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Contributions to Vortex Particle Methods for the Computation of Three-Dimensional Incompressible Unsteady Flows

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Recent contributions to vortex particle methods for the computation of three-dimensional incompressible unsteady flows are presented. Both singular and regularized vortex particle methods are reviewed, along with an investigation of different evolution equations for the particle strength vector. For the regularized method, a new algebraic smoothing is presented with convergence properties equal to those of Gaussian smoothing. A version of the regularized method which can account for viscous diffusion is developed using a scheme that redistributes the particle strength vectors. Finally, particle methods are investigated with respect to conservation laws, and new expressions for the quadratic diagnostics, energy, helicity, and enstrophy are derived.

1. INTRODUCTION

The momentum equation for a constant-density fluid can be written as

$$\frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\omega} \times \mathbf{u} = -\nabla\left(\frac{p}{\rho} + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right) + \nu\,\nabla^2\mathbf{u}, \qquad (1)$$

where $\mathbf{u}(\mathbf{x}, t)$ is the velocity field, $\boldsymbol{\omega}(\mathbf{x}, t) = \nabla \times \mathbf{u}(\mathbf{x}, t)$ is the vorticity field, $p(\mathbf{x}, t)$ is the pressure field, ρ is the density, and ν is the kinematic viscosity. The vorticity equation is obtained by taking the curl of Eq. (1),

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + \nabla \times (\boldsymbol{\omega} \times \mathbf{u}) = \nu\,\nabla^2\boldsymbol{\omega}, \qquad (2)$$

or equivalently,

$$\frac{D\boldsymbol{\omega}}{Dt} = \frac{\partial \boldsymbol{\omega}}{\partial t} + (\mathbf{u}\cdot\nabla)\,\boldsymbol{\omega} = (\boldsymbol{\omega}\cdot\nabla)\,\mathbf{u} + \nu\,\nabla^2\boldsymbol{\omega}. \qquad (3)$$

Recalling that the evolution equation for a material line element $\delta\mathbf{l}$ is given by (Batchelor [4])

$$\frac{D\,\delta\mathbf{l}}{Dt} = (\delta\mathbf{l}\cdot\nabla)\,\mathbf{u}, \qquad (4)$$

it follows that, for inviscid flows, vortex lines move as material lines (Helmholtz). A vortex tube is defined as the collection of vortex lines that pierce a given surface patch S. The circulation of a vortex tube is $\Gamma = \int_S \boldsymbol{\omega}\cdot d\mathbf{x} = \int_{\partial S} \mathbf{u}\cdot d\mathbf{x}$. Because $\nabla\cdot\boldsymbol{\omega} = 0$, the circulation of a vortex tube is the same for all oriented surface patches that define the vortex tube (Helmholtz). For inviscid flows, the circulation of a vortex tube is conserved (Kelvin). Vortex tubes are thus interesting entities in inviscid flows: they move as material volumes and they retain their circulation; i.e., they preserve their identity. These facts form the basis for the method of vortex filaments (see Leonard [30, 31] for reviews). For viscous flows, the concept of vortex tubes is not as useful. One can define vortex tubes at every instant and associate to each vortex tube a unique circulation. This is kinematics only, however. Vortex tubes do not necessarily retain their identity because of the possibility of reconnection of vortex tubes by viscous diffusion.

This paper is written from work which was part of a Ph.D. thesis (Winckelmans and Leonard [43, 44]; Winckelmans [45]). It is concerned with vortex particle methods for the computation of three-dimensional (3D) incompressible unsteady flows, both inviscid and viscous. Vortex particles, also called *vortex sticks* or *vortons*, are an alternative to the use vortex filaments. A position vector and a strength vector (= vorticity × volume) is associated to each element. Each element can be thought of as a small section of a vortex tube (= circulation × length). The element is convected by the local velocity and the strength vector is strained by the local velocity gradient. The method has the advantage that the particles are somewhat independent as they do not necessarily belong to a specific vortex filament for all times. This property also makes the method attractive because treatment of viscous diffusion using a scheme developed by Mas-Gallic [32], and Degond and Mas-Gallic [22] can be incorporated in the method (see also Fishelov [23] for an alternative way of incorporating diffusion in the method). With that scheme, processes involving the reconnection of vortex tubes (such as the fusion of two vortex rings) can be computed. The particle method presents, however, a problem: the particle representation of

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the vorticity field is not guaranteed to remain a good representation of a divergence-free field for all times. This issue is also addressed. In particular, a relaxation scheme is proposed which forces the particle vorticity field to remain nearly divergence-free for all times.

The paper is organized as follows: use of δ-function particles and weak solutions of the vorticity equation (Section 2); use of regularized particles and choice of the regularization function (Section 3); viscous diffusion by the redistribution of element strengths (Section 4); and conservation laws—how to evaluate them—are they satisfied? (Section 5 and Appendix C). Numerical results are also presented for the interaction of vortex rings.

2. SINGULAR VORTEX PARTICLES

The vorticity equation, Eq. (3), is a nonlinear transport equation which can be solved using a particle method (see, e.g., Raviart [37, 38]). In the singular vortex particle method (also called method of *point vortices* or *vortex sticks* or *vortons*: Rehbach [39], Chorin [9, 10], Saffman [41], Leonard [30, 31], Novikov [35], Aksman, Novikov, and Orszag [1], Anderson and Greengard [2], Mosher [34], Saffman and Meiron [42], Winckelmans and Leonard [43, 44], Winckelmans [45]), the particle representation of the vorticity field is taken as

$$\tilde{\boldsymbol{\omega}}(\mathbf{x}, t) = \sum_p \boldsymbol{\omega}^p(t)\, vol^p\, \delta(\mathbf{x} - \mathbf{x}^p(t)) = \sum_p \boldsymbol{\alpha}^p(t)\, \delta(\mathbf{x} - \mathbf{x}^p(t)), \tag{5}$$

where $\delta(\mathbf{x})$ is the 3D δ-function. The velocity field $\mathbf{u}(\mathbf{x}, t)$ is computed from $\tilde{\boldsymbol{\omega}}(\mathbf{x}, t)$ as the curl of a streamfunction which solves $\nabla^2 \tilde{\boldsymbol{\psi}}(\mathbf{x}, t) = -\tilde{\boldsymbol{\omega}}(\mathbf{x}, t)$. Recalling that the Green's function for $-\nabla^2$ in unbounded domain is $G(\mathbf{x}) = 1/(4\pi\,|\mathbf{x}|)$,

$$\tilde{\boldsymbol{\psi}}(\mathbf{x}, t) = G(\mathbf{x}) * \tilde{\boldsymbol{\omega}}(\mathbf{x}, t) = \sum_p G(\mathbf{x} - \mathbf{x}^p(t))\, \boldsymbol{\alpha}^p(t) = \frac{1}{4\pi} \sum_p \frac{\boldsymbol{\alpha}^p(t)}{|\mathbf{x} - \mathbf{x}^p(t)|}, \tag{6}$$

where $*$ stands for the convolution product. The velocity is obtained as

$$\begin{aligned}\mathbf{u}(\mathbf{x}, t) &= \nabla \times \tilde{\boldsymbol{\psi}}(\mathbf{x}, t) = \sum_p \nabla(G(\mathbf{x} - \mathbf{x}^p(t))) \times \boldsymbol{\alpha}^p(t) \\ &= -\frac{1}{4\pi} \sum_p \frac{1}{|\mathbf{x} - \mathbf{x}^p(t)|^3} (\mathbf{x} - \mathbf{x}^p(t)) \times \boldsymbol{\alpha}^p(t) \\ &= \sum_p \mathbf{K}(\mathbf{x} - \mathbf{x}^p(t)) \times \boldsymbol{\alpha}^p(t) \\ &= (\mathbf{K}(\mathbf{x}) \times) * \tilde{\boldsymbol{\omega}}(\mathbf{x}, t) \\ &= -\frac{1}{4\pi\,|\mathbf{x} - \mathbf{x}^p(t)|^3} (\mathbf{x} - \mathbf{x}^p(t)) \times \boldsymbol{\alpha}^p(t) + \mathbf{u}^p(\mathbf{x}, t),\end{aligned} \tag{7}$$

where $\mathbf{K}(\mathbf{x}) \times = -(\mathbf{x}/(4\pi\,|\mathbf{x}|^3)) \times$ is the Biot–Savart kernel and where $\mathbf{u}^p(\mathbf{x}, t)$ stands for the velocity field without the contribution of the p particle.

A few remarks should be made at this point:

- The particle field (5) is not generally divergence-free:

$$\nabla \cdot (\tilde{\boldsymbol{\omega}}(\mathbf{x}, t)) = \sum_p \nabla(\delta(\mathbf{x} - \mathbf{x}^p(t))) \cdot \boldsymbol{\alpha}^p(t). \tag{8}$$

Thus a "basis" which is not generally divergence-free is used to represent the divergence-free vorticity field $\boldsymbol{\omega}$.

- The streamfunction (6) is also not generally divergence-free:

$$\nabla \cdot (\tilde{\boldsymbol{\psi}}(\mathbf{x}, t)) = -\frac{1}{4\pi} \sum_p \frac{1}{|\mathbf{x} - \mathbf{x}^p(t)|^3} \times ((\mathbf{x} - \mathbf{x}^p(t)) \cdot \boldsymbol{\alpha}^p(t)). \tag{9}$$

This result is a direct consequence of the fact that $\nabla^2 \tilde{\boldsymbol{\psi}} = -\tilde{\boldsymbol{\omega}}$ is solved with $\tilde{\boldsymbol{\omega}}$ not generally divergence-free.

- The velocity field (7) is divergence-free since it is the curl of a streamfunction. Indeed,

$$\nabla \cdot (\mathbf{u}(\mathbf{x}, t)) = \frac{3}{4\pi} \sum_p \frac{1}{|\mathbf{x} - \mathbf{x}^p(t)|^5} (\mathbf{x} - \mathbf{x}^p(t)) \cdot ((\mathbf{x} - \mathbf{x}^p(t)) \times \boldsymbol{\alpha}^p(t)) = 0, \tag{10}$$

since $(\mathbf{x} - \mathbf{x}^p)$ is orthogonal to $(\mathbf{x} - \mathbf{x}^p) \times \boldsymbol{\alpha}^p$. At $\mathbf{x} = \mathbf{x}^p$, the singularity is of removable type so that $\nabla \cdot \mathbf{u} = 0$.

- As noted by Novikov [35], one can reconstruct the divergence-free vorticity field by taking the curl of the velocity field (7):

$$\begin{aligned}\boldsymbol{\omega}(\mathbf{x}, t) &= \nabla \times \mathbf{u}(\mathbf{x}, t) \\ &= \sum_p \left[\boldsymbol{\alpha}^p(t)\, \delta(\mathbf{x} - \mathbf{x}^p(t)) + \nabla\left(\boldsymbol{\alpha}^p(t) \cdot \nabla\left(\frac{1}{4\pi\,|\mathbf{x} - \mathbf{x}^p(t)|} \right) \right) \right]\end{aligned} \tag{11}$$

$$= \sum_p \left[\left(\delta(\mathbf{x} - \mathbf{x}^p(t)) - \frac{1}{4\pi\,|\mathbf{x} - \mathbf{x}^p(t)|^3} \right) \boldsymbol{\alpha}^p(t) + 3\, \frac{((\mathbf{x} - \mathbf{x}^p(t)) \cdot \boldsymbol{\alpha}^p(t))}{4\pi\,|\mathbf{x} - \mathbf{x}^p(t)|^5} (\mathbf{x} - \mathbf{x}^p(t)) \right]. \tag{12}$$

The added term in Eq. (11) corresponds to that which is needed to close the vortex lines and it decays as $1/r^3$. Thus, $\boldsymbol{\omega} = \nabla \times \mathbf{u} = \nabla \times (\nabla \times \tilde{\boldsymbol{\psi}}) = -\nabla^2 \tilde{\boldsymbol{\psi}} + \nabla(\nabla \cdot \tilde{\boldsymbol{\psi}})$. Recalling that $\nabla^2 \tilde{\boldsymbol{\psi}} = -\tilde{\boldsymbol{\omega}}$, it follows that $\nabla(\nabla \cdot \tilde{\boldsymbol{\psi}}) = \boldsymbol{\omega} - \tilde{\boldsymbol{\omega}}$. The second term in Eq. (11) does not contribute to the Biot–Savart velocity field as it is the gradient of a scalar.

