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Conservation properties of smoothed particle hydrodynamics applied to the shallow water equations

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Conservation Properties of Smoothed Particle Hydrodynamics Applied to the Shallow Water Equations

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ABSTRACT

Conservation of potential vorticity (PV) and Kelvin's circulation theorem express two of the fundamental concepts in ideal fluid dynamics. In this note, we discuss these two concepts in the context of the Smoothed Particle Hydrodynamics (SPH) method. We show that, if interpreted in an appropriate way, one can make a statement about conservation of circulation and PV in a particle fluid model such as SPH. We also indicate some limitations where the analogy with ideal fluid dynamics breaks down.

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1. INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) [7, 10] is a popular particle based method for computational fluid dynamics. It is well-known that the SPH method can be derived from a variational principle (see, e.g., [10]) or, in other words, can be given a Hamiltonian structure. In this note, we address the important question of conservation of potential vorticity and circulation in SPH simulations. These conserved quantities follow from the underlying relabeling symmetry of ideal fluid dynamics and are fundamental to the long-time solution behavior [8]. For simplicity of exposition, we consider the two-dimensional shallow water equations (SWEs):

$$\frac{D}{Dt}\mathbf{u} = -c_0\nabla_{\mathbf{x}}h, \quad (1.1)$$

$$\frac{D}{Dt}h = -h\nabla_{\mathbf{x}}\cdot\mathbf{u}, \quad (1.2)$$

where $\mathbf{u} = (u, v)^T$ is the horizontal velocity field, h is the layer depth, $c_0 > 0$ is an appropriate constant, and $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}}$ is the material time derivative.

2. CONSERVED QUANTITIES IN IDEAL SHALLOW WATER FLOWS

The SWEs (1.1)-(1.2) possess a number of conserved quantities which are important for the long-time dynamics. Let us start with the vorticity $\zeta = \nabla_{\mathbf{x}} \times \mathbf{u}$. Using

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

it is easy to conclude that vorticity satisfies the continuity equation

$$\frac{D}{Dt}\zeta = -\zeta \nabla_{\mathbf{x}} \cdot \mathbf{u}. \quad (2.1)$$

The ratio of ζ to h , i.e., $q = \zeta/h$, is called the potential vorticity (PV) [8]. The PV field q is materially conserved since

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

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

$$\frac{\partial}{\partial t}[hf(q)] = -\nabla_{\mathbf{x}} \cdot [hf(q)\mathbf{u}], \quad (2.2)$$

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

Next we introduce fluid particle labels $\mathbf{a} = (a, b) \in \mathbb{R}^2$ and define particle positions $\mathbf{x}(\mathbf{a}, t) \in \mathbb{R}^2$ via a diffeomorphism. The labels are fixed for each particle [8], i.e.

$$\frac{D}{Dt}\mathbf{a} = \mathbf{0}.$$

The determinant of the 2×2 Jacobian matrix

$$\mathbf{x}_{\mathbf{a}} = \frac{\partial(x, y)}{\partial(a, b)}$$

satisfies

$$h |\mathbf{x}_{\mathbf{a}}| = h_o,$$

where $h_o(\mathbf{a})$ is a time-independent function [8].

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

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

Kelvin's circulation theorem [8] states that

$$\frac{d}{dt} \oint \mathbf{u} \cdot \mathbf{x}_s ds = 0. \quad (2.3)$$

Indeed, we obtain

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

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

$$\frac{d}{dt} \int_{\mathcal{A}} (\nabla_{\mathbf{x}} \times \mathbf{u}) |\mathbf{x}_{\mathbf{a}}| da \wedge db = \frac{d}{dt} \int_{\mathcal{R}} (\nabla_{\mathbf{x}} \times \mathbf{u}) dx \wedge dy = 0. \quad (2.4)$$

Since \mathcal{A} is arbitrary, the left side of this equation yields another statement of PV conservation since

$$(\nabla_{\mathbf{x}} \times \mathbf{u})|_{\mathbf{x}_a} = h_o \frac{\zeta}{h} = h_o q,$$

and $Dh_o/Dt = 0$. Similarly, after applying the transport theorem [4] to the right equality in (2.4), a second appeal to the arbitrariness of \mathcal{A} yields the vorticity equation (2.1).

The SWEs also conserve energy

$$\mathcal{E} = \frac{1}{2} \int h_o \{\mathbf{u} \cdot \mathbf{u} + c_0 h\} da \wedge db = \frac{1}{2} \int h \{\mathbf{u} \cdot \mathbf{u} + c_0 h\} dx \wedge dy$$

and the symplectic two-form $\bar{\omega} := \int (d\mathbf{u} \wedge d\mathbf{x}) da \wedge db$ [8].

