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CONSERVATION PROPERTIES OF SMOOTHED PARTICLE HYDRODYNAMICS APPLIED TO THE SHALLOW WATER EQUATIONS

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Abstract.

Kelvin's circulation theorem and its implications for potential vorticity (PV) conservation are among the most fundamental concepts in ideal fluid dynamics. In this note, we discuss the numerical treatment of these concepts with the Smoothed Particle Hydrodynamics (SPH) and related methods. We show that SPH satisfies an exact circulation theorem in an interpolated velocity field, and that, when appropriately interpreted, this leads to statements of conservation of PV and generalized enstrophies. We also indicate some limitations where the analogy with ideal fluid dynamics breaks down. *AMS subject classification:* 76M28.

Key words: geophysical fluid dynamics, potential vorticity conserving methods, geometric methods, smoothed particle hydrodynamics.

1 Introduction and Lagrangian Equations of Motion

Large scale geophysical flows in the atmosphere and ocean are incompressible and nearly two-dimensional. As a result, vorticity plays a central role in geophysical fluid dynamics. In the Lagrangian fluid description, conservation of vorticity and circulation follow from the fact that fluid particles are identical and thus there is a great degree of freedom in labeling particles; that is, vorticity conservation follows from the particle nature of the fluid (§2). One might therefore expect that a Lagrangian, particle-based approach would lead to good vorticity conservation also in a computational setting. In this article, we consider the conservation properties of the popular Smoothed Particle Hydrodynamics method (SPH) [9, 14], as briefly outlined in §3. We will show that, indeed, the continuous velocity field that interpolates the SPH particle velocities exactly satisfies Kelvin's circulation theorem (§4). In turn, Stoke's theorem implies that absolute vorticity is also exactly conserved. Recently, Monaghan [10] has suggested that circulation is conserved approximately by SPH due to a "discrete relabeling symmetry". We stress that in this article we prove *exact conservation of circulation* for a *continuous* interpolated velocity field, which implies the convergence of the discrete integral introduced in [10]. The Hamiltonian Particle-Mesh method developed by the authors in [7] inherits conservation of circulation from SPH, and in §5 we provide a numerical illustration of this result using the HPM method.

Additional conservation properties of importance in geophysical fluid dynamics are mass and energy conservation. Mass conservation is intrinsic to the SPH formulation. It is also well-known that SPH can be derived from a variational principle (see, e.g., [14, 3, 10]); i.e. it can be given a Hamiltonian structure, for which symplectic integrators may be used to obtain excellent energy conservation [13].

For simplicity of exposition, we consider the two-dimensional shallow water equations (SWEs):

$$\frac{D}{Dt}\mathbf{u} = -c_0 \boldsymbol{\nabla}_{\boldsymbol{x}} h, \tag{1.1}$$

$$\frac{D}{Dt}h = -h \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \mathbf{u}, \tag{1.2}$$

where $\mathbf{u} = (u, v)^T$ is the horizontal velocity field, h is the layer depth, $c_0 > 0$ is an appropriate constant, and $\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}$ is the material time derivative. The results of this paper immediately generalize to the rotating SWEs. This is briefly discussed in §6.

In the Lagrangian description [12], the positions of all fluid particles are given as a time dependent diffeomorphism from the fluid label space $\mathbb{A} \subset \mathbb{R}^2$ to $\mathbb{R}^2$:

$$\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{a}, t), \quad \boldsymbol{a} = (a, b) \in \mathbb{A}, \quad \boldsymbol{X} = (X, Y) \in \mathbb{R}^2.$$

The labels are fixed for each particle, i.e. $\frac{D}{Dt}\boldsymbol{a} = \boldsymbol{0}$, and the fluid layer depth h is defined, as a function of the determinant of the 2×2 Jacobian matrix

$$\boldsymbol{X}_{\boldsymbol{a}} = \frac{\partial(X, Y)}{\partial(a, b)},$$

through the relation

$$h(\boldsymbol{X}(\boldsymbol{a}, t), t)\, |\boldsymbol{X}_{\boldsymbol{a}}| = h_o(\boldsymbol{a}), \tag{1.3}$$

where $h_o(\boldsymbol{a})$ is a time-independent function [12]. Differentiation of (1.3) with respect to time yields an expression that is equivalent to the continuity equation (1.2). Hence (1.3) and (1.2) are essentially equivalent statements.

A natural choice for the labels $\boldsymbol{a}$ is given by $\boldsymbol{a} = \boldsymbol{X}(0) = \boldsymbol{x}$ which we assume from now on. Then the matrix $\boldsymbol{X}_{\boldsymbol{a}}$ is the identity and h_o the layer-depth at $t = 0$.

Consider the integral identity defining the layer-depth h at time t and Eulerian position $\boldsymbol{x}$

$$h(\boldsymbol{x}, t) = \int h(\boldsymbol{X}, t)\, \delta(\boldsymbol{x} - \boldsymbol{X})\, d\boldsymbol{X},$$

where δ is the Dirac delta function. Using (1.3) we can pull this integral back to label space, arriving at the relation

$$h(\boldsymbol{x}, t) = \int h_o(\boldsymbol{a})\, \delta(\boldsymbol{x} - \boldsymbol{X}(\boldsymbol{a}, t))\, d\boldsymbol{a}, \tag{1.4}$$

which can be taken as the definition of the layer depth in the Eulerian reference frame.