2.1. *Evolution Equations*

In the *classical scheme*, the evolution equations for the particle position and strength vector are taken as

$$\frac{d}{dt}\mathbf{x}^p(t) = \mathbf{u}^p(\mathbf{x}^p(t), t), \tag{13}$$

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t) = (\boldsymbol{\alpha}^p(t) \cdot \nabla)\, \mathbf{u}^p(\mathbf{x}^p(t), t). \tag{14}$$

As noted by Rehbach [39] (see also Cantaloube and Huberson [8], Choquin [12], and Choquin and Cottet [13]), alternative forms of the vorticity equation (3) can be written as

$$\frac{D\boldsymbol{\omega}}{Dt} = (\boldsymbol{\omega} \cdot \nabla^{\mathrm{T}})\, \mathbf{u}, \tag{15}$$

$$= \frac{1}{2}(\boldsymbol{\omega} \cdot (\nabla + \nabla^{\mathrm{T}}))\, \mathbf{u}. \tag{16}$$

This is so because $(\nabla \mathbf{a} - (\nabla \mathbf{a})^{\mathrm{T}}) \cdot \mathbf{b} = (\nabla \times \mathbf{a}) \times \mathbf{b}$ for any vector fields $\mathbf{a}$ and $\mathbf{b}$. Here, we have that $\mathbf{a} = \mathbf{u}$, $\mathbf{b} = \boldsymbol{\omega}$, with $\boldsymbol{\omega} = \nabla \times \mathbf{u}$. Note that $\frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) = \mathrm{Def}(\mathbf{u}) = \{e_{ij}\}$ is the classical deformation tensor. The formulation (15) suggests the *transpose scheme*,

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t) = (\boldsymbol{\alpha}^p(t) \cdot \nabla^{\mathrm{T}})\, \mathbf{u}^p(\mathbf{x}^p(t), t), \tag{17}$$

while the formulation (16) suggests the *mixed scheme*,

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t) = \frac{1}{2}(\boldsymbol{\alpha}^p(t) \cdot (\nabla + \nabla^{\mathrm{T}}))\, \mathbf{u}^p(\mathbf{x}^p(t), t). \tag{18}$$

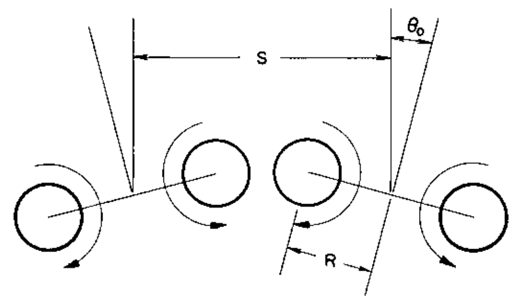

FIG. 1. Initial condition for the computation of the collision of two vortex rings.

This scheme was favored by Rehbach because the symmetry of the deformation tensor yields computational savings. All three schemes would be equivalent if the particle vorticity field, Eq. (5), were equal to the curl of the velocity field (7). Unfortunately, this is not the case as a consequence of the nonzero divergence of the field (5). Thus, although Eqs. (14), (15), and (16) are equivalent when $\boldsymbol{\omega} = \nabla \times \mathbf{u}$, they are not equivalent otherwise. Consequently, Eqs. (14), (17), and (18) may lead to different results when solving the 3D vorticity equation with vortex particles.

The transpose scheme Eq. (17) appears to be special. First, it leads to the exact conservation of the total vorticity (Choquin and Cottet [13]), a property not satisfied by the classical scheme (14) or the mixed scheme (18). Second, it leads to a weak solution of Eq. (15) as shown by Winckelmans and Leonard [43]. (By contrast, the classical scheme does not lead to a weak solution of Eq. (3) (Saffman and Meiron [42]), and the mixed scheme does not lead to a weak solution of Eq. (16).) The proof is however "fragile" because the integrals, evaluated in the principal value sense, are bounded only for a radially symmetric regularization of the δ-function. (Greengard and Thomann [24]). Nevertheless, that property and the conservation of total vorticity lead to the belief that the transpose scheme is more suited than the classical scheme to the representation of 3D flows using vortex singularities. This point is reenforced by numerical results on the inviscid collision of two vortex rings, Figs. 1 to 4 (see also Knio and Ghoniem [28] for a numerical study of the placement of vortex particles within a vortex ring cross section).

Although the computations fail to go through the fusion process (a process which requires viscous diffusion!), the transpose scheme yields a particle field $\tilde{\boldsymbol{\omega}}$ which remains a good representation of $\boldsymbol{\omega}$ for the longest time and hence nearly conserves linear impulse, I, and kinetic energy,

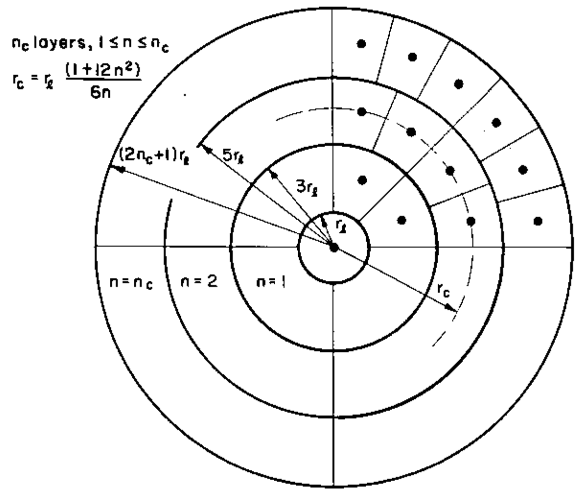

FIG. 2. Discretization of the core of a vortex tube. Each cell has an equal area πr_l^2.

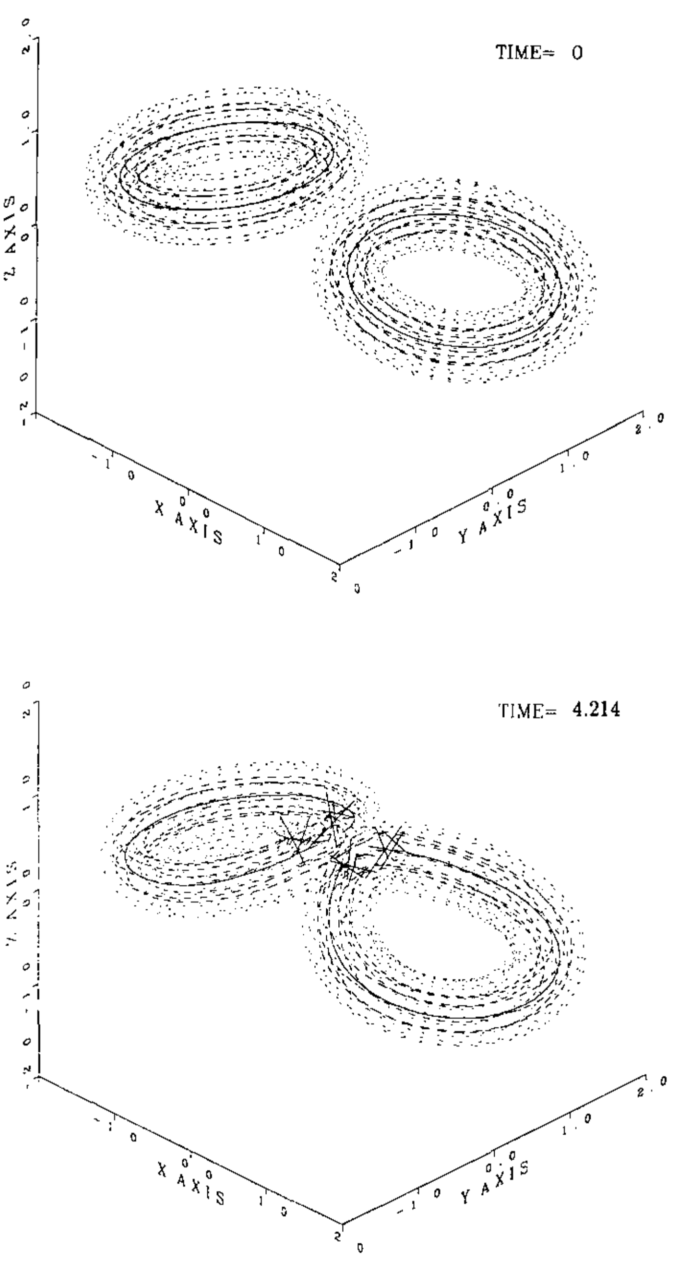

FIG. 3. Collision of two vortex rings computed with the method of singular vortex particles and using the transpose scheme. View of particle strength vectors. Initial conditions: $\Gamma = 1$, $R = 1$, $s = 3$, $\theta_0 = 10°$, $r_l = 0.08$, $n_c = 2(\rightarrow N_s = 25)$, $N_\varphi = 44$, and particle strength vectors in ratio [1 : 0.54 : 0.16].

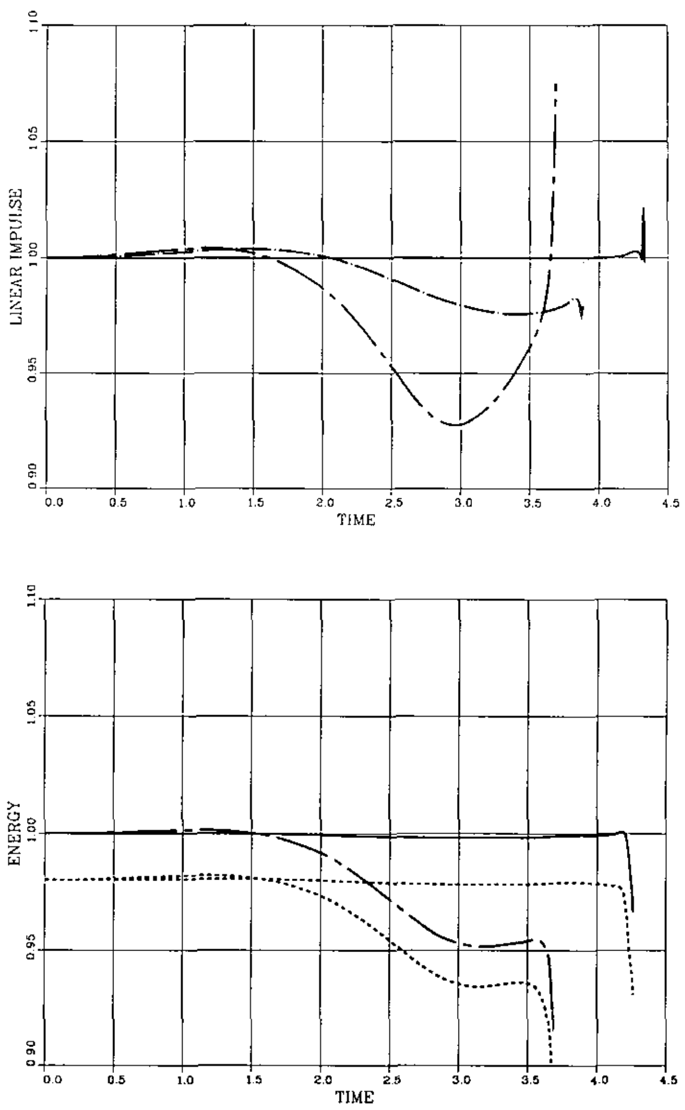

FIG. 4. Collision of two vortex rings computed with the method of singular vortex particles. Diagnostics I, E, and $\tilde{E}$ (dash). Transpose scheme (solid), classical scheme (chain-dash), and mixed scheme (chain-dot).

E_σ, up to numerical blowup (see also Section 5 and Appendix C).

Finally, it should be mentioned that, regardless of the choice for the stretching operator, convergence of the 3D point vortex method to the incompressible Euler equations with smooth solutions was recently proven by Hou and Lowengrub [26], and Cottet, Goodman, and Hou [19]). The method of regularized vortex particles was also shown to converge in 3D and is now considered.