3. RADIAL BASIS FUNCTIONS AND SMOOTHED PARTICLE HYDRODYNAMICS

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

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

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

$$\frac{\partial}{\partial t} g = -\nabla_{\mathbf{x}} \cdot [g\mathbf{u}],$$

can be approximated by

$$g(\mathbf{x}, t) = \sum_k \gamma_k \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|^2).$$

Here $\{\gamma_k\}$ are constants determined by the initial $g(\mathbf{x})$ field and $\psi(r)$ is an appropriate radial basis function [3], for example,

$$\psi(r^2) = \left(\left(\frac{r}{R} \right)^2 + c^2 \right)^{-1/2},$$

$c, R > 0$ two parameters.

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

$$h(\mathbf{x}, t) = \sum_k m_k \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|^2) \tag{3.2}$$

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

$$\rho_k(\mathbf{x}, t) := \frac{m_k \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|^2)}{h(\mathbf{x}, t)} \tag{3.3}$$

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

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

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

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

and a layer depth flux density

$$h(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) = \sum_k m_k \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|^2) \mathbf{U}_k(t).$$

Using (3.1), it is now easily verified that

$$\frac{\partial}{\partial t} h(\mathbf{x}, t) + \nabla_{\mathbf{x}} \cdot [h(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)] = 0. \quad (3.5)$$

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 interpolated velocity, i.e $\mathbf{U}_k \neq \mathbf{u}(\mathbf{X}_k)$. We note that the modification suggested in [6] to avoid penetration in SPH corresponds¹ 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

$$\frac{d}{dt} \mathbf{U}_k = -c_0 \nabla_{\mathbf{x}} h(\mathbf{x} = \mathbf{X}_k, t) = -c_0 \sum_j m_j \nabla_{\mathbf{X}_k} \psi(\|\mathbf{X}_k - \mathbf{X}_j\|^2). \quad (3.6)$$

The equations (3.1), (3.2), and (3.6) are commonly known as a smoothed particle hydrodynamics (SPH) approximation [7] to the SWEs (1.1)-(1.2). A variant of these equations is obtained by replacing (3.6) by

$$\frac{d}{dt} \mathbf{U}_k = -\frac{c_0}{2} \sum_j (m_k + m_j) \nabla_{\mathbf{X}_k} \psi(\|\mathbf{X}_k - \mathbf{X}_j\|^2). \quad (3.7)$$

The equations (3.1), (3.2), and (3.7) are now canonical with Hamiltonian (energy)

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

and symplectic structure $\bar{\omega} = \sum_k d\mathbf{U}_k \wedge d\mathbf{X}_k$. If we assume that the particle locations $\{\mathbf{X}_k\}$ have been chosen such that $m_k = m = \text{const.}$, then (3.6) and (3.7) coincide.

A numerical time-stepping scheme is obtained by noting that

$$\frac{d}{dt} \mathbf{X}_k = \mathbf{U}_k, \quad \frac{d}{dt} \mathbf{U}_k = \mathbf{0}$$

can be solved exactly and that the associated time evolution of $h(\mathbf{x}, t)$ exactly satisfies (3.5). Similarly, equation (3.7) and $\frac{d}{dt} \mathbf{X}_k = \mathbf{0}$ can also be integrated exactly since $h_t = 0$. A composition of these exact propagators leads to a symplectic time-stepping scheme [9] implying good long-time energy conservation [2]. The same approach using (3.6) can be made time-symmetric but is not symplectic, in general.

4. CONSERVATION OF ENSTROPY AND CIRCULATION

The PV field q is materially conserved. This suggests assigning a constant PV value q_k to each particle location \mathbf{X}_k , thereby trivially enforcing the PV conservation law $Dq/Dt = 0$. Using the fractions ρ_k , we obtain the interpolated fields

$$f(q(\mathbf{x}, t)) := \sum_k f(q_k) \rho_k(\mathbf{x}, t), \quad (4.1)$$

¹More precisely, the formulation Eqn. (2.6) in [6] advocates particle advection in an interpolated velocity field based on a generic kernel. Taking this kernel to be ψ yields the advection field $\mathbf{u}(\mathbf{X}_k)$.

where f is again an arbitrary function of q . It is easily verified that the approximation (4.1) satisfies the continuity equation

$$\frac{\partial}{\partial t}[hf(q)](\mathbf{x}, t) = -\nabla_{\mathbf{x}} \cdot \left\{ \sum_k m_k f(q_k) \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|^2) \mathbf{U}_k \right\}$$

corresponding to (2.2). Under the given periodic boundary conditions, this discrete conservation law implies the exact conservation of the generalized enstrophies

$$\mathcal{Q}_f = \int hf(q) dx \wedge dy.$$

Since this is also true for the split equations of motion used for the time-stepping, the overall space-time discretization conserves enstrophy independently of whether (3.6) or (3.7) is used. One should, however, be aware that the product hq is not equivalent to the vorticity of the interpolated velocity field \mathbf{u} as is true for the SWEs. See below.