The motion of the SWEs is given as the stationary state $\delta\mathcal{L} = 0$ of the action integral

$$\mathcal{L} = \iint h_o \left\{ \frac{1}{2}\dot{\boldsymbol{X}} \cdot \dot{\boldsymbol{X}} - \frac{c_0}{2} h \right\} d\boldsymbol{a}\, dt \tag{1.5}$$

with respect to admissible variations $\delta\boldsymbol{X}(\boldsymbol{a}, t)$, where the dot notation refers to time differentiation for fixed label, i.e. the material time derivative $\frac{D}{Dt}$. The equations of motion become

$$\frac{D}{Dt}\boldsymbol{X} = \boldsymbol{u} \tag{1.6}$$

$$\frac{D}{Dt}\boldsymbol{u} = -c_0 \boldsymbol{\nabla}_{\boldsymbol{X}} h \tag{1.7}$$

where h is defined by (1.3) or (1.4).

Since the SWEs (1.6)–(1.7) are derived from a Lagrangian variational form, they are Hamiltonian, conserving the energy

$$\mathcal{E} = \frac{1}{2} \int h_o \left\{ \mathbf{u} \cdot \mathbf{u} + c_0 h \right\} d\boldsymbol{a} = \frac{1}{2} \int \frac{\mathbf{p} \cdot \mathbf{p}}{h_o} d\boldsymbol{a} + \frac{c_0}{2} \int h^2 d\boldsymbol{x},$$

$\mathbf{p} = h_o \mathbf{u}$, and the symplectic two-form $\bar{\omega} := \int (d\mathbf{p} \wedge d\boldsymbol{X})\, d\boldsymbol{a}$ [11].

2 Vorticity Conservation in Ideal Shallow Water Flows

The action integral (1.5) depends on the labels $\boldsymbol{a}$ explicitly only through the layer depth

$$h = h_o |\boldsymbol{X}_{\boldsymbol{a}}|^{-1}.$$

As a result, the action is invariant to any transformation of label space (i.e. "relabeling") that leaves the determinant $|\boldsymbol{X}_{\boldsymbol{a}}|$ unchanged (e.g. any divergence-free relabeling $|\partial(a', b')/\partial(a, b)| = 1$ will suffice.) By Noether's theorem, this *particle relabeling symmetry* implies a conserved quantity of the dynamics, which turns out to be the conservation of vorticity in its many forms as outlined below. Note, however, that this symmetry with implied conservation law is very much tied into the particle nature of the flow in the Lagrangian description; it follows essentially because particles are indistinguishable from one other. It is this observation which motivates us to consider the vorticity conservation properties of Lagrangian methods such as SPH in this article. For further discussion of the particle relabeling symmetry and its relation to vorticity, we highly recommend Salmon's monograph [12].

Consider the vorticity $\zeta = \boldsymbol{\nabla}_{\boldsymbol{x}} \times \mathbf{u}$. Using

$$\boldsymbol{\nabla}_{\boldsymbol{x}} \times \frac{D}{Dt}\mathbf{u} = \boldsymbol{\nabla}_{\boldsymbol{x}} \times \mathbf{u}_t + (\boldsymbol{\nabla}_{\boldsymbol{x}} \times \mathbf{u})(\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \mathbf{u}) + \mathbf{u} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}}(\boldsymbol{\nabla}_{\boldsymbol{x}} \times \mathbf{u}) = 0,$$

it is easy to conclude that vorticity satisfies the continuity equation

$$\frac{D}{Dt}\zeta = -\zeta \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot \mathbf{u}. \tag{2.1}$$

The ratio of ζ to h, i.e., $q = \zeta/h$, is called the potential vorticity (PV) [12]. The PV field q is materially conserved since, using (1.2) and (2.1),

$$\frac{D}{Dt}q = h^{-1}\left\{\frac{D}{Dt}\zeta - q\frac{D}{Dt}h\right\} = 0.$$

As a result, it follows that (1.2) and (2.1) are special cases of an infinite family of continuity equations

$$\frac{\partial}{\partial t}[hf(q)] = -\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot [hf(q)\mathbf{u}], \tag{2.2}$$

where f is an arbitrary (smooth) function of q.

Let us now discuss the concept of circulation. Take a closed loop $\mathcal{S} = \{\boldsymbol{a}(s)\}_{s\in S^1}$ in label space and consider the particle locations $\boldsymbol{X}(s) = \boldsymbol{X}(\boldsymbol{a}(s))$ parameterized by $s \in S^1$. By definition, the loop $\{\boldsymbol{X}(s)\}_{s\in S^1}$ in configuration space is advected along the velocity field, i.e.

$$\frac{d}{dt}\boldsymbol{X}(s) = \mathbf{u}(\boldsymbol{X}(s)).$$

Kelvin's circulation theorem [12] states that

$$\frac{d}{dt}\oint \mathbf{u}\cdot \boldsymbol{X}_s\, ds = 0. \tag{2.3}$$

Indeed, we obtain

$$\begin{aligned}
\frac{d}{dt}\oint \mathbf{u}\cdot\boldsymbol{X}_s\,ds &= \oint\left(\frac{D}{Dt}\mathbf{u}\right)\cdot\boldsymbol{X}_s\,ds + \oint \mathbf{u}\cdot\left(\frac{\partial}{\partial s}\frac{D}{Dt}\boldsymbol{X}\right)ds \\
&= -c_0\oint \boldsymbol{\nabla}_{\boldsymbol{X}} h\cdot\boldsymbol{X}_s\,ds + \oint \mathbf{u}\cdot\mathbf{u}_s\,ds \\
&= \oint\left(\frac{1}{2}(\mathbf{u}\cdot\mathbf{u})_s - c_0 h_s\right)ds \\
&= 0.
\end{aligned}$$

Let $\mathcal{V}$ denote the area enclosed by $\mathcal{S}$ in label space and $\mathcal{R}$ its image in $\boldsymbol{x}$-space. Then Stokes' theorem applied to (2.3) yields

$$\frac{d}{dt}\int_{\mathcal{V}}(\boldsymbol{\nabla}_{\boldsymbol{X}}\times\mathbf{u})|\boldsymbol{X}_{\boldsymbol{a}}|\,d\boldsymbol{a} = \frac{d}{dt}\int_{\mathcal{R}}(\boldsymbol{\nabla}_{\boldsymbol{x}}\times\mathbf{u})\,d\boldsymbol{x} = 0. \tag{2.4}$$

Because $\mathcal{V}$ is arbitrary, the left side of this equation yields another statement of PV conservation, since

$$(\boldsymbol{\nabla}_{\boldsymbol{X}}\times\mathbf{u})|\boldsymbol{X}_{\boldsymbol{a}}| = h_o\frac{\zeta}{h} = h_o q,$$

and $Dh_o/Dt = 0$. Similarly, after applying the transport theorem [5] to the right equality in (2.4), a second appeal to the arbitrariness of $\mathcal{V}$ yields the vorticity equation (2.1).