3. REGULARIZED VORTEX PARTICLES

In the regularized version of the vortex particle method, the particle representation of the vorticity field is taken as (Rehbach [39], Chorin [9, 10], Saffman [41], Leonard [30, 31], Beale and Majda [6, 7], Anderson and Greengard [2], Mosher [34], Beale [5], Choquin [12], Cottet [17, 18], Choquin and Cottet [13], Winckelmans and Leonard [43, 44], Chua *et al.* [15], Winckelmans [45], Knio and Ghoniem [28], Chua [16]

$$\begin{aligned}\tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}, t) &= \zeta_\sigma(\mathbf{x}) * \tilde{\boldsymbol{\omega}}(\mathbf{x}, t) \\ &= \sum_p \boldsymbol{\alpha}^p(t)\, \zeta_\sigma(\mathbf{x} - \mathbf{x}^p(t)). \qquad (19)\end{aligned}$$

where ζ_σ is a regularization function which is usually taken as radially symmetric, and σ is a smoothing radius (i.e., a cutoff length or core size), i.e.,

$$\zeta_\sigma(\mathbf{x}) = \frac{1}{\sigma^3}\,\zeta\left(\frac{|\mathbf{x}|}{\sigma}\right), \tag{20}$$

with the normalization

$$4\pi \int_0^\infty \zeta(\rho)\,\rho^2\,d\rho = 1. \tag{21}$$

The velocity field is computed from the particle representation of the vorticity fields as the curl of a streamfunction which solves $\nabla^2 \tilde{\boldsymbol{\psi}}_\sigma(\mathbf{x}, t) = -\tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}, t)$. Defining $G(\rho)$ such that

$$\begin{aligned} -\zeta(\rho) = \nabla^2 G(\rho) &= \frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2 \frac{dG}{d\rho}\right) \\ &= \frac{1}{\rho}\frac{d^2}{d\rho^2}(\rho G(\rho)), \end{aligned} \tag{22}$$

one obtains

$$\begin{aligned} \tilde{\boldsymbol{\psi}}_\sigma(\mathbf{x}, t) = G(\mathbf{x}) * \tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}, t) &= G_\sigma(\mathbf{x}) * \tilde{\boldsymbol{\omega}}(\mathbf{x}, t) \\ &= \sum_p G_\sigma(\mathbf{x} - \mathbf{x}^p(t))\,\boldsymbol{\alpha}^p(t), \end{aligned} \tag{23}$$

where $G_\sigma(\mathbf{x}) = G(|\mathbf{x}|/\sigma)/\sigma$. A function $q(\rho)$ is now defined:

$$q(\rho) = \int_0^\rho \zeta(t)\,t^2\,dt. \tag{24}$$

From the normalization condition (21), $4\pi q(\rho) \to 1$ as $\rho \to \infty$. Since $\zeta(\rho)$ is $\mathcal{O}(1)$ for small ρ, $q(\rho)$ is $\mathcal{O}(\rho^3)$ for small ρ. The following relations between $\zeta(\rho)$, $G(\rho)$, and $q(\rho)$ are useful. First, from the definition of $q(\rho)$,

$$\frac{1}{\rho^2}\frac{d}{d\rho}\,q(\rho) = \zeta(\rho). \tag{25}$$

Second, from the definition of $G(\rho)$ and $q(\rho)$,

$$\begin{aligned} q(\rho) = \int_0^\rho \zeta(t)\,t^2\,dt &= -\int_0^\rho \frac{d}{dt}\left(t^2 \frac{d}{dt} G(t)\right) dt \\ &= -\rho^2 \frac{d}{d\rho} G(\rho), \end{aligned} \tag{26}$$

so that

$$-\frac{1}{\rho}\frac{d}{d\rho}\,G(\rho) = \frac{q(\rho)}{\rho^3}. \tag{27}$$

Finally, from Eq. (25),

$$-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right) = \frac{1}{\rho^2}\left(\zeta(\rho) - 3\,\frac{q(\rho)}{\rho^3}\right). \tag{28}$$

From Eq. (27), $G(\rho)$ is $\mathcal{O}(\rho^2)$ for small ρ and $4\pi G(\rho) \to 1/\rho$ as $\rho \to \infty$. The velocity field is obtained as

$$\begin{aligned} \mathbf{u}_\sigma(\mathbf{x}, t) &= \nabla \times \tilde{\boldsymbol{\psi}}_\sigma(\mathbf{x}, t) \\ &= \sum_p \nabla(G_\sigma(\mathbf{x} - \mathbf{x}^p(t))) \times \boldsymbol{\alpha}^p(t) \\ &= -\sum_p \frac{q_\sigma(\mathbf{x} - \mathbf{x}^p(t))}{|\mathbf{x} - \mathbf{x}^p(t)|^3}(\mathbf{x} - \mathbf{x}^p(t)) \times \boldsymbol{\alpha}^p(t) \\ &= \sum_p \mathbf{K}_\sigma(\mathbf{x} - \mathbf{x}^p(t)) \times \boldsymbol{\alpha}^p(t) \\ &= (\mathbf{K}_\sigma(\mathbf{x}) \times\,) * \tilde{\boldsymbol{\omega}}(\mathbf{x}, t), \end{aligned} \tag{29}$$

where $q_\sigma(\mathbf{x}) = q(|\mathbf{x}|/\sigma)$ and $\mathbf{K}_\sigma(\mathbf{x}) \times\, = -(q_\sigma(\mathbf{x})/|\mathbf{x}|^3)\,\mathbf{x} \times$ is the regularized Biot–Savart kernel.

The evolution equations for the particle position and strength vector are, with the classical scheme, taken as

$$\frac{d}{dt}\mathbf{x}^p(t) = \mathbf{u}_\sigma(\mathbf{x}^p(t), t), \tag{30}$$

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t) = (\boldsymbol{\alpha}^p(t) \cdot \nabla)\,\mathbf{u}_\sigma(\mathbf{x}^p(t), t). \tag{31}$$

Again, the transpose scheme

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t) = (\boldsymbol{\alpha}^p(t) \cdot \nabla^{\mathrm{T}})\,\mathbf{u}_\sigma(\mathbf{x}^p(t), t) \tag{32}$$

or the mixed scheme

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t) = \frac{1}{2}(\boldsymbol{\alpha}^p(t) \cdot (\nabla + \nabla^{\mathrm{T}}))\,\mathbf{u}_\sigma(\mathbf{x}^p(t), t) \tag{33}$$

can be used instead of Eq. (31). The details of the evolutions equations are provided in Appendix A.

Remarks made in Section 2 concerning singular vortex particles also apply here:

- The particle field (19) is not generally divergence-free:

$$\nabla \cdot (\tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}, t)) = \sum_p \nabla(\zeta_\sigma(\mathbf{x} - \mathbf{x}^p(t))) \cdot \boldsymbol{\alpha}^p(t). \tag{34}$$

Thus, a basis which is not generally divergence-free is used to represent the divergence-free field $\boldsymbol{\omega}$. Initially, $\tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}, 0)$ can be set to be a good representation of $\boldsymbol{\omega}(\mathbf{x}, 0)$, but nothing guarantees that, as time evolves, $\tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}, t)$ remains a good representation of $\boldsymbol{\omega}(\mathbf{x}, t)$.

• The streamfunction (23) is also not generally divergence-free:

$$\nabla \cdot (\tilde{\boldsymbol{\psi}}_\sigma(\mathbf{x}, t)) = -\sum_p \frac{q_\sigma(\mathbf{x} - \mathbf{x}^p(t))}{|\mathbf{x} - \mathbf{x}^p(t)|^3} \times ((\mathbf{x} - \mathbf{x}^p(t)) \cdot \boldsymbol{\alpha}^p(t)). \quad (35)$$

This result is a direct consequence of the fact that $\nabla^2 \tilde{\boldsymbol{\psi}}_\sigma = -\tilde{\boldsymbol{\omega}}_\sigma$ is solved with $\tilde{\boldsymbol{\omega}}_\sigma$ not generally divergence-free.

• The velocity field (29) is divergence-free since it is the curl of a streamfunction.

• The divergence-free vorticity field can be reconstructed by taking the curl of the velocity field (29):

$$\begin{aligned} \boldsymbol{\omega}_\sigma(\mathbf{x}, t) &= \nabla \times \mathbf{u}_\sigma(\mathbf{x}, t) \\ &= \sum_p [\boldsymbol{\alpha}^p(t)\, \zeta_\sigma(\mathbf{x} - \mathbf{x}^p(t)) \\ &\quad + \nabla(\boldsymbol{\alpha}^p(t) \cdot \nabla(G_\sigma(\mathbf{x} - \mathbf{x}^p(t))))] \quad (36) \\ &= \sum_p \Bigg[\left(\zeta_\sigma(\mathbf{x} - \mathbf{x}^p(t)) - \frac{q_\sigma(\mathbf{x} - \mathbf{x}^p(t))}{|\mathbf{x} - \mathbf{x}^p(t)|^3}\right) \boldsymbol{\alpha}^p(t) \\ &\quad + \left(3\,\frac{q_\sigma(\mathbf{x} - \mathbf{x}^p(t))}{|\mathbf{x} - \mathbf{x}^p(t)|^3} - \zeta_\sigma(\mathbf{x} - \mathbf{x}^p(t))\right) \\ &\quad \times \frac{((\mathbf{x} - \mathbf{x}^p(t)) \cdot \boldsymbol{\alpha}^p(t))}{|\mathbf{x} - \mathbf{x}^p(t)|^2} (\mathbf{x} - \mathbf{x}^p(t))\Bigg]. \quad (37) \end{aligned}$$

The added term in Eq. (36) corresponds to that which is needed to close the vortex lines and it decays as $1/r^3$. Thus, $\boldsymbol{\omega}_\sigma = \nabla \times \mathbf{u}_\sigma = \nabla \times (\nabla \times \tilde{\boldsymbol{\psi}}_\sigma) = -\nabla^2 \tilde{\boldsymbol{\psi}}_\sigma + \nabla(\nabla \cdot \tilde{\boldsymbol{\psi}}_\sigma)$. Recalling that $\nabla^2 \tilde{\boldsymbol{\psi}}_\sigma = -\tilde{\boldsymbol{\omega}}_\sigma$, it follows that $\nabla(\nabla \cdot \tilde{\boldsymbol{\psi}}_\sigma) = \boldsymbol{\omega}_\sigma - \tilde{\boldsymbol{\omega}}_\sigma$. The second term in Eq. (36) does not contribute to the Biot–Savart velocity field as it is the gradient of a scalar.

Beale and Majda [6] have proven convergence of the regularized vortex particle method to the Euler equations with smooth solutions when the stretching term, $\nabla \mathbf{u}$, is approximated by a finite difference operator, $\nabla^h \mathbf{u}$, evaluated on a grid (see also Anderson and Greengard [2]). Beale [5] and Cottet [18] (see also Choquin and Cottet [13]) have proven independently the convergence of the above regularized vortex particle method (also called a *grid-free method*). These convergence proofs hold for any of the choices Eqs. (31), (32), or (33). Beale [5] has also obtained improved error estimates when using the mixed scheme (33), due to the symmetry of the stretching operator. It is not intended to review the various convergence proofs. It is only recalled that the appropriate error norms for the vorticity and velocity fields go to zero as the number of particles is increased and the core size σ is decreased, subject to the constraint that cores overlap (i.e., $\sigma/h > 1$, where h is a typical distance between neighbor particles). The error norm for the vorticity is composed of two terms: one term which is $\mathcal{O}((\sigma/L)^r)$ (where L is a global length scale) and another term which is $\mathcal{O}((\sigma/L)(h/\sigma)^m)$. The exponent m is related to the number of derivatives that exist of $\zeta(\rho)$. For most functions used in practice, m is large so that it is essential that cores do overlap for the second error term to vanish as $\sigma \to 0$. The exponent r is related to the moment properties of $\zeta(\rho)$; that is, $\zeta(\rho)$ has to satisfy the normalization constraint (21), together with

$$\int_0^\infty \zeta(\rho)\, \rho^{2+s}\, d\rho = 0, \qquad 2 \leqslant s \leqslant r-1 \qquad s \text{ even}, \quad (38)$$

$$\int_0^\infty |\zeta(\rho)|\, \rho^{2+r}\, d\rho < \infty. \quad (39)$$

In particular, it can be shown that $r \geqslant 2$ as soon as $\int_0^\infty |\zeta(\rho)|\, \rho^4\, d\rho < \infty$. If, moreover, $\zeta(\rho)$ is positive, then $r = 2$.

3.1. *Regularization Functions*

A number of 3D regularization functions $\zeta(\rho)$ and their associated $G(\rho)$ and $q(\rho)$ functions are collected in Table I. Note that the smoothings that are $r > 2$, such as the super-Gaussian, are also not strictly positive. The related 2D regularization functions (obtained by projecting a straight 3D (vortex) filament onto a 2D plane) are useful for 2D (vortex) particle methods and are collected in Table II. See also Huberson [27] and Hald [25] for additional 2D smoothings.