The circulation is also conserved, but for a different velocity field $\mathbf{U}(\mathbf{x}, t)$ defined as follows: Let $\mathbf{U}(\mathbf{x}, 0)$ be any initial velocity field satisfying $\mathbf{U}(\mathbf{X}_k, 0) = \mathbf{U}_k(0)$ at the particle locations. (For example, suppose the particle velocities at $t = 0$ are given as a continuous function.) And let $\mathbf{U}(\mathbf{x}, t)$ evolve—under the solution of the SPH flow due to (3.6)—according to

$$\frac{D}{Dt} \mathbf{U}(\mathbf{x}) = -c_0 \nabla_{\mathbf{x}} h(\mathbf{x}, t) = -c_0 \sum_k m_k \nabla_{\mathbf{x}} \psi(\|\mathbf{x} - \mathbf{X}_k(t)\|^2).$$

Note that for this velocity field it *does* hold that $\mathbf{U}(\mathbf{X}_k(t)) = \mathbf{U}_k(t)$. Figure 1 illustrates the relationship between the velocity fields \mathbf{u} and \mathbf{U} .

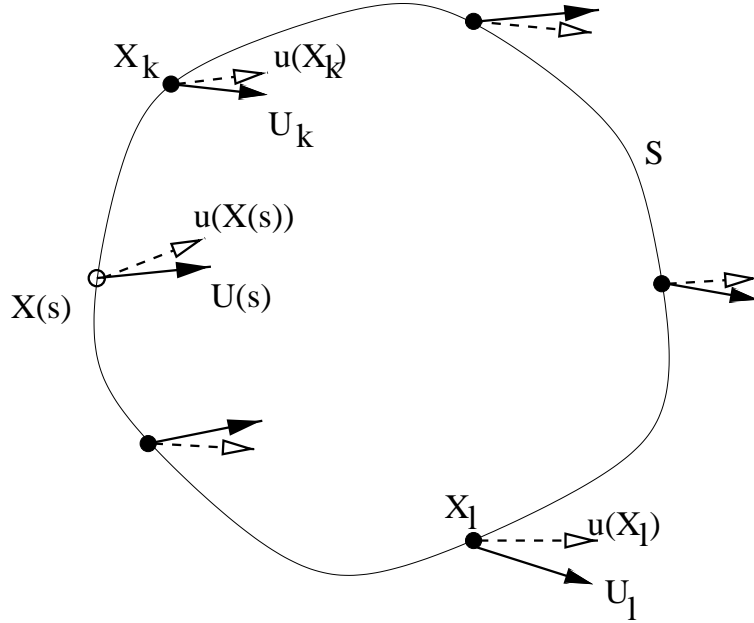


Figure 1: A closed curve advected with the flow, illustrating the velocity fields \mathbf{u} and \mathbf{U} .

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

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

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

$$\frac{d}{dt} \oint \mathbf{U} \cdot \mathbf{X}_s ds = 0. \quad (4.2)$$

Indeed, we obtain

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

This reasoning is no longer valid if the momentum equation (3.7) is used. Conservation of circulation is thus in conflict with conservation of symplectic structure.

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

$$\frac{d}{dt} \int_{\mathcal{A}} (\nabla_{\mathbf{x}} \times \mathbf{U}) | \mathbf{X}_{\mathbf{a}} | da \wedge db = \frac{d}{dt} \int_{\mathcal{R}} (\nabla_{\mathbf{x}} \times \mathbf{U}) dx \wedge dy = 0, \quad (4.3)$$

for which the left side implies

$$\frac{D}{Dt} \{ (\nabla_{\mathbf{x}} \times \mathbf{U}) | \mathbf{X}_{\mathbf{a}} | \} = 0, \quad (4.4)$$

since \mathcal{A} is arbitrary. Note that, in principle, the determinant $| \mathbf{X}_{\mathbf{a}} |$ can be computed along a given particle path $\mathbf{X}_k(t)$ by integrating the linearized SPH equations along $\mathbf{X}_k(t)$. However, the product of $| \mathbf{X}_{\mathbf{a}} |$ and h is not equivalent to a time-independent function $h_o(\mathbf{a})$ and, hence, equation (4.4) is not equivalent to conservation of PV in the standard sense, i.e. $Dq/Dt = 0$.

