any spatial variation in density and h inside the volume defined by the smoothing kernel for any given particle, we obtain:

$$
(\mathbf{F}\cdot\mathbf{A})_{ij} \approx \frac{m_i m_j P_i}{\rho_i^2} \nabla_i W(\mathbf{x}_i - \mathbf{x}_j, h_i) - \frac{m_i m_j P_j}{\rho_j^2} \nabla_j W(\mathbf{x}_j - \mathbf{x}_i, h_j). \qquad (25)
$$

To obtain this equation we used an approximation to the effective volume derived above, $V_i = m_i/\rho_i$. Finally, if we substitute this approximation to $(\mathbf{F}\cdot\mathbf{A})_{ij}$ into Eq. 21 (in which we write $q = \rho\mathbf{v}$ for the momentum), then we obtain the following result

$$
\frac{d}{dt}(m_i\mathbf{v}_i) = -m_i \sum_j m_j \left(\frac{P_i}{\rho_i^2}\nabla_i W_{ij}(h_i) + \frac{P_j}{\rho_j^2}\nabla_j W_{ij}(h_j)\right) + \frac{m_i S_i}{\rho_i}. \qquad (26)
$$

Here, we used standard SPH notation $W_{ij}(h_i) = W(\mathbf{x}_i - \mathbf{x}_j, h_i)$ and the identity $\nabla_j W(\mathbf{x}_j - \mathbf{x}_i, h_j) = -\nabla_j W(\mathbf{x}_i - \mathbf{x}_i, h_j)$. Since in Lagrangian fluid dynamics the flux of mass across cell boundaries is zero, which implies $dm_i/dt = 0$, Eq. 26 reduces to the standard form of the SPH equations of motion

$$
\frac{d\mathbf{v}_i}{dt} = -\sum_j m_j \left(\frac{P_i}{\rho_i^2}\nabla_i W_{ij}(h_i) + \frac{P_j}{\rho_j^2}\nabla_j W_{ij}(h_j)\right) + \frac{S_i}{\rho_i}. \qquad (27)
$$

With a more careful analysis that takes into account variations of density inside the smoothing kernel one can derive additional correction terms due to the varying smoothing length.

1.2 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. One of the properties of utmost importance is local conservation, which means that the amount of 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. A careful inspection of Eq. 21 and Eq. 5, demonstrates that the necessary and sufficient condition for local conservation is the antisymmetry identity $(\mathbf{F}\cdot\mathbf{A})_{ij} = -(\mathbf{F}\cdot\mathbf{A})_{ji}$. In the case of the SPH equations of motion, Eq. 27, it becomes clear that local conservation guarantees that Newton's third law is satisfied exactly for any particle distribution. The reader can now check why we added the extra, identically zero, term to Eq. 13 in continuous form. Without including that term then applying the approximations that lead to the SPH equations of motion results in the violation of Newton's third law in the final discretized equations; in that form, Newton's third law would only have been satisfied to the truncation error.

Another property of the equations, which we call the closure condition, is that 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, $\sum_j \mathbf{A}_{ij} = 0$. 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 (which is gradient of the pressure) on each particle or mesh cell is zero for any mesh or particle distribution. While the sum $\sum_j \mathbf{A}_{ij} = 0$ can be geometrically proven when referring to a mesh, this identity is not intuitive in case of particles; however, it can be easily proven. Starting with Eq. 16, we write

$$\begin{aligned}\sum_j \mathbf{A}_{ij} &= \sum_j \int \left[\psi_j(\mathbf{x})\nabla\psi_i(\mathbf{x}) - \psi_i\nabla\psi_j(\mathbf{x})\right] dV \\ &= \sum_j \int \left[\nabla(\psi_j(\mathbf{x})\psi_i(\mathbf{x})) - 2\psi_i\nabla\psi_j(\mathbf{x})\right] dV = 0. \end{aligned} \tag{28}$$

Here we applied integration by parts to the first term of the integral. Applying the divergence theorem to the first integral on the right-hand side, we can rewrite it as a surface integral over the boundary between overlapping regions of the corresponding partition of unity. Therefore, by construction this integral vanishes, because the value of the partition of unity at its boundary is zero. In the second term, we include the sum inside the integral, $\sum_j \int 2\psi_i(\mathbf{x})\nabla\psi_j(\mathbf{x}) = 2\int \psi_i(\mathbf{x})\sum_j \nabla\psi_j(\mathbf{x})$. Applying the identity $\sum_j \nabla\psi_j(\mathbf{x}) \equiv 0$, we can demonstrate that this term vanishes as well, therefore completing the proof that $\sum_j \mathbf{A}_{ij} = 0$ in mesh-less schemes.