The 3D *Gaussian* smoothing

$$\zeta(\rho) = \frac{1}{(2\pi)^{3/2}} e^{-\rho^2/2} \quad (40)$$

corresponds to $m = \infty$, $r = 2$. It yields the 2D *Gaussian* smoothing when projected in 2D. The 3D *low-order algebraic* smoothing (proposed by Rosenhead [40] in the context of vortex filaments)

$$\zeta(\rho) = \frac{3}{4\pi} \frac{1}{(\rho^2 + 1)^{5/2}} \quad (41)$$

gives $m = \infty$, but $r = 0$ because the inequality (39) is not satisfied. Thus, this smoothing might not lead to convergence as the number of particles is increased. When projected in 2D, it yields the 2D *low order algebraic* smoothing (which might also not lead to convergence).

A new 3D smoothing is proposed which will be referred to as the *high order algebraic* smoothing:

$$\zeta(\rho) = \frac{15}{8\pi} \frac{1}{(\rho^2 + 1)^{7/2}}. \quad (42)$$

TABLE I

3D Regularization Functions

$4\pi\zeta(\rho)$	$4\pi G(\rho)$	$4\pi \frac{q(\rho)}{\rho^3}$	m	r
$\frac{3}{(\rho^2+1)^{5/2}}$	$\frac{1}{(\rho^2+1)^{1/2}}$	$\frac{1}{(\rho^2+1)^{3/2}}$	∞	0
Low order algebraic smoothing; $\zeta(\rho), \eta(\rho) > 0$; note that $r = 0$; yields 2D low order algebraic smoothing when projected from 3D to 2D				
$\frac{15/2}{(\rho^2+1)^{7/2}}$	$\frac{(\rho^2+3/2)}{(\rho^2+1)^{3/2}}$	$\frac{(\rho^2+5/2)}{(\rho^2+1)^{5/2}}$	∞	2
High order algebraic smoothing; $\zeta(\rho), \eta(\rho) > 0$; yields 2D high order algebraic smoothing				
$\left(\frac{2}{\pi}\right)^{1/2} e^{-\rho^2/2}$	$\frac{1}{\rho}\operatorname{erf}\left(\frac{\rho}{2^{1/2}}\right)$	$\frac{1}{\rho^3}\left(\operatorname{erf}\left(\frac{\rho}{2^{1/2}}\right) - \left(\frac{2}{\pi}\right)^{1/2} \rho e^{-\rho^2/2}\right)$	∞	2
Gaussian smoothing; $\zeta(\rho), \eta(\rho) > 0$; yields 2D Gaussian smoothing				
$3e^{-\rho^3}$		$\frac{1}{\rho^3}(1-e^{-\rho^3})$	∞	2
$\zeta(\rho) > 0, \eta(\rho) \ngtr 0$				
$3\,\operatorname{sech}^2(\rho^3)$		$\frac{1}{\rho^3}\tanh(\rho^3)$	∞	2
$\zeta(\rho) > 0, \eta(\rho) \ngtr 0$				
$\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{5}{2}-\frac{\rho^2}{2}\right) e^{-\rho^2/2}$	$\frac{1}{\rho}\left(\operatorname{erf}\left(\frac{\rho}{2^{1/2}}\right) + \frac{1}{(2\pi)^{1/2}} \rho e^{-\rho^2/2}\right)$	$\frac{1}{\rho^3}\left(\operatorname{erf}\left(\frac{\rho}{2^{1/2}}\right) - \left(\frac{2}{\pi}\right)^{1/2}\left(1-\frac{\rho^2}{2}\right) \rho e^{-\rho^2/2}\right)$	∞	4
Super-Gaussian smoothing; $\zeta(\rho), \eta(\rho) \ngtr 0$				
The functions below have, for $\rho > 1$:				
0	$\frac{1}{\rho}$	$\frac{1}{\rho^3}$		
and, for $\rho < 1$:				
3	$\frac{1}{2}(3-\rho^2)$	1	1	2
Hat smoothing; does not yield 2D hat smoothing				
$\frac{4}{\pi}\frac{1}{(1-\rho^2)^{1/2}}$	$\frac{2}{\pi}\left(\frac{\arcsin\rho}{\rho} + (1-\rho^2)^{1/2}\right)$	$\frac{2}{\pi}\frac{1}{\rho^3}(\arcsin\rho - \rho(1-\rho^2)^{1/2})$	—	2
Smoothing that yields 2D hat smoothing				

In the context of particle and filament methods (not necessarily vortex methods), this new smoothing (42) is special in many respects:

- It has convergence properties equal to those of the Gaussian smoothing (40).
- It yields the previously known 2D high order algebraic smoothing when projected to 2D.
- The associated $G(\rho)$ and $q(\rho)$ functions are numerically more convenient to use than those associated with Gaussian smoothing (see Appendix A).
- For vortex particles, this smoothing is a case for which closed form expressions for all quadratic diagnostics can be obtained: kinetic energy, helicity, and enstrophy (see Appendix C).

TABLE II

2D Regularization Functions

$2\pi\zeta(\rho)$	$2\pi G(\rho)$	$2\pi \frac{q(\rho)}{\rho^2}$	m	r
$\frac{2}{(\rho^2+1)^2}$	$\frac{1}{2}\log(\rho^2+1)$	$\frac{1}{\rho^2+1}$	∞	0
Low order algebraic smoothing; $\zeta(\rho), \eta(\rho) > 0$; note that $r=0$				
$\frac{4}{(\rho^2+1)^3}$	$\frac{1}{2}\left(\log(\rho^2+1)+\frac{\rho^2}{\rho^2+1}\right)$	$\frac{(\rho^2+2)}{(\rho^2+1)^2}$	∞	2
High order algebraic smoothing; $\zeta(\rho), \eta(\rho) > 0$				
$e^{-\rho^2/2}$	$\frac{1}{2}\left(\log\left(\frac{\rho^2}{2}\right)+E_1\left(\frac{\rho^2}{2}\right)\right)$	$\frac{1}{\rho^2}(1-e^{-\rho^2/2})$	∞	2
Gaussian smoothing; $\zeta(\rho), \eta(\rho) > 0$				
$2\,\mathrm{sech}^2(\rho^2)$		$\frac{1}{\rho^2}\tanh(\rho^2)$	∞	2
$\zeta(\rho) > 0, \eta(\rho) \not> 0$				
$4\frac{(2-\rho^2)}{(\rho^2+1)^4}$		$\frac{(\rho^4+3\rho^2+4)}{(\rho^2+1)^3}$	∞	3
Super-algebraic smoothing; $\zeta(\rho), \eta(\rho) \not> 0$				
$\left(2-\frac{\rho^2}{2}\right)e^{-\rho^2/2}$	$\frac{1}{2}\left(\log\left(\frac{\rho^2}{2}\right)+E_1\left(\frac{\rho^2}{2}\right)-e^{-\rho^2/2}\right)$	$\frac{1}{\rho^2}\left(1-\left(1-\frac{\rho^2}{2}\right)e^{-\rho^2/2}\right)$	∞	4
Super-Gaussian smoothing; $\zeta(\rho), \eta(\rho) \not> 0$				
$\frac{J_1(\rho)}{\rho}$		$\frac{1}{\rho^2}(1-J_0(\rho))$	∞	∞
Spectral smoothing; $\zeta(\rho), \eta(\rho) \not> 0$; spectral-like convergence since $r=\infty$				
The functions below have, for $\rho > 1$:				
0	$\log\rho$	$\frac{1}{\rho^2}$		
and, for $\rho < 1$:				
2	$\frac{1}{2}(\rho^2-1)$	1	1	2
Hat smoothing				
$3(1-\rho^2)^{1/2}$	$\log(1+(1-\rho^2)^{1/2})-\frac{1}{3}(1-\rho^2)^{3/2}-(1-\rho^2)^{1/2}$	$\frac{1}{\rho^2}(1-(1-\rho^2)^{3/2})$	2	2
Projection of 3D hat smoothing				
$\frac{2}{E_2(1)}e^{-1/(1-\rho^2)}$		$\frac{1}{\rho^2}\left(1-(1-\rho^2)\frac{E_2(1/(1-\rho^2))}{E_2(1)}\right)$	∞	2
Smoothing which is $\mathscr{C}^\infty$ and of compact support				

3.2. *Relaxation of the Particle Vorticity Field Divergence*

The particle method has no built-in control on keeping the particle vorticity field, $\tilde{\boldsymbol{\omega}}_\sigma$, nearly divergence-free as time evolves. This weakness may get the method into trouble in long time computations. Moreover, the need for particle redistribution and/or addition may also arise due to intense vortex stretching.

This point is illustrated by numerical results on the inviscid collision of two vortex rings, Figs. 5 and 6. Although the computations fail to go through the fusion process (a viscous process!), the reconnection of vortex tubes has nearly occurred. The classical and transpose schemes do not, however, lead to the same "flow picture" before numerical blowup, Fig. 5. This accumulated effect is due to $\tilde{\boldsymbol{\omega}}_\sigma$ not remaining nearly divergence-free as time evolves, Fig. 6. Note that both methods perform equally well/bad on the conservation of linear impulse and kinetic energy (see also Section 5 and Appendix C). This is in contrast to the simulations with singular particles for which the transpose scheme is clearly superior.

These regularized vortex particle computations can be compared with regularized vortex filament computations of the same problem: Chua, Leonard, Pépin, and Winckelmans [15], Winckelmans [45], Anderson and Greengard [3]. Since both methods are inviscid, they both fail to go through the fusion process. Vortex filaments, however, are divergence-free by construction. Hence they

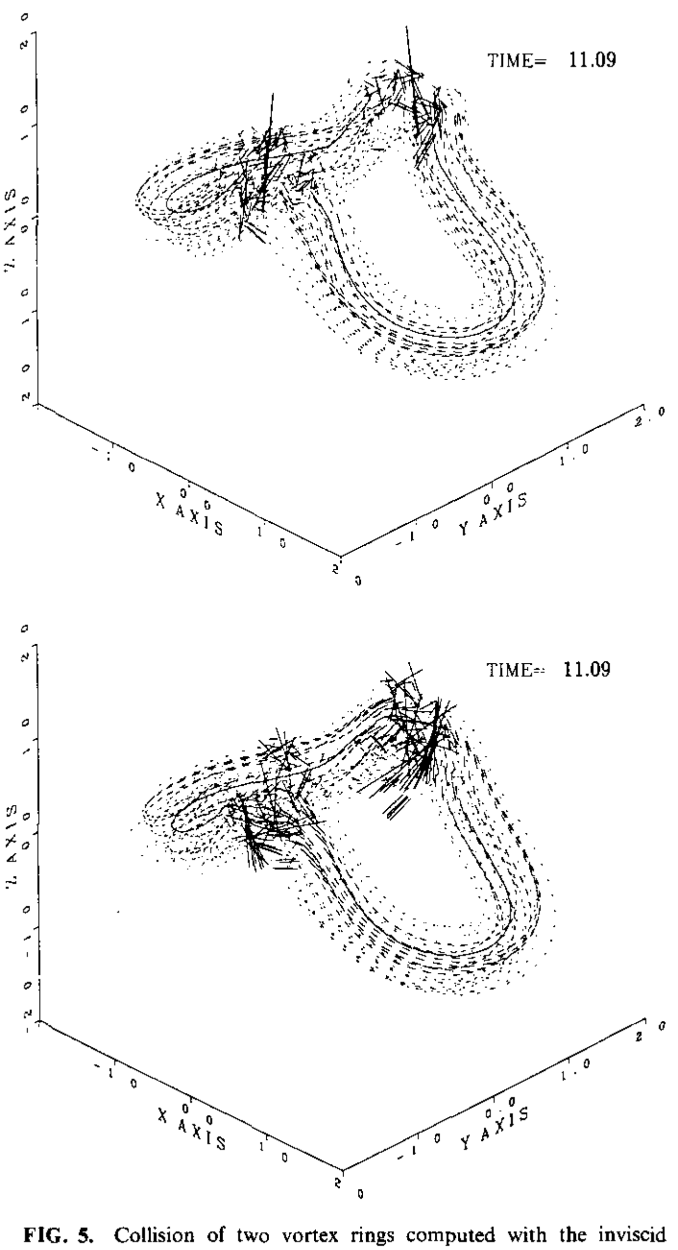

FIG. 5. Collision of two vortex rings computed with the inviscid method of regularized vortex particles. View of particle strength vectors: (a) classical scheme; (b) transpose scheme. Initial conditions: same as Fig. 3, $\sigma = 0.2$.