3 Review of Smoothed Particle Hydrodynamics

The Smoothed Particle Hydrodynamics (SPH) method [9] is a Lagrangian method for fluid dynamics, in which the fluid mass is distributed over a number of smooth, compactly supported, particle-centered basis functions. A similar method is the Finite Mass Method [14].

Assume that a set of Lagrangian particles with positions $\{\boldsymbol{X}_k(t);\ \boldsymbol{X}_k \in \mathbb{R}^2\}$ is given as a function of time and that

$$\frac{d}{dt}\boldsymbol{X}_k = \mathbf{u}_k, \tag{3.1}$$

where $\mathbf{u}_k$ is the velocity of the particle. Then the time evolution of a quantity g, satisfying a continuity equation

$$\frac{\partial}{\partial t} g = -\boldsymbol{\nabla}_{\boldsymbol{x}} \cdot [g\boldsymbol{u}],$$

can be approximated by

$$\bar{g}(\boldsymbol{x}, t) = \sum_k \gamma_k \psi(\boldsymbol{x} - \boldsymbol{X}_k(t)).$$

Here $\{\gamma_k\}$ are constants determined by the initial $g(\boldsymbol{x})$ field and ψ is an appropriate basis function. Typically, SPH is implemented with radially symmetric basis functions, i.e. $\psi(\boldsymbol{x}) = \Psi(\|\boldsymbol{x}\|)$ and $\Psi(r)$ is either a Gaussian, a compactly supported radial basis function [4], or a radial spline [9].

Let us apply this idea to the layer-depth h, i.e., we introduce the approximation

$$\bar{h}(\boldsymbol{x}, t) = \sum_k m_k \psi(\boldsymbol{x} - \boldsymbol{X}_k(t)) \tag{3.2}$$

and assume that $\bar{h}(\boldsymbol{x}, t) > 0$. Then each particle contributes the fraction

$$\rho_k(\boldsymbol{x}, t) := \frac{m_k \psi(\boldsymbol{x} - \boldsymbol{X}_k(t))}{\bar{h}(\boldsymbol{x}, t)} \tag{3.3}$$

to the total layer-depth. These fractions form a partition of unity, i.e.

$$\sum_k \rho_k(\boldsymbol{x}, t) = 1.$$

Hence they can be used to approximate data from the particle locations to any $\boldsymbol{x} \in \mathbb{R}^2$. In particular, we define an approximate Eulerian velocity field

$$\bar{\mathbf{u}}(\boldsymbol{x}, t) := \sum_k \rho_k(\boldsymbol{x}, t)\, \mathbf{u}_k(t) \tag{3.4}$$

with layer depth flux density (inserting (3.3))

$$\bar{h}(\boldsymbol{x}, t)\, \bar{\mathbf{u}}(\boldsymbol{x}, t) = \sum_k m_k \psi(\boldsymbol{x} - \boldsymbol{X}_k(t))\, \mathbf{u}_k(t).$$

Using (3.1), it is now easily verified that

$$\frac{\partial}{\partial t}\bar{h}(\boldsymbol{x},t) + \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot [\bar{h}(\boldsymbol{x},t)\bar{\mathbf{u}}(\boldsymbol{x},t)] = 0. \tag{3.5}$$

It follows that the layer depth approximation (3.2) exactly satisfies the continuity equation (1.2) under the flow of the formally defined velocity field (3.4). In general the particle advection velocity is different from the approximated velocity, i.e $\mathbf{u}_k \neq \bar{\mathbf{u}}(\boldsymbol{X}_k)$. We note that the modification suggested in [8] to avoid penetration in SPH corresponds[1] to advecting the particles in the velocity field (3.4).

Hence, (3.1) and (3.2) provide an approximation to the continuity equation (1.2). To get a closed system of discretized equations, we still have to approximate the momentum equation (1.1). For example, one can use

$$\frac{d}{dt}\mathbf{u}_k = -c_0 \boldsymbol{\nabla}_{\boldsymbol{x}}\bar{h}(\boldsymbol{x},t)\big|_{\boldsymbol{x}=\boldsymbol{X}_k} = -c_0 \sum_j m_j \boldsymbol{\nabla}_{\boldsymbol{X}_k}\psi(\boldsymbol{X}_k - \boldsymbol{X}_j). \tag{3.6}$$

The equations (3.1), (3.2), and (3.6) comprise the standard SPH approximation to the SWEs (1.1)–(1.2). We introduce the canonical momenta $\mathbf{p}_k = m_k\mathbf{u}_k$. The equations (3.1), (3.2), and (3.6) are now canonical with Hamiltonian (energy)

$$\mathcal{H} = \frac{1}{2}\sum_k \frac{1}{m_k}||\mathbf{p}_k||^2 + \frac{c_0}{2}\sum_{l,k} m_k m_l \psi(\boldsymbol{X}_l - \boldsymbol{X}_k) \tag{3.7}$$

and symplectic structure $\bar{\omega} = \sum_k d\mathbf{p}_k \wedge d\boldsymbol{X}_k$.