The approximations that lead to Eq. 27 may result in the loss of some properties. Indeed, while the equations maintain their local conservative character (Newton's third law is still exactly satisfied), the closure condition does not hold anymore. Indeed, setting

$P_{ij} = P_0 = \text{const}$, we obtain

$$\frac{d}{dt}(m_i \mathbf{v}_i) = -m_i P_0 \sum_j m_j \left(\frac{\nabla_i W_{ij}(h_i)}{\rho_i^2} + \frac{\nabla_j W_{ij}(h_j)}{\rho_j^2} \right) = -m_i P_0 C_i, \tag{29}$$

where $C_i = 0$ only when particles are distributed on a regular lattice. It is well known in SPH that for irregular particle distributions there is a net force proportional to the mean pressure of the system. This effect, called 'pressure leak', tends to regularize the particle distribution (which in turn tends to decrease the strength of the effect). This pressure leak can be attributed to the violation of the exact closure condition, and it becomes more damaging with increasing degrees of particle irregularity. One manifestation of this pressure leak is the presence of "surface tension" forces at a discontinuity in the particle distribution. It is possible to reduce this effect by more accurate evaluation of the volumes and areas in Eq. 23 and Eq. 25 respectively either by numerical quadratures (e.g. Junk 2002) or using an inter-particle model for the density distribution (Inutsuka, 2002).

1.2.1 Angular momentum conservation

Spatially discrete Euler equations exactly conserve the total mass, linear momentum and energy of the system. However, conservation of these quantities does not automatically guarantee conservation of angular momentum, even though it is guaranteed in a continuous approximation. Let consider a system of particles or mesh points with coordinates $\mathbf{x}_i$. To check whether a discretized form of the equations conserves angular momentum, we compute

$$\sum_i \dot{\mathbf{L}}_i = \sum_i \frac{d}{dt} (\mathbf{x}_i \times m_i \mathbf{v}_i) = \sum_i \dot{\mathbf{x}}_i \times m_i \mathbf{v}_i + \sum_i \mathbf{x}_i \times \frac{d}{dt}(m_i \mathbf{v}_i), \tag{30}$$

where $\dot{\mathbf{x}}_i = \mathbf{w}_i$ is the velocity of a particle or a mesh point. Using Eq. 5 with $q = \rho_i \mathbf{v}_i$ together with momentum flux form Eq 2, we obtain

$$\begin{aligned} \frac{d}{dt}(m_i v_i^\alpha) &= -\sum_j \left[(P \delta^{\alpha\beta} A^\beta)_{ij} + (\rho v^\alpha (v - w)^\beta A^\beta)_{ij} \right] \\ &= -\sum_j \left[(P A^\alpha)_{ij} + (\rho v^\alpha (\mathbf{v} - \mathbf{w}) \cdot \mathbf{A})_{ij} \right], \end{aligned} \tag{31}$$

where we use Einstein summation convention over Greek indices (which here denote the three-dimensional components of a vector). Substituting this into Eq. 30, we obtain an equation for the time evolution of the angular momentum in component form:

$$\sum_i \dot{L}_i^\alpha = \epsilon^{\alpha\beta\gamma} \sum_i m_i w^\beta v^\gamma - \epsilon^{\alpha\beta\gamma} \sum_i x_i^\beta \sum_j \left[(P A^\gamma)_{ij} + (\rho v^\gamma (\mathbf{v} - \mathbf{w}) \cdot \mathbf{A})_{ij} \right] \tag{32}$$

where we write a cross product of two vectors as $(\mathbf{v} \times \mathbf{w})^\alpha = \epsilon^{\alpha\beta\gamma} v^\beta w^\gamma$, and $\epsilon^{\alpha\beta\gamma}$ is the three-dimensional Levi-Civita symbol. The second term in this equation can be rewritten in the following form

$$\epsilon^{\alpha\beta\gamma} \frac{1}{2} \sum_{i,j} (x_i - x_j)^\beta (PA^\gamma)_{ij} + \epsilon^{\alpha\beta\gamma} \frac{1}{2} \sum_{i,j} (x_i - x_j)^\beta (\rho v^\gamma (\mathbf{v} - \mathbf{w}) \cdot \mathbf{A})_{ij}. \tag{33}$$