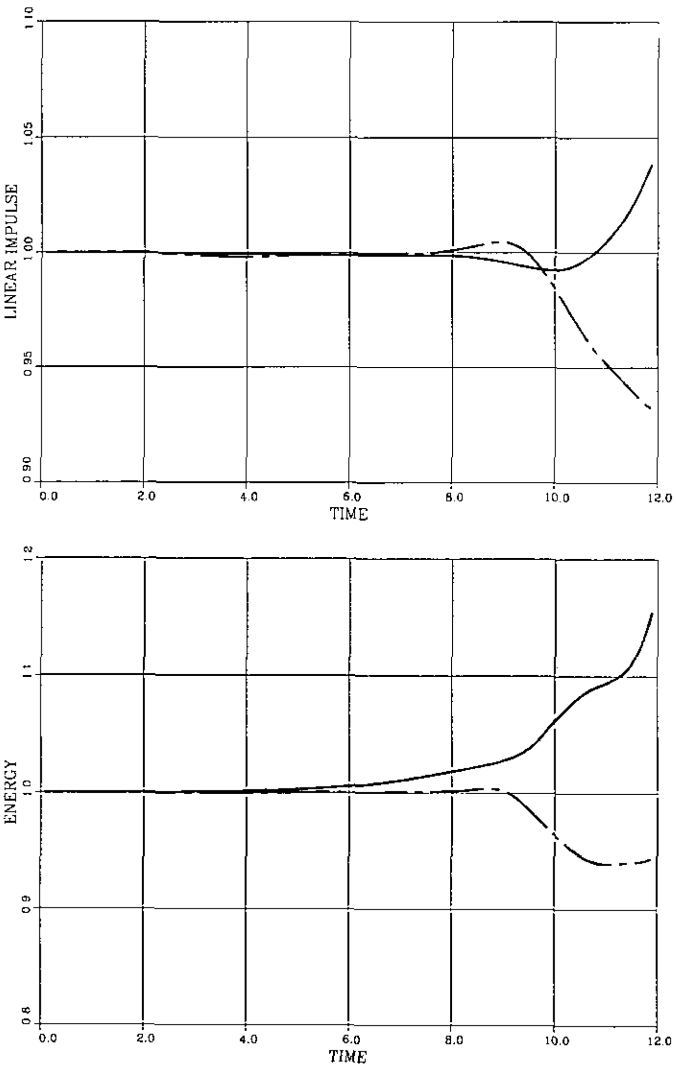

FIG. 6. Collision of two vortex rings computed with the inviscid method of regularized vortex particles. Diagnostics I and $\tilde{E}_\sigma$ (E_σ not evaluated). Transpose scheme (solid), classical scheme (chain-dash).

remain a good representation of the vorticity field during this inviscid collision process.

A relaxation scheme is proposed which forces the particle field, $\tilde{\boldsymbol{\omega}}_\sigma$, to remain nearly divergence-free for all times, and hence it makes the method well-suited to long time computations. The procedure is as follows: if and when $\tilde{\boldsymbol{\omega}}_\sigma$ becomes a poor representation of the divergence-free field, $\boldsymbol{\omega}_\sigma$, assign new particle strengths $\boldsymbol{\alpha}^p_{\text{new}}(t)$ by imposing that $\tilde{\boldsymbol{\omega}}_\sigma(\mathbf{x}^p(t), t) = \boldsymbol{\omega}_\sigma(\mathbf{x}^p(t), t)$, namely by solving the system of linear equations for all p:

$$\sum_q \boldsymbol{\alpha}^q_{\text{new}}(t)\,\zeta_\sigma(\mathbf{x}^q(t) - \mathbf{x}^q(t)) = \sum_q \left[\boldsymbol{\alpha}^q_{\text{old}}(t)\,\zeta_\sigma(\mathbf{x}^p(t) - \mathbf{x}^q(t)) + \nabla(\boldsymbol{\alpha}^q_{\text{old}}(t)\cdot\nabla(G_\sigma(\mathbf{x}^p(t) - \mathbf{x}^q(t))))\right]. \tag{43}$$

Different formulas for the evaluation of global quadratic diagnostics (energy, helicity, and enstrophy) based on both $\boldsymbol{\omega}_\sigma$ and $\tilde{\boldsymbol{\omega}}_\sigma$ are derived in Appendix C. The comparison between $\boldsymbol{\omega}_\sigma$-based quadratic diagnostics and their $\tilde{\boldsymbol{\omega}}_\sigma$-based

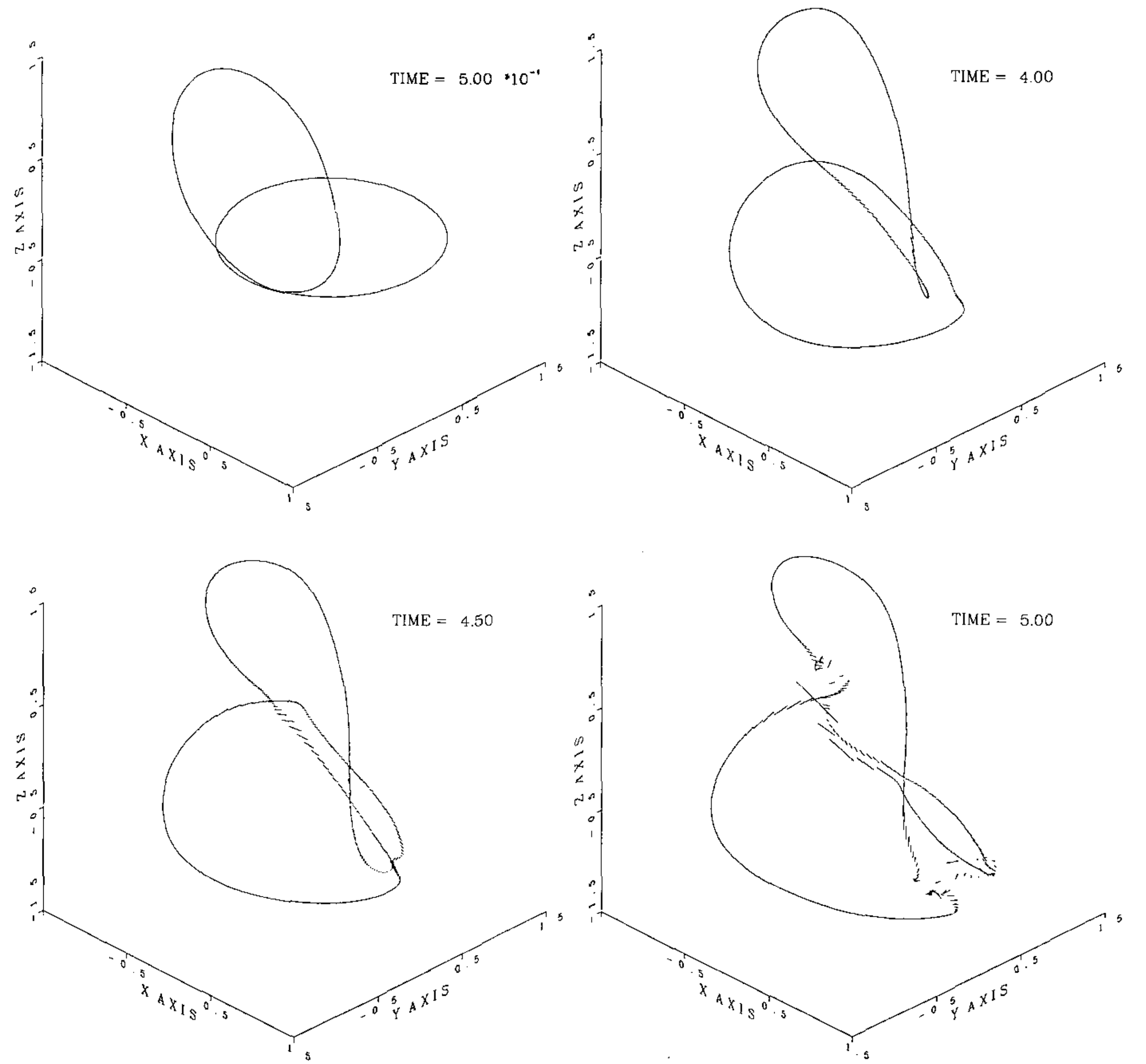

FIG. 7. The "knot" problem computed with the method of regularized vortex particles and using the transpose scheme. No particle addition and no relaxation of $\nabla\cdot\tilde{\boldsymbol{\omega}}_\sigma$. Perspective view of particle strength vectors. Initial conditions: $\Gamma = 1$, $R = 1$, $s = 1$, $N_\varphi = 250$, $\sigma = 0.1$.

counterparts provides global criteria as to when the need for applying the relaxation scheme arises during the course of a computation. Other global criteria can be used, e.g., criteria based on monitoring the conservation of total vorticity and/or linear impulse and/or angular impulse (see Section 5 and Appendix B). Finally, local criteria can also be used, e.g., local monitoring of $\nabla \cdot (\tilde{\omega}_\sigma(\mathbf{x}^p(t), t))$ for each particle p.

Since $\boldsymbol{\alpha}^q_{\text{old}}$ is close to $\boldsymbol{\alpha}^q_{\text{new}}$, the above system is of the form $A\boldsymbol{\alpha}_{\text{new}} = \boldsymbol{\alpha}_{\text{old}}$ with A close to the identity matrix. Writing $A = I + (A - I)$, it can be solved by iteration using the convergent scheme:

$$\boldsymbol{\alpha}^{p\;(0)}_{\text{new}} = \boldsymbol{\alpha}^p_{\text{old}}, \qquad 1 \leqslant p \leqslant N,$$

$$\boldsymbol{\alpha}^{p\;(n)}_{\text{new}} = (\boldsymbol{\alpha}^p_{\text{old}} + \boldsymbol{\alpha}^{p\;(n-1)}_{\text{new}}) - \sum_q a^{pq} \boldsymbol{\alpha}^{q\;(n-1)}_{\text{new}}, \tag{44}$$

$$1 \leqslant p \leqslant N, \qquad n \geqslant 1.$$

Note that this method is not the Jacobi iterative method (which would be obtained by writing $A = D + (A - D)$). Actually, because A is not diagonally dominant (when the core overlapping condition is satisfied as it should be), Jacobi or Gauss–Seidel usually fail to converge even with a good first guess. Only highly underrelaxed versions of Jacobi or Gauss–Seidel sometimes converge!

A convergent "Gauss–Seidel" version of the above method is obtained by simply making use of the latest values of $\boldsymbol{\alpha}^p_{\text{new}}$ (i.e., overwriting of the vector $\boldsymbol{\alpha}_{\text{new}}$):

$$\boldsymbol{\alpha}^p_{\text{new}} = \boldsymbol{\alpha}^p_{\text{old}}, \qquad 1 \leqslant p \leqslant N,$$

$$\boldsymbol{\alpha}^p_{\text{new}} = (\boldsymbol{\alpha}^p_{\text{old}} + \boldsymbol{\alpha}^p_{\text{new}}) - \sum_q a^{pq} \boldsymbol{\alpha}^q_{\text{new}}, \tag{45}$$