A numerical time-stepping scheme is obtained by noting that

$$\frac{d}{dt}\boldsymbol{X}_k = \mathbf{u}_k, \qquad \frac{d}{dt}\mathbf{u}_k = \mathbf{0}$$

can be solved exactly and that the implied time evolution of $\bar{h}(\boldsymbol{x},t)$ exactly satisfies (3.5). Similarly, equation (3.6) and $\frac{d}{dt}\boldsymbol{X}_k = \mathbf{0}$ can also be integrated exactly since in this case $\bar{h}_t = 0$. A composition of these exact propagators leads to a symplectic time-stepping scheme [13] implying good long-time energy conservation [2].

Bonet & Lok [3] have also discussed conservation properties of SPH in a variational formulation. In particular they show conservation of linear and angular momentum, provided the basis function ψ is radially symmetric. These follow from the fact that the Hamiltonian (3.7) is invariant under translations and rotations in the Lagrangian particle positions $\{\boldsymbol{X}_k\}$ and subsequent application of Noether's theorem [11].

[1] More precisely, the formulation Eqn. (2.6) in [8] advocates particle advection in an approximated velocity field based on a generic kernel. Taking this kernel to be ψ yields the advection field $\bar{\mathbf{u}}(\boldsymbol{X}_{\boldsymbol{k}})$.

4 Vorticity Conservation Properties of SPH

Circulation is conserved, using SPH, for an interpolated velocity field $\mathbf{u}(\boldsymbol{X})$ defined as follows: at time $t = 0$, let $\mathbf{u}(\boldsymbol{X})$ be any initial velocity field satisfying $\mathbf{u}(\boldsymbol{X}_k) = \mathbf{u}_k(0)$ at the particle locations $\boldsymbol{X}_k$. (For example, suppose the particle velocities at $t = 0$ are given as a continuous function.) Define natural labels $\boldsymbol{a} = \boldsymbol{X}(0) = \boldsymbol{x}$ and let the field of particle locations $\boldsymbol{X}(\boldsymbol{a})$ and particle velocities $\mathbf{u}(\boldsymbol{a}) = \mathbf{u}(\boldsymbol{X}(\boldsymbol{a}))$ evolve—under the solution of the SPH flow due to (3.6)—according to the ordinary differential equations (i.e. decoupled in label space)

$$(4.1)\quad \frac{D}{Dt}\mathbf{u} = -c_0 \boldsymbol{\nabla}_{\boldsymbol{X}} \bar{h}(\boldsymbol{X}, t) = -c_0 \sum_k m_k \boldsymbol{\nabla}_{\boldsymbol{X}} \psi(||\boldsymbol{X} - \boldsymbol{X}_k(t)||), \qquad \frac{D}{Dt}\boldsymbol{X} = \mathbf{u}.$$

Note that for this velocity field it *does* hold that $\mathbf{u}(\boldsymbol{X}_k) = \mathbf{u}_k$ for all time t, in contrast to the approximated velocity field $\bar{\mathbf{u}}(\boldsymbol{x})$ of the continuity equation (3.4). Figure 4.1 illustrates the relationship between the velocity fields $\mathbf{u}$ and $\bar{\mathbf{u}}$.

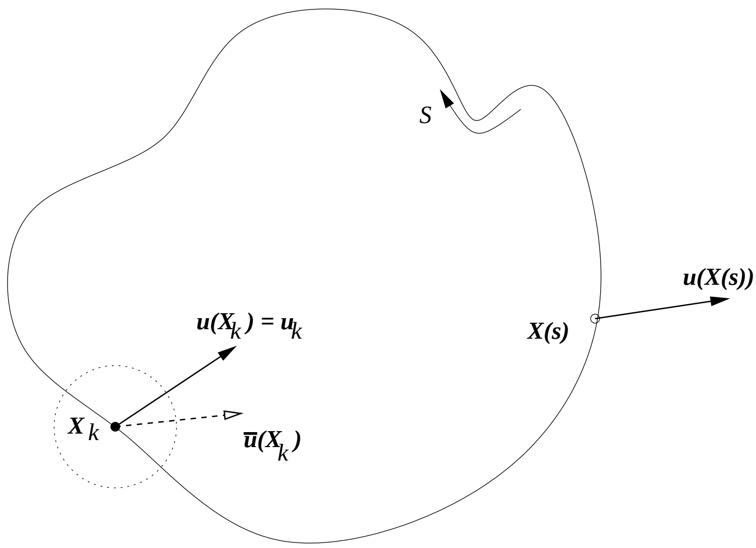

Figure 4.1: A closed curve $\boldsymbol{X}(s)$ advected with the flow, illustrating the velocity fields $\mathbf{u}$ and $\bar{\mathbf{u}}$. The SPH particle at $\boldsymbol{X}_k$ (support indicated by the dotted line) with velocity $\boldsymbol{u}_k$ remains on the curve throughout the integration.