Applying the transport theorem to the right equality of (4.3), and again noting that \mathcal{A} is arbitrary, yields a continuity equation for the relative vorticity of the velocity field \mathbf{U} :

$$\zeta_t = -\nabla_{\mathbf{x}} \cdot (\zeta \mathbf{U}), \quad \zeta = \nabla_{\mathbf{x}} \times \mathbf{U},$$

cf. (2.1). However, the vorticity $\zeta(\mathbf{x}, t)$ will be different from the quantity

$$h(\mathbf{x}, t) q(\mathbf{x}, t) = \sum_k q_k m_k \psi(\| \mathbf{x} - \mathbf{X}_k(t) \|^2),$$

even if the two are initially equal, because the latter is advected by the interpolated velocity field \mathbf{u} . Hence the agreement between \mathbf{u} and \mathbf{U} is a fundamental measure of the quality of an SPH simulation.

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 has to represent the loop $\{ \mathbf{X}(s) \}$ by a sufficient number of particles $\{ \bar{\mathbf{X}}_l \}$ with associated velocities $\{ \bar{\mathbf{U}}_l \}$. The integral (4.2) is then approximated by

$$\oint \mathbf{U} \cdot \mathbf{X}_s ds \approx \sum_l \bar{\mathbf{U}}_l \cdot (\bar{\mathbf{X}}_{l+1} - \bar{\mathbf{X}}_l).$$

Note that the particles $\{ \bar{\mathbf{X}}_l \}$ are not part of the SPH discretization but are instead obtained via "post-processing" of the SPH solutions.

5. CONCLUDING REMARKS

In this note, we have shown that the SPH method with (3.6) satisfies a Kelvin circulation law. However, conservation of circulation is in conflict with conservation of symplecticness unless the weights m_k are all equal. We have also shown that conservation of circulation implies a form of PV conservation and that the generalized enstrophies \mathcal{Q}_f are also preserved. Note that the numerical approximations do not, in general, satisfy the fundamental relations $\zeta = hq$ and $h|\mathbf{x}_\alpha| = h_o$. The consequences of this limitation require further investigations.

The results of this paper easily generalize to the rotating SWEs

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

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

$$q = \frac{\nabla_{\mathbf{x}}\times\mathbf{u} + f_0}{h}$$

and Kelvin's circulation theorem becomes

$$\frac{d}{dt}\oint\left(\mathbf{u} + \frac{f_0}{2}\mathbf{x}^\perp\right)\cdot\mathbf{x}_s ds = \frac{d}{dt}\int_{\mathcal{A}}(\nabla_{\mathbf{x}}\times\mathbf{u} + f_0)|\mathbf{x}_\alpha| da \wedge db = \frac{d}{dt}\int_{\mathcal{R}}(\nabla_{\mathbf{x}}\times\mathbf{u} + f_0) dx \wedge dy = 0.$$

We wish to mention the Balanced Particle-Mesh (BPM) method of [5] which uses radial basis functions to approximate the absolute vorticity $\omega = \nabla_{\mathbf{x}}\times\mathbf{u} + f_0$. See [5] 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 [8]). 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

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

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

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

and note that Newton's law is equivalent to

$$\frac{d}{dt}\mathbf{P}_k = -\nabla_{\mathbf{X}_k}\mathcal{H} = -\nabla_{\mathbf{x}}\rho(\mathbf{x} = \mathbf{X}_k, t).$$

We also have

$$\frac{d}{dt}\mathbf{X}_k = \frac{1}{m}\mathbf{P}_k.$$

Applying the notations of §4 and replacing \mathbf{U} by \mathbf{P} , we obtain the circulation theorem

$$\frac{d}{dt}\oint\mathbf{P}\cdot\mathbf{X}_s ds = 0$$

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

$$\frac{d}{dt}\int_{\mathcal{R}}(\nabla_{\mathbf{x}}\times\mathbf{P}) dx \wedge dy.$$

One should keep in mind that $\phi(r)$ is often singular at $r = 0$ and, hence, $\rho(\mathbf{x}, t)$ is not defined for $\mathbf{x} = \mathbf{X}_k$. 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 $\bar{\phi}'(0) = 0$, $\bar{\rho}(0) < \infty$. Here r_o is chosen such that $\|\mathbf{X}_i(t) - \mathbf{X}_j(t)\| > r_o$ for all $t \geq 0$ and all $i \neq j$.

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