$$1 \leqslant p \leqslant N, \qquad n \geqslant 1.$$

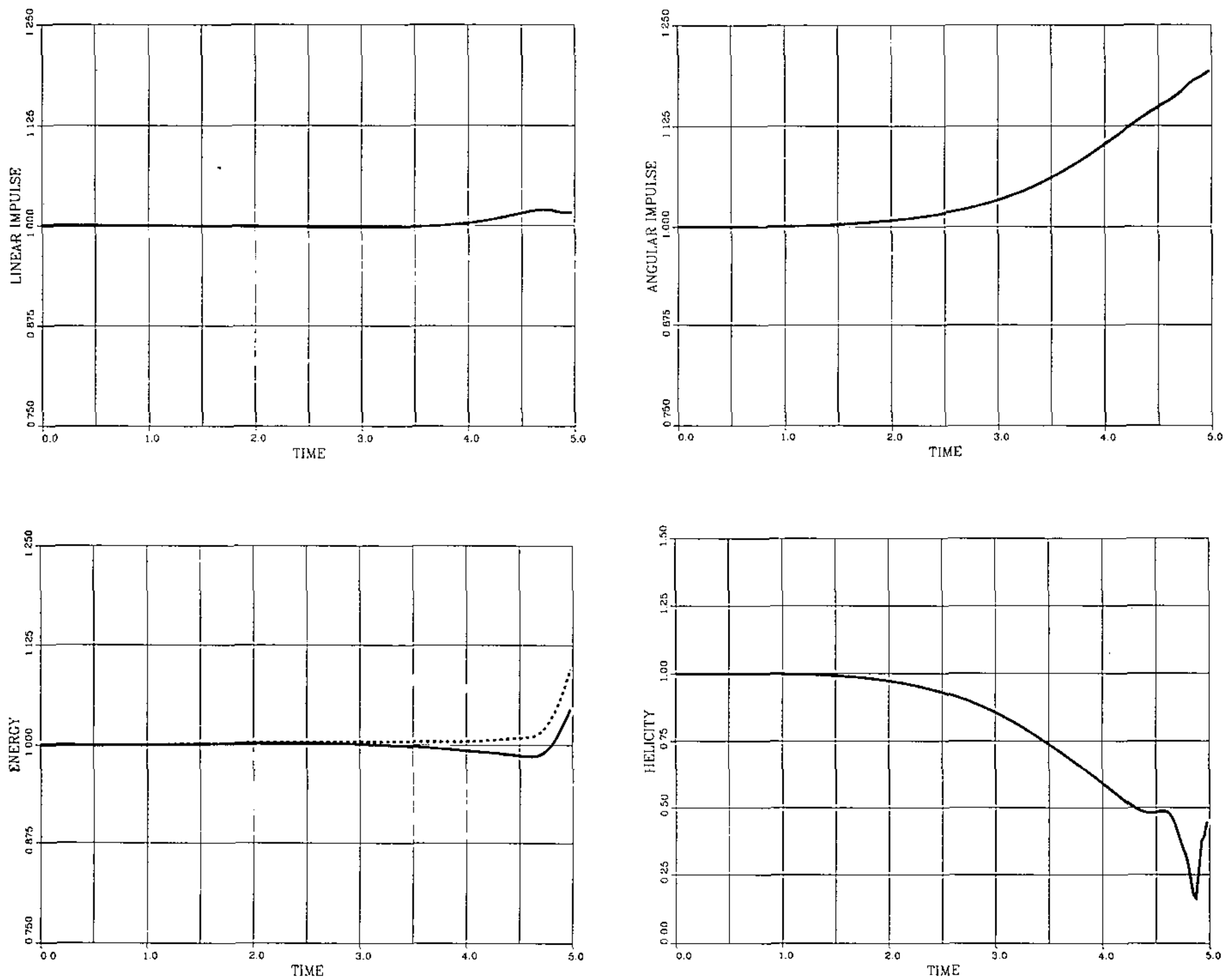

FIG. 8. The "knot" problem computed with the method of regularized vortex particles and using the transpose scheme. No particle addition and no relaxation of $\nabla \cdot \tilde{\omega}_\sigma$. Diagnostics I, A, E_σ (solid) and $\tilde{E}_\sigma$ (dash), $\mathscr{H}_\sigma$.

Finally, convergent overrelaxed versions of both methods can also be used.

It should be mentioned that Pedrizzetti [36] also proposed, in the context of singular particles, a relaxation scheme called the "divergence filtering method." This scheme can also be used in the context of regularized particles: At every time step, the updated particle strength vector, $\boldsymbol{\alpha}^p(t)$, is modified using the filtering,

$$\boldsymbol{\alpha}^p_{\text{new}}(t) = (1 - f\,\delta t)\,\boldsymbol{\alpha}^p(t) + f\,\delta t\,\frac{\boldsymbol{\omega}_\sigma(\mathbf{x}^p(t), t)}{\|\boldsymbol{\omega}_\sigma(\mathbf{x}^p(t), t)\|}\,\|\boldsymbol{\alpha}^p(t)\|, \tag{46}$$

where f is a frequency factor; i.e., the time scale $1/f$ is "tuned" with respect to the time scale(s) of the physical phenomena under study to give satisfactory results.

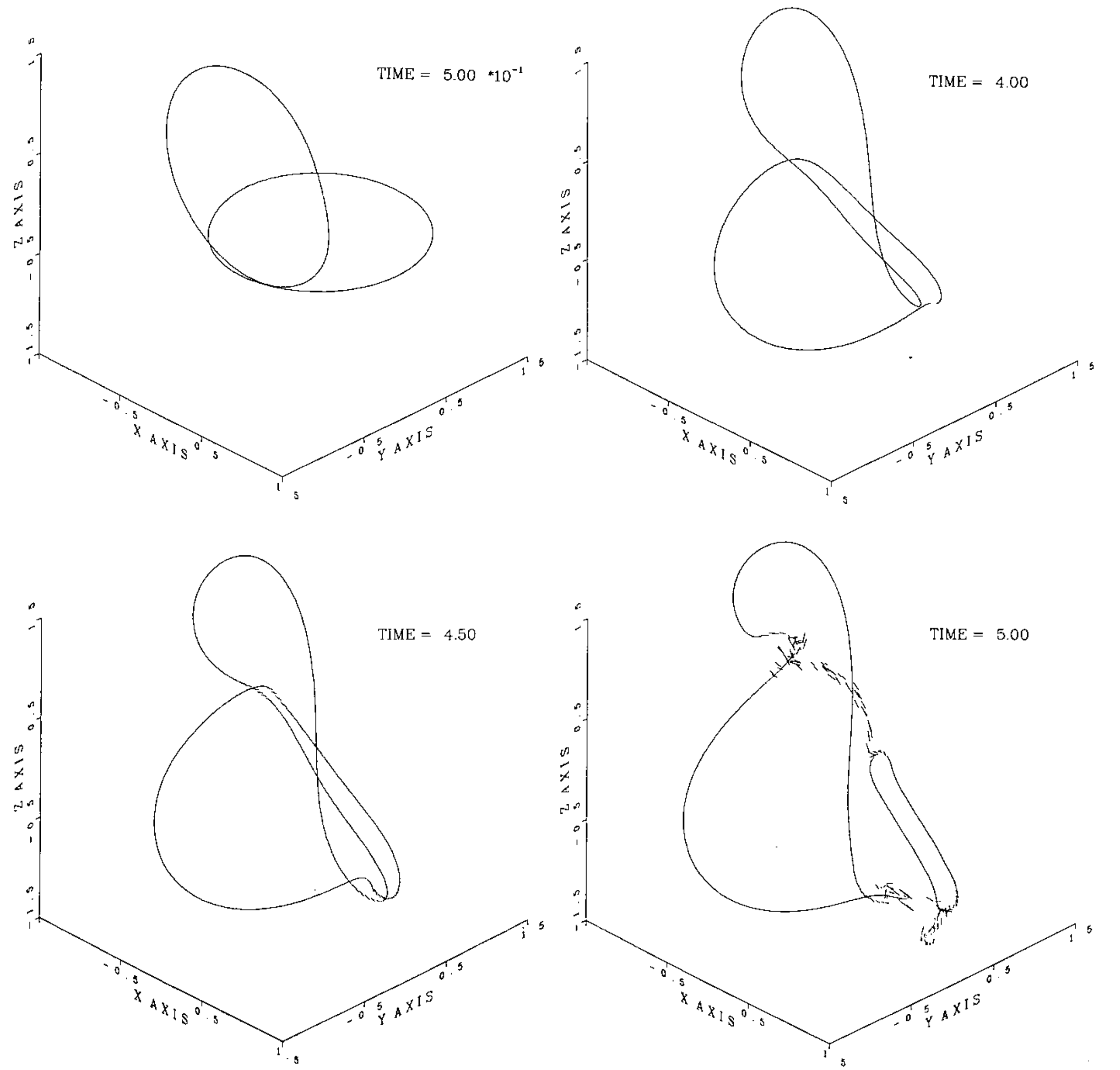

FIG. 9. The "knot" problem computed with the method of regularized vortex particles and using the transpose scheme. Particle addition (every $\Delta t = 0.125$) and relaxation of $\nabla \cdot \tilde{\boldsymbol{\omega}}_\sigma$ (every $\Delta t = 0.25$). Perspective view of particle strength vectors. Initial conditions: $\Gamma = 1$, $R = 1$, $s = 1$, $N_\varphi = 175$, $\sigma = 0.1$. Final $N_\varphi(t = 5) = 541$.

To be most effective, our relaxation scheme must be accompanied by the addition of particles wherever vortex stretching is intense. This has to do with ensuring the core overlapping condition, $\sigma/h > 1$, for all times. Recalling that, in inviscid flows, vortex lines move as material lines, one assumes that $h(t) \propto \|\boldsymbol{\alpha}(t)\|$. A simple local procedure is then to split a particle $\boldsymbol{\alpha}$ into two particles $\boldsymbol{\alpha}/2$ when $\|\boldsymbol{\alpha}(T)\| \geqslant 2\, \|\boldsymbol{\alpha}(0)\|$. This ensures the same overlap as that initially. The new particles are placed at $\mathbf{x} \pm c_r \sigma \boldsymbol{\alpha}/\|\boldsymbol{\alpha}\|$. This choice ensures the conservation of total vorticity and linear impulse. Angular impulse is not generally conserved by this scheme. (A scheme exists which conserves all three linear invariants but it requires the solution of a set of nine nonlinear equations for the nine unknowns $\boldsymbol{\alpha}^1$, $\boldsymbol{\alpha}^2$, and $\Delta\mathbf{x}$.) The parameter c_r is chosen so that the new particles smoothly replace the old ones (e.g., $c_r \sigma = 0.25 h(T)$).

The above procedures are applied to the computation of the inviscid "knot" problem, Figs. 7 to 10, and use only a single line of elements to define each vortex ring. This purely "computational" problem includes complex vortex interactions with intense vortex stretching and also has nonzero angular impulse, $\mathbf{A}$, and helicity, $\mathscr{H}$. Here, $I_y = -I_z$ with $I = (I_y^2 + I_z^2)^{1/2}$, and $A_y = -A_z$ with $A = (A_y^2 + A_z^2)^{1/2}$. As seen in Figs. 7 and 8, the computation without relaxation of $\nabla \cdot \tilde{\boldsymbol{\omega}}_\sigma$ and without addition of particles performs poorly, mainly because particles become misaligned from the direction of the vortex tube they are supposed to discretize. This phenomenon surely happens, no matter how many particles

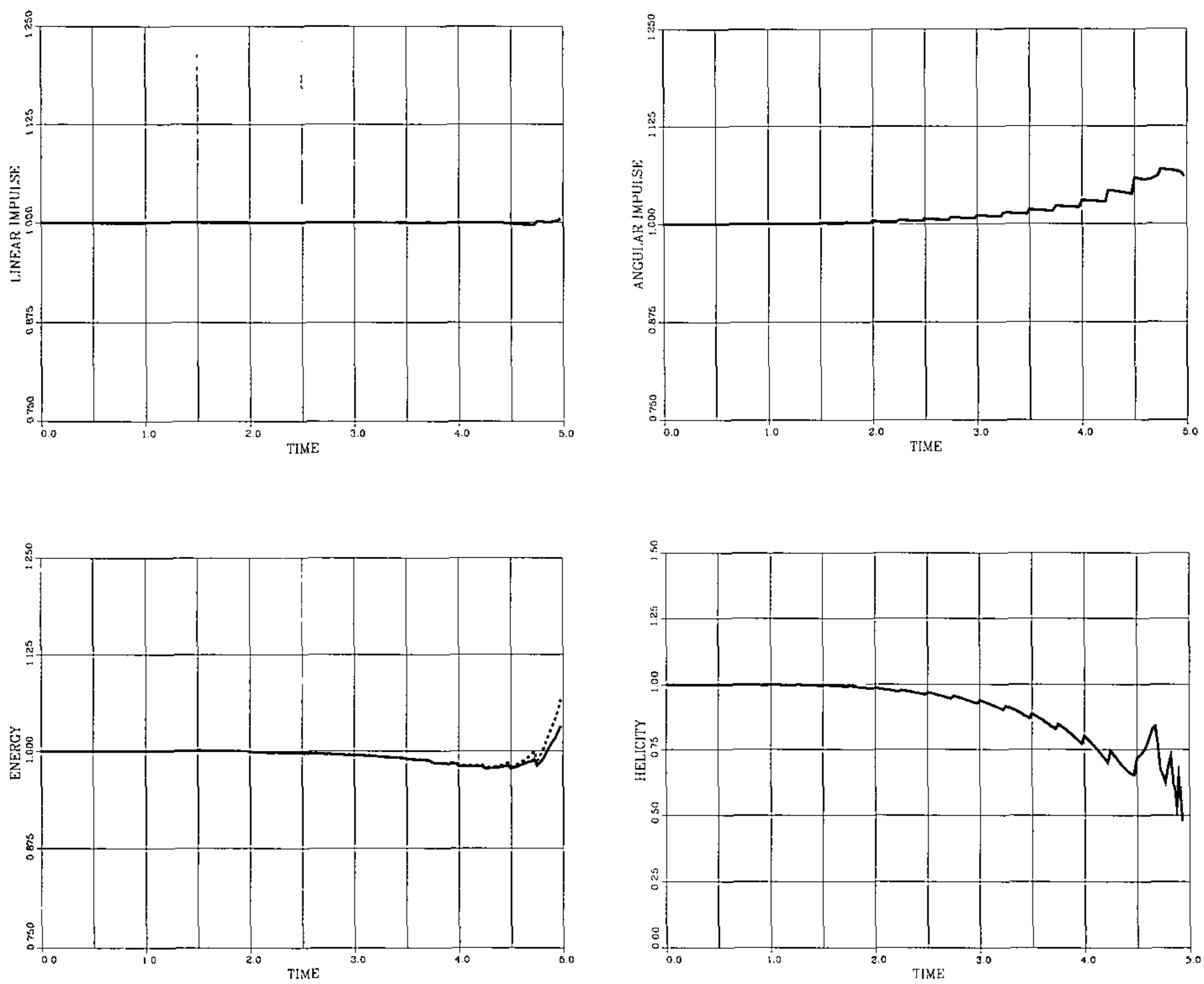

FIG. 10. The "knot" problem computed with the method of regularized vortex particles and using the transpose scheme. Particle addition and relaxation of $\nabla \cdot \tilde{\boldsymbol{\omega}}_\sigma$. Diagnostics I, A, E_σ (solid) and $\tilde{E}_\sigma$ (dash), $\mathscr{H}_\sigma$.

are used. If the relaxation of $\nabla \cdot \tilde{\omega}_\sigma$ is applied, together with the addition of particles wherever stretching is intense, the computation performs much better, Figs. 9 and 10. Invariants are better conserved (see also Section 5 and Appendix C).