Now, we define a curve of Lagrangian points $\boldsymbol{X}(s) = \boldsymbol{X}(\boldsymbol{a}(s))$ with $s \in S^1$ and $\mathcal{S} = \{\boldsymbol{a}(s)\}_{s \in S^1}$ being a closed loop in label space. The associated loop $\{\boldsymbol{X}(s)\}_{s \in S^1}$ in configuration space is propagated in the velocity field $\mathbf{u}(s) = \mathbf{u}(\boldsymbol{X}(s))$ according to

$$\frac{D}{Dt}\boldsymbol{X}(s) = \mathbf{u}(s).$$

We assume that $\boldsymbol{X}(s)$ and $\mathbf{u}(s)$ are sufficiently differentiable. Then Kelvin's circulation theorem (2.3) becomes

$$\frac{d}{dt}\oint \mathbf{u}\cdot \boldsymbol{X}_s\,ds = 0. \tag{4.2}$$

Indeed, we obtain

$$\begin{aligned}
\frac{d}{dt}\oint \mathbf{u}\cdot \boldsymbol{X}_s\,ds &= \oint \left(\frac{D}{Dt}\mathbf{u}\right)\cdot \boldsymbol{X}_s\,ds + \oint \mathbf{u}\cdot\left(\frac{\partial}{\partial s}\frac{D}{Dt}\boldsymbol{X}\right)ds\\
&= -c_0\oint \boldsymbol{\nabla}_{\boldsymbol{X}}\bar{h}\cdot \boldsymbol{X}_s\,ds + \oint \mathbf{u}\cdot\mathbf{u}_s\,ds\\
&= \oint\left(\frac{1}{2}(\mathbf{u}\cdot\mathbf{u})_s - c_0\bar{h}_s\right)ds\\
&= 0.
\end{aligned}$$

It is important to notice that the circulation theorem above induces a true constraint on the numerical solution, since any SPH particle that is initially located on the loop $\mathcal{S}$ will remain on the loop as the integration proceeds, and furthermore, the particle velocity $\mathbf{u}_k$ will be exactly interpolated by $\mathbf{u}(\boldsymbol{X}_k)$.

If we now give each particle inside $\mathcal{S}$ a label $\boldsymbol{a}$ and let $\mathcal{V}$ denote the area enclosed by $\mathcal{S}$ and let $\mathcal{R}$ denote the image of $\mathcal{V}$ in $\boldsymbol{x}$-space, then applying Stokes' theorem to (4.2) yields

$$\frac{d}{dt}\int_{\mathcal{V}}(\boldsymbol{\nabla}_{\boldsymbol{X}}\times\mathbf{u})|\boldsymbol{X}_a|\,d\boldsymbol{a} = \frac{d}{dt}\int_{\mathcal{R}}(\boldsymbol{\nabla}_{\boldsymbol{x}}\times\mathbf{u})\,d\boldsymbol{x} = 0, \tag{4.3}$$

for which the left side implies

$$\frac{D}{Dt}\{(\boldsymbol{\nabla}_{\boldsymbol{X}}\times\mathbf{u})|\boldsymbol{X}_{\boldsymbol{a}}|\} = 0, \tag{4.4}$$

since $\mathcal{V}$ is arbitrary.

Let $h(\boldsymbol{X}(\boldsymbol{a}))$ denote the layer-depth approximation obtained as the solution of the continuity equation (1.2) along the interpolated velocity field $\mathbf{u}(\boldsymbol{X}(\boldsymbol{a}))$. Then $h|\boldsymbol{X}_a| = h_o$ and equation (4.4) implies conservation of the PV field $q = (\boldsymbol{\nabla}_{\boldsymbol{X}}\times\mathbf{u})/h$, i.e. $Dq/Dt = 0$.

Furthermore, applying the transport theorem to the right equality of (4.3), and again noting that $\mathcal{V}$ is arbitrary, yields a continuity equation for the absolute vorticity of the velocity field $\mathbf{u}$:

$$\frac{\partial}{\partial t}\zeta = -\boldsymbol{\nabla}_{\boldsymbol{x}}\cdot(\zeta\mathbf{u}), \quad \zeta = \boldsymbol{\nabla}_{\boldsymbol{x}}\times\mathbf{u},$$

cf. (2.1).

We would add that (4.2) and (4.3) are preserved under time discretization via a splitting as described in the previous section.

For a numerical verification of (4.2) one can represent the loop $\{\boldsymbol{X}(s)\}$ by a sufficient number of particles $\{\hat{\boldsymbol{X}}_l\}$ with associated velocities $\{\hat{\mathbf{u}}_l\}$ satisfying

(4.1). Note that the particles $\{\hat{\boldsymbol{X}}_l\}$ may be computed along with the SPH simulation as passive tracers with zero mass. The integral (4.2) is approximated by

$$\oint \mathbf{u} \cdot \boldsymbol{X}_s \, ds \approx \sum_l \hat{\mathbf{u}}_l \cdot (\hat{\boldsymbol{X}}_{l+1} - \hat{\boldsymbol{X}}_l). \tag{4.5}$$

One should observe that the variation of this integral in time converges to zero as the number of points discretizing the loop is increased. Such a verification is included in §5 for the Hamiltonian Particle-Mesh method. Monaghan [10] motivates the approximate conservation of (4.5), appealing to Noether's theorem for a discrete relabeling (change of index) of particles of equal mass. This reasoning is limited because Noether's theorem applies only to continuous symmetries. However, our result shows that the approximate conservation of (4.5) is an implication of a stronger result, namely the exact conservation of (4.2).

We have seen that the PV field $q = (\boldsymbol{\nabla}_{\boldsymbol{X}} \times \mathbf{u})/h$ is exactly conserved in SPH. It is also easy to verify that the product $hf(q)$, where f is an arbitrary function of q, exactly satisfies the continuity equation (1.2) in the interpolated velocity field $\boldsymbol{u}(\boldsymbol{X})$. For diagnostic purposes, one can obtain a computable continuous approximation of $hf(q)$ by again taking a sufficient number of passive tracer particles $\{\hat{\boldsymbol{X}}_l\}$ with associated velocities $\{\hat{\mathbf{u}}_l\}$ satisfying (4.1). Following the discussion for the layer-depth $\bar{h}$ in §3, we define a continuous approximation

$$\overline{hf(q)}(\boldsymbol{x}, t) = \sum_l \alpha_l \psi(\boldsymbol{x} - \hat{\boldsymbol{X}}_l(t).$$

Given a particle mass m_l and PV value q_l for each tracer particle $\hat{\boldsymbol{X}}_l$, as determined by the initial data, the weights $\{\alpha_l\}$ can be defined by $\alpha_l = m_l f(q_l)$. It is straightforward to show that $\overline{hf(q)}$ satisfies a modified continuity equation of type (3.5). Under periodic boundary conditions, this continuity equation implies the exact conservation of the generalized enstrophies

$$\mathcal{Q}_f = \int \overline{hf(q)} \, d\boldsymbol{x}.$$

Since this is also true for the split equations of motion used for the time-stepping, the overall space-time approximation conserves enstrophy. The number of tracer particles can be chosen to be quite large if, for example, the statistical/spectral properties of the SPH approximation to hq^2 are of interest.