Several properties can be derived from this equation. The first term vanishes if the normal to the surface between mesh-cell (or particles) i and j, $\mathbf{A}_{ij}/A_{ij}$, is parallel to the their separation vector, $\mathbf{x}_i - \mathbf{x}_j$. The second term, however, only automatically and generally vanishes if the mesh points move with the fluid velocity, i.e. $\mathbf{w} = \mathbf{v}$. So, in general the necessary condition for angular momentum conservation to be guaranteed is a Lagrangian formulation of hydrodynamics,[2] in which case we have

$$\sum_i \dot{\mathbf{L}}_i = -\frac{1}{2} \sum_{i,j} (\mathbf{x}_i - \mathbf{x}_j) \times (P\mathbf{A})_{ij}. \tag{34}$$

It becomes clear that, in order to conserve angular momentum exactly, the normal vector to the area between particle i and j must be directed along the line connecting these two particles. In the mesh-based Lagrangian method that uses a Voronoi mesh (Trease, 1988; Heß & Springel, 2010), these normal vectors are always parallel to the separation vector between two particles, as required. In the case of mesh-less schemes, however, it cannot be proven from Eq. 25 that $(P\mathbf{A})_{ij}$ is, in general, parallel to the separation vector. Nevertheless, the nature of the approximation that led to the SPH equations of motion, although sacrificing the closure condition, does guarantee exact conservation of angular momentum.

1.3 Discussion

We have presented a generic formalism for the mesh-less discretization of finite-volume equations. Formally, the spatially discrete equations (Eq. 21) have the same form as mesh-based equations (Eq. 5), and therefore posses the same properties, such as local conservation and the closure condition. The former property is of the utmost importance, as the violation of it will most likely produce incorrect results in problems involving strong shocks.

We have shown that, with few approximation, Eq. 21 reduces to the SPH equations of motion. While the resulting equations conserve angular momentum exactly, the closure condition is no longer satisfied for generic particle distribution. This will result in a pressure leak effect. In a positive pressure system with a random particle distribution, this pressure leak will tend to regularize the particle distribution such as to minimise the leak, whilst it will cause tensile instability in the case of negative stresses. Amongst other issues,

[2] In the special case of a cylindrical coordinate system, only the z-component of angular momentum is conserved.

this pressure leak causes the inability of SPH to resolve certain fluid instabilities, such as the Kelvin-Helmholtz and Rayleigh-Taylor instabilities. A more accurate approximation Eq. 25 can substantially reduce the damaging effects of pressure leak and the associated surface tension forces (Inutsuka, 2002; Cha et al., 2010). Alternatively, one may apply a high order numerical quadrature to integrate Eq. 25, and therefore enforce satisfaction of the closure conditions to high order (Junk, 2002), but this may still result in violation of angular momentum conservation.

Particle-based scheme require various approximations to derive equations that can be numerically integrated. On the other hand, the mesh-based schemes require a rather complex process of construction of the unstructured mesh in order to obtain the necessary geometrical quantities. The advantage of the latter is that the geometry is exact and well-defined, which means that local conservation and the closure condition are satisfied by construction. On the contrary, to achieve these properties with mesh-less schemes, one needs to invoke high-order numerical quadrature over complex spatial domains, such as the overlapping regions of two partitions of unity; these are conceptually simple but computationally expensive. Therefore both methods can reach comparable degrees of accuracy, and the eventual computational cost and overall complexity of each of the methods might also be comparable. Furthermore, as we have shown, there is no well-defined line separating the underlying principles of mesh-based and mesh-less methods. Hence we expect that the generalisation outlined here will help future simulations to take advantage of the best properties of both kinds of scheme.

References

Abel, T. 2011, MNRAS, 413, 271

Cha, S.-H., Inutsuka, S.-I., & Nayakshin, S. 2010, MNRAS, 403, 1165

Dilts, G. A. 1999, International Journal for Numerical Methods in Engineering, 44, 1115

—. 2000, International Journal for Numerical Methods in Engineering, 48, 1503

Gaburov, E. & Nitadori, K. 2011, MNRAS, 414, 129

Heß, S. & Springel, V. 2010, MNRAS, 406, 2289

Hietel, D., Steiner, K., & Struckmeier, J. 2000, Math. Models Methods Appl. Sci, 10, 1363

Inutsuka, S.-I. 2002, Journal of Computational Physics, 179, 238

Junk, M. 2002, in Lecture Notes in Computational Science and Engineering, Vol. 26, Meshfree Methods for Partial Differential Equations, ed. M. Griebel & M. A. Schweitzer (Springer Berlin Heidelberg), 223–238

Lanson, N. & Vila, J.-P. 2008, SIAM J. Numer. Anal., 46, 1912

Trease, H. E. 1988, Computer Physics Communications, 48, 39

Vila, J. P. 1999, Mathematical models and Methods in Applied Sciences, 9, 161