Note that the relaxation scheme has a diffusive character which makes the inviscid particle method "robust": vortex lines that would reconnect in high Re number flows because of finite viscous diffusion reconnect artificially when the inviscid particle method is combined with the relaxation scheme. Vortex lines reconnect artificially because, if two vortex lines of opposite sign vorticity are locally in close proximity, applying the relaxation scheme results in partial mutual cancelation of the particle strengths in that region. This results in a new topology, where the previous vortex lines have "reconnected" locally. The resulting topology is likely to be close to the one that would be obtained in high Re number flows.

4. VISCOUS DIFFUSION BY THE REDISTRIBUTION OF PARTICLE STRENGTHS

Despite the lack of built-in control on the particle vorticity divergence, there is the unique feature that the particle method allows for and that cannot be achieved with a filament method: the possibility of taking into account viscous diffusion, Eq. (3). This property is very attractive because viscous diffusion is a necessary ingredient for the successful reconnection of vortex tubes.

Diffusion can be dealt with using an approach in which *the strength vectors $\boldsymbol{\alpha}^p(t)$ are redistributed among particles* in a manner that is consistent and accurate. This approach was introduced by Mas-Gallic [32], and Degond and Mas-Gallic [22] (see also Cottet and Mas-Gallic [20, 21], Huberson [27], and Choquin and Huberson [14]) in the general framework of solving convection–diffusion equations using particle methods. Another particle exchange scheme for discretizing the diffusion terms was introduced by Fishelov [23]. The former scheme was used for the present work. It was applied to the 3D vortex particle method.

In essence, they showed that the diffusion operator (i.e., the Laplacian) can be approximated by an integral operator which can, in turn, be discretized using the particle representation of the function of interest. Consider a smoothing function with radial symmetry as described in Section 3 and which satisfies the integral constraints (21), (38), and (39), together with

$$\int_0^\infty |\zeta'(\rho)|\, \rho^{3+r}\, d\rho < \infty. \tag{47}$$

Define

$$-\frac{1}{\rho}\frac{d}{d\rho}\zeta(\rho) = \eta(\rho) \tag{48}$$

and $\eta_\sigma(\mathbf{x}) = \eta(|\mathbf{x}|/\sigma)/\sigma^3$. Then a good approximation to $\nabla^2 f(\mathbf{x})$ is given by

$$\nabla^2 f(\mathbf{x}) \simeq \frac{2}{\sigma^2}\int (f(\mathbf{y}) - f(\mathbf{x}))\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{y} \tag{49}$$

in the sense that, in the appropriate norm, the difference between $\nabla^2 f(\mathbf{x})$ and Eq. (49) is $\mathcal{O}((\sigma/L)^r)$. Again, the classical smoothing (41) does not satisfy the constraint (47) and is therefore a poor choice for the diffusion term. The function $\eta_\sigma(\mathbf{x})$ is essentially an approximation to the kernel for the heat equation. The nature of the approximation may be understood as follows: For the purpose of illustration, consider the Gaussian smoothing (40) which is such that $\eta(\rho) = \zeta(\rho)$. Then, the Fourier transform of Eq. (49) gives

$$\begin{aligned} \frac{2}{\sigma^2}(\hat{\eta}_\sigma(\mathbf{k}) - 1)\hat{f}(\mathbf{k}) &= \frac{2}{\sigma^2}(e^{-k^2\sigma^2/2} - 1)\hat{f}(\mathbf{k}) \\ &\simeq -k^2(1 + \mathcal{O}(k^2\sigma^2))\hat{f}(\mathbf{k}) \qquad \text{for small } \mathbf{k} \\ &\simeq \mathcal{F}(\nabla^2 f(\mathbf{x})), \end{aligned} \tag{50}$$

thus showing that, in the Fourier space, the integral operator is a second-order approximation to the Laplacian when $\eta(\rho)$ is the Gaussian. This conclusion is consistent with the above error estimate since the Gaussian smoothing corresponds to $r = 2$.

Consider now the general convection-diffusion equation written in conservative form (i.e., $\nabla \cdot \mathbf{u}$ not necessarily zero),

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{u}) = \nu\, \nabla^2 f, \tag{51}$$

and the equation approximating (51),

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{u}) = \frac{2\nu}{\sigma^2}\int (f(\mathbf{y}) - f(\mathbf{x}))\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{y}. \tag{52}$$

Acceptable error estimates are obtained for the difference in time between the solutions of the two problems for all ν, provided that $\eta(\rho) \geqslant 0$ for all ρ (which implies that $r \leqslant 2$). (The case $\eta(\rho) \ngeqslant 0$ is more obscure and will not be addressed here.)

Consider a particle approximation of $f(\mathbf{x}, t)$,

$$f_\sigma(\mathbf{x}, t) = \sum_p (f^p(t)\, vol^p(t))\, \zeta_\sigma(\mathbf{x} - \mathbf{x}^p(t)), \tag{53}$$

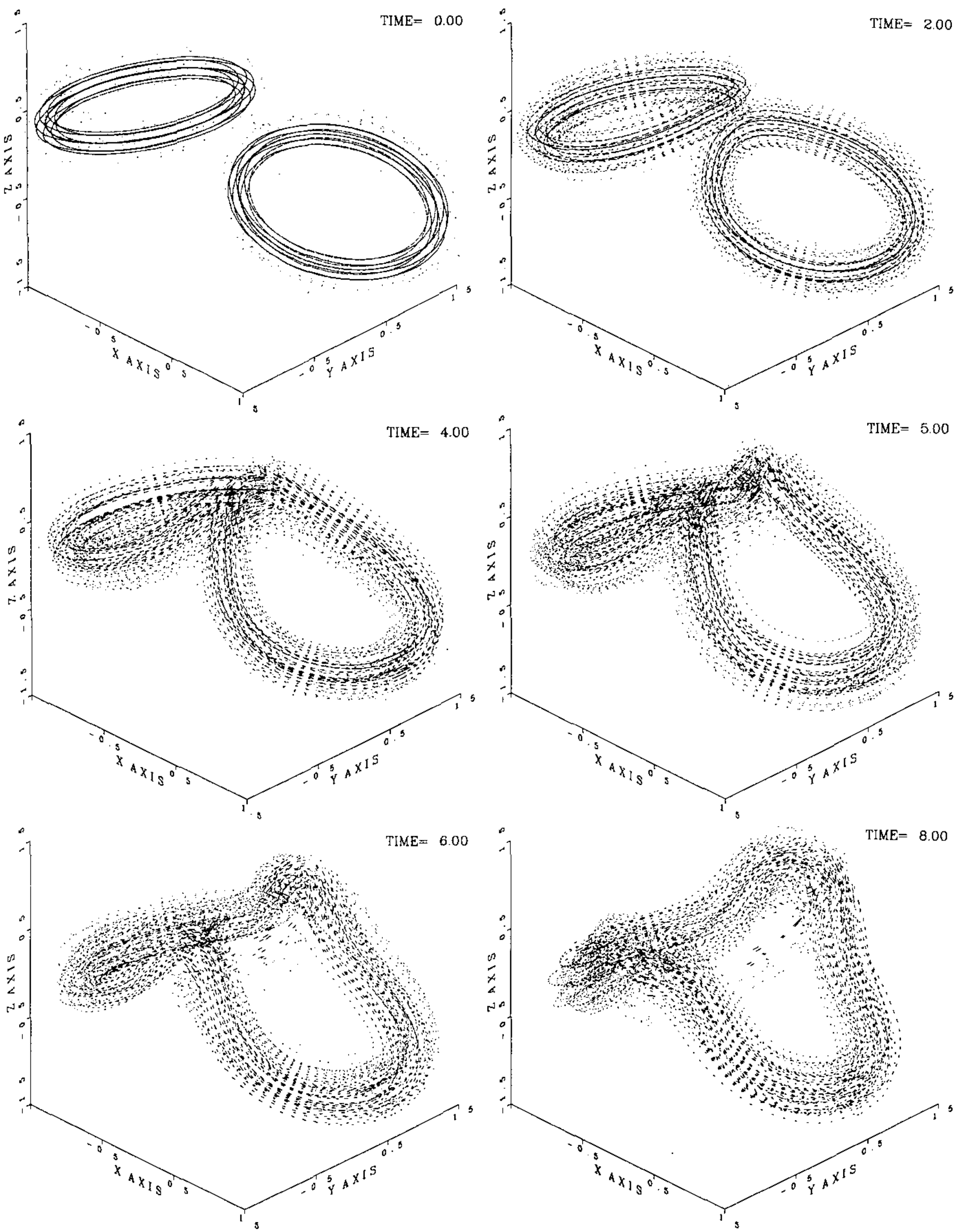

FIG. 11. Fusion of two vortex rings computed with the viscous method of regularized vortex particles and using the transpose scheme. View of particle strength vectors. Initial conditions: $\Gamma = 1$, $R = 1$, $s = 2.7$, $\theta_0 = 15°$, $r_l = 0.05$, $n_c = 3(\rightarrow N_s = 49)$, $N_\varphi = 64$, $\sigma = 0.065$, $\mathrm{Re} = \Gamma/\nu = 400$, and $\omega_\varphi = (\Gamma/2\pi a^2)(1 + (r/R)\cos\theta)\, e^{-r^2/2a^2}$ with $a = 0.1$.

and solve the approximate convection–diffusion problem (52), using a particle discretization of the integral operator:

$$\frac{d}{dt}\mathbf{x}^p(t)=\mathbf{u}(\mathbf{x}^p(t),t),$$

$$\frac{d}{dt}\,vol^p(t)=vol^p(t)\,\nabla\cdot\mathbf{u}(\mathbf{x}^p(t),t),$$

$$\frac{d}{dt}(f^p(t)\,vol^p(t))=\frac{2\nu}{\sigma^2}\,vol^p(t)\sum_q vol^q(t)(f^q(t)-f^p(t))\times\eta_\sigma(\mathbf{x}^p(t)-\mathbf{x}^q(t)). \tag{54}$$

For $\eta(\rho)\geqslant 0$, the error estimates show that the replacement of the integral operator by a discrete sum leads to an error of $\mathcal{O}((h/\sigma)^m/(\sigma/L))$. Thus, the particle approximation of the diffusion term leads to a global error of $\mathcal{O}(\nu((\sigma/L)^r+(h/\sigma)^m/(\sigma/L)))$. For arbitrary ν, this error is higher than the error $\mathcal{O}((\sigma/L)^r+(h/\sigma)^m)$ due to the particle approximation of the convective term, but, for small ν, this error is lower.

An important remark is in order: $\zeta(\rho)\not> 0$ implies that $\eta(\rho)\not> 0$ but $\zeta(\rho)>0$ does not guarantee that $\eta(\rho)>0$ (see Tables I and II). For viscous computations, it is a good policy to use functions for which both $\zeta(\rho)>0$ and $\eta(\rho)>0$. This limits the choice to functions that have $r=2$, but it leaves the freedom of arbitrary viscosity.