5 Hamiltonian Particle-Mesh Method and Numerical Verification

The SPH equations of motion are equivalent to the simulation of a molecular fluid with a softened repulsive pair potential given by the SPH basis function $\psi(\boldsymbol{x}) = \Psi(\|\boldsymbol{x}\|)$ [1]. In general, such flows tend to a statistically uniform state of disorder. In practice, therefore, SPH is used with some form of artificial viscosity, and this results in a monotone decrease in circulation along any loop, and a monotone loss of energy.

To improve the stability of SPH, we suggested in [7] working with an averaged SWE

$$\frac{D}{Dt}\boldsymbol{X} = \boldsymbol{u}, \tag{5.1}$$

$$\frac{D}{Dt}\boldsymbol{u} = -c_0 \boldsymbol{\nabla}_{\boldsymbol{X}} (\mathcal{A} * h), \tag{5.2}$$

where $\mathcal{A}$ is some smoothing operator. These equations are still canonical with Hamiltonian

$$\mathcal{H} = \frac{1}{2}\int \frac{\mathbf{p}\cdot\mathbf{p}}{h_o}\, d\boldsymbol{a} + \frac{c_0}{2}\int h(\mathcal{A} * h)\, d\boldsymbol{x} \tag{5.3}$$

and circulation preserving. Let $\{\boldsymbol{X}_k\}$ be an initially equi-distributed set of points with an associated area ΔA. Numerically the layer-depth h is now approximated by the singular measure

$$\tilde{h}(\boldsymbol{x}, t) = \sum_k m_k\, \delta(\boldsymbol{x} - \boldsymbol{X}_k(t)), \qquad m_k = h_o(\boldsymbol{a}_k)\, \Delta A,$$

$\boldsymbol{a}_k = \boldsymbol{X}_k(0)$, which approximates the integral (1.4) in a weak sense. If, for example, $\mathcal{A}$ is chosen to be convolution with the SPH basis function ψ such that

$$(\mathcal{A} * \tilde{h})\,(\boldsymbol{x}, t) = \bar{h}(\boldsymbol{x}, t) = \sum_k m_k \psi(\boldsymbol{x} - \boldsymbol{X}_k(t)),$$

then the layer-depth dependent part of the Hamiltonian (5.3) becomes

$$\frac{c_0}{2}\int \tilde{h}(\mathcal{A} * \tilde{h})\, d\boldsymbol{x} = \frac{c_0}{2}\int \tilde{h}\bar{h}\, d\boldsymbol{x} = \frac{c_0}{2}\sum_{l,k} m_k m_l \psi(\boldsymbol{X}_k - \boldsymbol{X}_l)$$

and the standard SPH method is recovered. However, typical SPH basis functions ψ do not provide enough smoothing, which results in the above mentioned tendency to a state of disorder.

The layer-depth approximation $\tilde{h}$ satisfies the continuity equation (1.2) in a weak sense. Furthermore, the following integral version of (1.3) is easily shown:

$$\int_{\mathcal{V}} \tilde{h}|\boldsymbol{X}_{\boldsymbol{a}}|\, d\boldsymbol{a} = \int_{\mathcal{R}} \tilde{h}\, d\boldsymbol{x} = \sum_{k:\boldsymbol{X}_k \in \mathcal{R}} m_k$$

and

$$\sum_{k:\boldsymbol{X}_k \in \mathcal{R}} m_k \approx \int_{\mathcal{V}} h_o(\boldsymbol{a})\, d\boldsymbol{a}.$$

The set of particles over which the sum is performed is constant provided no particle enters or leaves the domain $\mathcal{R}$ which would correspond to a singular $\boldsymbol{X}_{\boldsymbol{a}}$ and, hence, to a non-physical state.

The Hamiltonian Particle-Mesh method (HPM), introduced in [7], differs from SPH primarily in the construction of the smoothed layer depth $\mathcal{A}*\tilde{h}$. Specifically, we define a uniform grid with grid points $\boldsymbol{x}_{ij}$ and grid spacing Δx. Let $\bar{h}_{\mathrm{SPH}}(\boldsymbol{x},t)$ be the SPH approximation to the layer depth (3.2) with the SPH basis function replaced by a tensor product basis function

$$\psi(\boldsymbol{x}-\boldsymbol{X}_k) := \phi(|x-X_k|)\phi(|y-Y_k|),$$

where $\phi(r)$ is given by the cubic spline

$$\phi(r) = \begin{cases} \frac{2}{3} - r^2 + \frac{1}{2}r^3, & r \le R \\ \frac{1}{6}(2-r)^3, & R < r \le 2R \\ 0, & r > 2R \end{cases}$$

for $R = \Delta x$. Define the gridded layer depth values

$$\bar{h}^{ij}_{\mathrm{SPH}}(t) = \bar{h}_{\mathrm{SPH}}(\boldsymbol{x}_{ij}, t)$$

and let the matrix $\mathbf{S} = \{S^{mn}_{ij}\}$ denote the representation of a spatial averaging operator $\mathcal{S}$ over the given grid $\{\boldsymbol{x}_{ij}\}$. Since the cubic splines form a partition of unity on the grid, we can define a continuous approximation of a smoothed/averaged layer-depth in space

$$(\mathcal{A}*\tilde{h})\,(\boldsymbol{x},t) = \bar{h}_{\mathrm{HPM}}(\boldsymbol{x},t) = \sum_{ij,mn} \bar{h}^{ij}_{\mathrm{SPH}}(t)\, S^{mn}_{ij}\, \psi(\boldsymbol{x}_{mn}-\boldsymbol{x}).$$

This approximation, used in the HPM method, can be viewed as a spatial averaging over short wave-length disturbances in standard SPH. One can also think of the HPM method as an efficient implementation of the SPH method for a globally supported basis function $\tilde{\psi}$ defined by

$$\mathcal{A}*\delta = \tilde{\psi} := \mathcal{S}*\psi,$$

ψ a standard SPH basis function. For a more detailed description of the HPM method, including its Hamiltonian structure, see [7].

The HPM method conserves circulation using the same proof as for SPH in §4. The essential observation is that particles are advected in a velocity field that exactly evolves in some continuous approximate layer depth.

We have performed an experiment with HPM to verify the conservation of circulation. The flow models the interaction of two positively oriented vortices in a rotating reference plane. We discretized this flow using HPM on a 32×32 grid with 128^2 particles. We intentionally chose a fairly coarse discretization for this problem to illustrate that the circulation theorem holds independent of the precision of the discretization.

Initially a circular loop of M evenly spaced particles of zero mass was placed in the flow. The solution including the loop particles was evolved over time intervals of $T=3$, $T=6$ and $T=15$ revolutions of the plane. The experiments were repeated, each time refining the discretization, for $M = 100$, 200, 400, 800 and 1600 particles. The circulation integral was approximated using (cf. (4.5))

$$C_M(t) = \sum_m \hat{\mathbf{u}}_m \cdot (\hat{\boldsymbol{X}}_{m+1} - \hat{\boldsymbol{X}}_{m-1})$$

Figure 5.1 shows the deformation of the loop at time $T = 15$, computed using $M = 3200$ particles. The loop is superimposed over a contour plot of potential vorticity, and its interior is shaded. In Figure 5.2 we see second order convergence of $(C_M(t) - C_M(0))/C_M(0)$ to zero as M increases. Convergence of this sum as $M \to \infty$ is implied by (4.2).

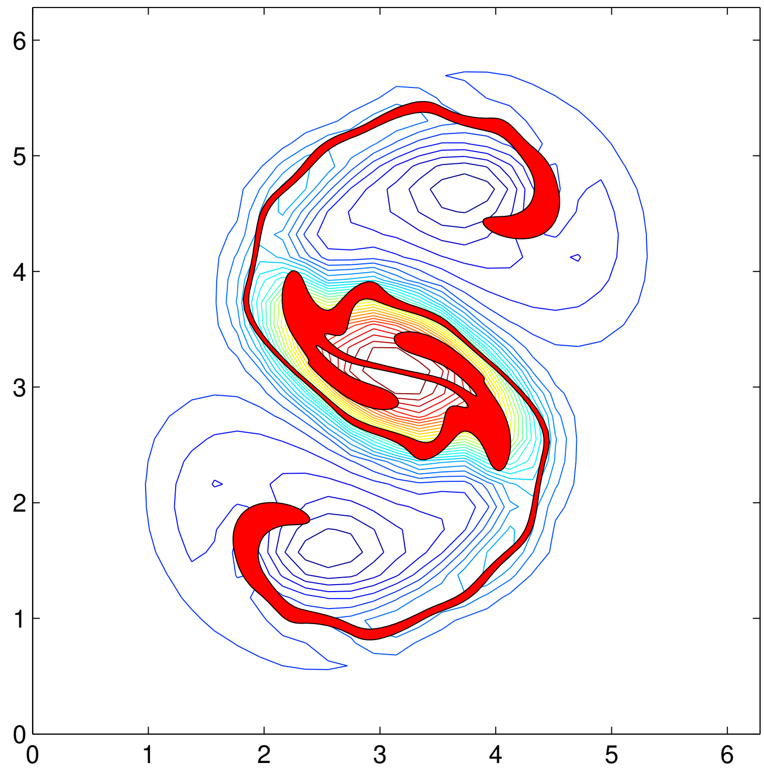

Figure 5.1: Final deformation of the circular loop at time $T = 15$, using $M = 3200$ particles.

6 Concluding Remarks

In this article, we have shown that the SPH method with (3.6) satisfies a Kelvin circulation law. The results are based on the introduction of a continuous velocity field $\boldsymbol{u}(\boldsymbol{X})$ which interpolates the particle velocities $\boldsymbol{u}_k$ for all time

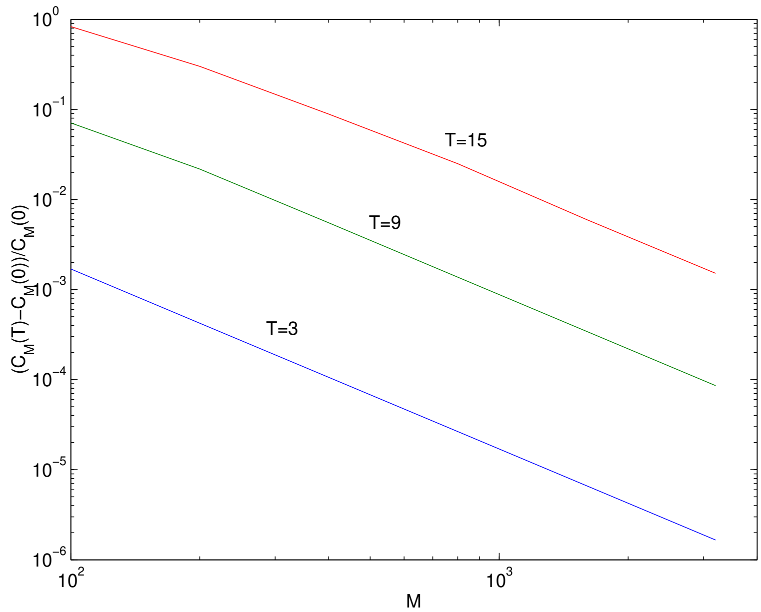

Figure 5.2: Convergence of the discretization of the circulation integral.

and is advected in the flow of the continuous SPH approximation (4.1). This velocity field conserves circulation (4.2) and, by Stokes' theorem, absolute vorticity (4.3). Furthermore, we can formally define a layer depth approximation h such that h satisfies the continuity equation (1.2) in the interpolated velocity field. Defining the potential vorticity with respect to this layer depth yields exact PV conservation.

One can expect a particle method to converge to the solutions of the averaged SWEs (5.1)-(5.2) for an appropriate smoothing operator $\mathcal{A}$ and in the limit of large particle numbers. The necessary amount of regularity and the impact of the smoothing operator $\mathcal{A}$ on the long term dynamics of the SWEs are not yet clear.

The results of this paper easily generalize to the rotating SWEs

$$\begin{aligned} \frac{D}{Dt}\mathbf{u} &= -f_0\mathbf{u}^{\perp} - c_0\boldsymbol{\nabla}_{\boldsymbol{x}}h, \\ \frac{D}{Dt}h &= -h\boldsymbol{\nabla}_{\boldsymbol{x}}\cdot\mathbf{u}, \end{aligned}$$

where $\mathbf{u}^{\perp} = (-v, u)^T$ and $f_0/2$ is the angular velocity of the reference plane. Potential vorticity is now defined by

$$q = \frac{\boldsymbol{\nabla}_{\boldsymbol{x}} \times \mathbf{u} + f_0}{h}$$

and Kelvin's circulation theorem becomes

$$\begin{aligned} 0 &= \frac{D}{Dt}\oint \left(\mathbf{u} + \frac{f_0}{2}\boldsymbol{X}^{\perp}\right)\cdot \boldsymbol{X}_s\,ds \\ &= \frac{D}{Dt}\int_{\mathcal{V}} \left(\boldsymbol{\nabla}_{\boldsymbol{X}}\times \mathbf{u} + f_0\right)|\boldsymbol{X}_{\boldsymbol{a}}|\,d\boldsymbol{a} \\ &= \frac{D}{Dt}\int_{\mathcal{R}} \left(\boldsymbol{\nabla}_{\boldsymbol{x}}\times \mathbf{u} + f_0\right)\,d\boldsymbol{x}. \end{aligned}$$

We wish to mention the Balanced Particle-Mesh (BPM) method of [6] which uses radial basis functions to approximate the absolute vorticity $\omega = \boldsymbol{\nabla}_{\boldsymbol{x}}\times\mathbf{u} + f_0$. See [6] for the geometric properties of the BPM method.

Kelvin's circulation theorem also applies to three-dimensional ideal fluids while conservation of PV takes a more complicated form (see [12]). Again, conservation of circulation can be shown for the SPH method in the same manner as outlined in this note for two-dimensional fluids. In fact, the concept of circulation even applies to molecular simulations of a mono-atomic liquid [1] with Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\sum_k ||\mathbf{p}_k||^2 + \sum_{l>k}\phi(||\boldsymbol{X}_k - \boldsymbol{X}_l||),$$

where m is the atomic mass and $\phi(r)$ an interaction potential. We introduce the function

$$\rho(\boldsymbol{x},t) = \sum_l \phi(||\boldsymbol{x} - \boldsymbol{X}_l(t)||), \qquad \boldsymbol{x}\in\mathbb{R}^3,$$

and note that Newton's law is equivalent to

$$\frac{D}{Dt}\mathbf{p}_k = -\boldsymbol{\nabla}_{\boldsymbol{X}_k}\mathcal{H} = -\boldsymbol{\nabla}_{\boldsymbol{x}}\rho(\boldsymbol{x} = \boldsymbol{X}_k, t).$$

We also have

$$\frac{D}{Dt}\boldsymbol{X}_k = \frac{1}{m}\mathbf{p}_k.$$

Applying the notations of §4 and defining $\mathbf{u} = \mathbf{p}/m$, we obtain the circulation theorem

$$\frac{D}{Dt}\oint \mathbf{u}\cdot\boldsymbol{X}_s\,ds = 0$$

and, in two dimensions, conservation of vorticity per control area, i.e.,

$$\frac{D}{Dt}\int_{\mathcal{R}}(\boldsymbol{\nabla}_{\boldsymbol{x}}\times\mathbf{u})\,d\boldsymbol{x}.$$

One should keep in mind that $\phi(r)$ is often singular at $r = 0$ and, hence, $\rho(\boldsymbol{x},t)$ is not defined for $\boldsymbol{x} = \boldsymbol{X}_k$. However, one can replace $\phi(r)$ by a smooth truncation $\bar{\phi}(r)$ such that $\bar{\phi}(r) = \phi(r)$ for $r \geq r_o$ and $\bar{\rho}'(0) = 0$, $\bar{\rho}(0) < \infty$. Here r_o is chosen such that $||\boldsymbol{X}_i(t) - \boldsymbol{X}_j(t)|| > r_o$ for all $t \geq 0$ and all $i \neq j$. One should also note that, contrary to fluid dynamics, the product $\rho|\boldsymbol{X}_a|$ need not to be approximately conserved and that $\boldsymbol{X}_{\boldsymbol{a}}$ can become singular.

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