Degond and Mas-Gallic [22] have generalized the formulation to an operator of the form $\nabla\cdot(\nu(\mathbf{x},t)\nabla)$ instead of $\nu\nabla^2$ with ν constant. This generalization could prove useful if one wishes to use this method in the context of *large eddy simulations* with a subgrid turbulent eddy viscosity.

Applying the above method to solving the incompressible

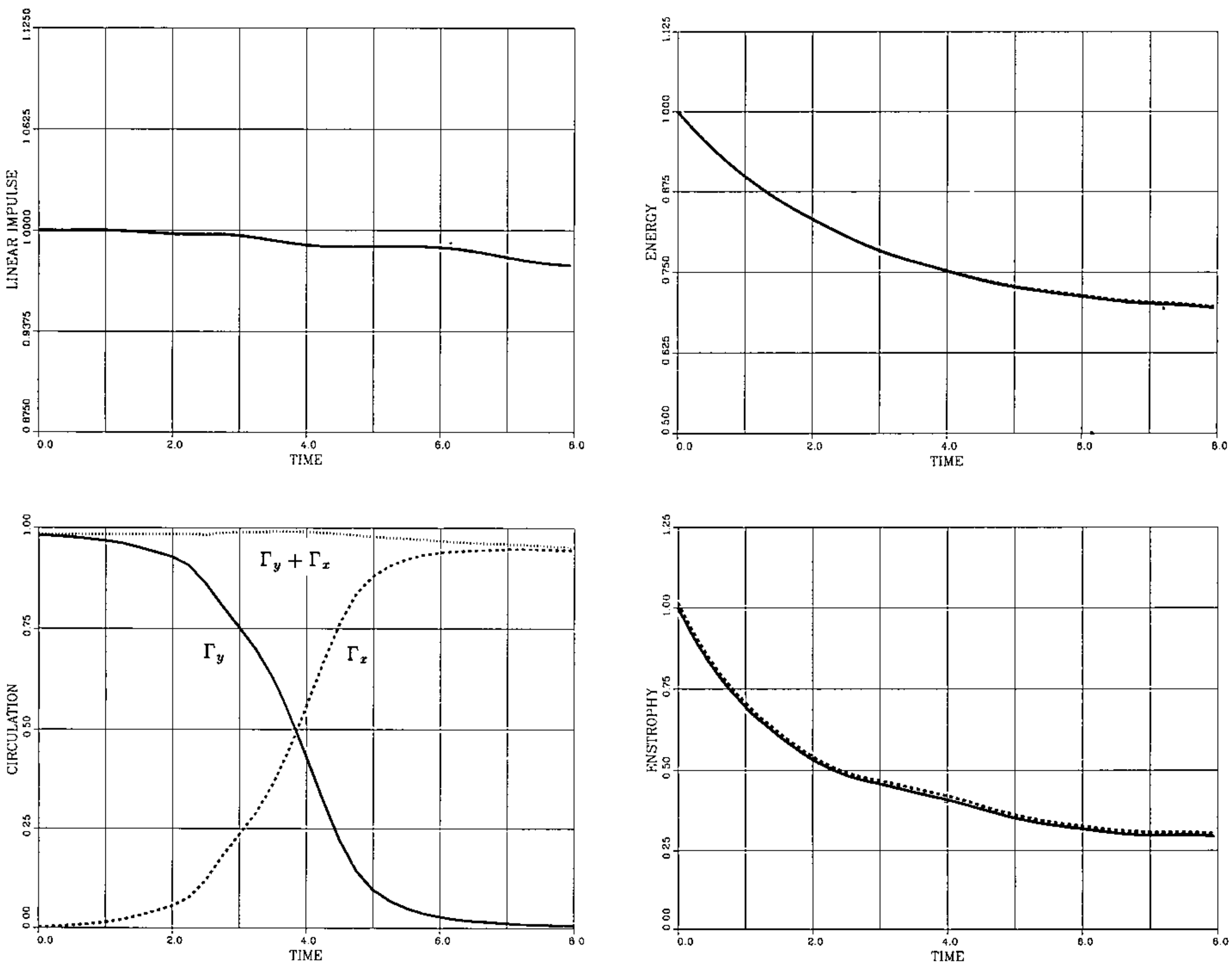

FIG. 12. Fusion of two vortex rings computed with the viscous method of regularized vortex particles and using the transpose scheme. Diagnostics I, Γ, E_σ (solid) and $\tilde{E}_\sigma$ (dash), $\mathcal{E}_\sigma$ (solid), and $\tilde{\mathcal{E}}_\sigma$ (dash).

vorticity equation, Eq. (3), with regularized vortex particles leads to the following scheme (see also Appendix A):

$$\frac{d}{dt}\mathbf{x}^p(t)=\mathbf{u}_\sigma(\mathbf{x}^p(t),t), \tag{55}$$

$$\frac{d}{dt}\boldsymbol{\alpha}^p(t)=(\boldsymbol{\alpha}^p(t)\cdot\nabla)\,\mathbf{u}_\sigma(\mathbf{x}^p(t),t)+\frac{2\nu}{\sigma^2}\sum_q (vol^p\boldsymbol{\alpha}^q(t)-vol^q\boldsymbol{\alpha}^p(t))\times\eta_\sigma(\mathbf{x}^p(t)-\mathbf{x}^q(t)). \tag{56}$$

The viscous method (using the transpose scheme) was applied to the computation of the fusion of two vortex rings at $\mathrm{Re}=\Gamma/\nu=400$, Figs. 11 and 12. (This computation is presented here for the sake of illustration. It is intended to present the results in more depth and to put them in the context of other researchers' work in another paper.) The computation goes through the entire fusion process with successful reconnection of the vortex tubes. No particle addition or relaxation of $\nabla\cdot\tilde{\boldsymbol{\omega}}_\sigma$ was used. Nevertheless, (1) linear impulse is nearly conserved (98%); (2) E_σ and $\tilde{E}_\sigma$; and (3) $\mathscr{E}_\sigma$ and $\tilde{\mathscr{E}}_\sigma$ remain nearly identical (see Appendix C). Hence, it appears that viscous diffusion helps maintain a nearly divergence-free particle field $\tilde{\boldsymbol{\omega}}_\sigma$. The decay rate of the kinetic energy follows Eq. (96). Finally, the circulation of the reconnecting vortex tubes is also nearly conserved: curves of Γ_y and Γ_x. (Note that, because the Gaussian vorticity distributions of the two rings overlap slightly at $t=0$, $\Gamma_y(0)$ is not exactly equal to unity.)

5. VORTEX PARTICLES AND CONSERVATION LAWS

The behavior of the method with respect to conservation laws is now examined. Conservation laws for 3D unbounded flows are reviewed in Appendix B.

First, the conservation of the linear invariants is examined. (These will be referred to as *invariants* when the real physical flow is understood and as *diagnostics* when the computed flow is understood.) For a system of singular vortex particles, the linear diagnostics (89), (90), and (91) become

$$\boldsymbol{\Omega}=\sum_p \boldsymbol{\alpha}^p(t), \tag{57}$$

$$\mathbf{I}=\tfrac{1}{2}\sum_p \mathbf{x}^p(t)\times\boldsymbol{\alpha}^p(t), \tag{58}$$

$$\mathbf{A}=\tfrac{1}{3}\sum_p \mathbf{x}^p(t)\times(\mathbf{x}^p(t)\times\boldsymbol{\alpha}^p(t)). \tag{59}$$

For a system of regularized vortex particles, the above expressions for $\boldsymbol{\Omega}$ and $\mathbf{I}$ still hold. $\mathbf{A}$ is obtained as

$$\mathbf{A}=\tfrac{1}{3}\sum_p \mathbf{x}^p(t)\times(\mathbf{x}^p(t)\times\boldsymbol{\alpha}^p(t))-\tfrac{2}{9}C\sigma^2\boldsymbol{\Omega}, \tag{60}$$

where

$$C=4\pi\int_0^\infty \zeta(\rho)\,\rho^4\,d\rho. \tag{61}$$

With the high order algebraic smoothing (42), $C=\frac{3}{2}$. With the low order algebraic smoothing (41), the right-hand side of Eq. (61) diverges logarithmically. Since $\boldsymbol{\Omega}=0$ for 3D unbounded flows, A reduces to Eq. (59).

The conservation of total vorticity $\boldsymbol{\Omega}$ and linear impulse $\mathbf{I}$ of a system of vortex particles is now examined. First define the notation

$$\mathbf{K}^{pq}=\mathbf{K}(\mathbf{x}-\mathbf{x}^q(t))\big|_{\mathbf{x}=\mathbf{x}^p(t)};\qquad \frac{\partial\mathbf{K}^{pq}}{\partial x_i}=\frac{\partial}{\partial x_i}\mathbf{K}(\mathbf{x}-\mathbf{x}^q(t))\big|_{\mathbf{x}=\mathbf{x}^p(t)}, \tag{62}$$

where $\mathbf{K}$ is the Biot–Savart kernel (Eq. (7) for singular particles, and Eq. (29) for regularized particles). Note that $\mathbf{K}^{pq}=-\mathbf{K}^{qp}$ and that $\partial\mathbf{K}^{pq}/\partial x_i=\partial\mathbf{K}^{qp}/\partial x_i$. With the transpose scheme, the evolution equations for the particle position and strength vector become

$$\frac{d}{dt}x_i^p=\sum_q(\mathbf{K}^{pq}\times\boldsymbol{\alpha}^q)_i, \tag{63}$$

$$\frac{d}{dt}\alpha_i^p=\boldsymbol{\alpha}^p\cdot\left(\sum_q\frac{\partial\mathbf{K}^{pq}}{\partial x_i}\times\boldsymbol{\alpha}^q\right)=-\sum_q\frac{\partial\mathbf{K}^{pq}}{\partial x_i}\cdot(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q). \tag{64}$$

The total vorticity is conserved by the transpose scheme as noted by Choquin and Cottet [13]. Indeed,

$$\frac{d}{dt}\boldsymbol{\Omega}=\frac{d}{dt}\left(\sum_p\alpha_i^p\right)=-\sum_{p,q}\frac{\partial\mathbf{K}^{pq}}{\partial x_i}\cdot(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q)=0, \tag{65}$$

since one sums on all pairs (p,q) and $\partial\mathbf{K}^{pq}/\partial x_i=\partial\mathbf{K}^{qp}/\partial x_i$. It is easy to see that the classical scheme or the mixed scheme do not conserve total vorticity in general.

The investigation of the linear impulse is more complicated (Cottet and Winckelmans 1987, private communication). One must examine

$$\frac{d}{dt}\mathbf{I}=\frac{d}{dt}\left(\frac{1}{2}\sum_p\mathbf{x}^p\times\boldsymbol{\alpha}^p\right)=\frac{1}{2}\sum_p\left(\frac{d}{dt}\mathbf{x}^p\times\boldsymbol{\alpha}^p\right)+\frac{1}{2}\sum_p\left(\mathbf{x}^p\times\frac{d}{dt}\boldsymbol{\alpha}^p\right). \tag{66}$$

The first term in Eq. (66) is equal to

$$\tfrac{1}{2}\sum_{p,q} (\mathbf{K}^{pq}\times\boldsymbol{\alpha}^q)\times\boldsymbol{\alpha}^p = -\tfrac{1}{2}\sum_{p,q} \boldsymbol{\alpha}^p\times(\mathbf{K}^{pq}\times\boldsymbol{\alpha}^q). \quad (67)$$

The second term in Eq. (67) must be examined in more detail. Using suffix notation, this term becomes

$$\begin{aligned}\frac{1}{2}\sum_p\left(\mathbf{x}^p\times\frac{d}{dt}\boldsymbol{\alpha}^p\right)_i &= -\frac{1}{2}\sum_{p,q}\varepsilon_{ijk}x_j^p\frac{\partial\mathbf{K}^{pq}}{\partial x_k}\cdot(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q)\\ &= -\frac{1}{4}\sum_{p,q}\varepsilon_{ijk}(x_j^p-x_j^q)\frac{\partial\mathbf{K}^{pq}}{\partial x_k}\cdot(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q)\\ &\quad -\frac{1}{4}\sum_{p,q}\varepsilon_{ijk}(x_j^p+x_j^q)\frac{\partial\mathbf{K}^{pq}}{\partial x_k}\cdot(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q). \quad (68)\end{aligned}$$

The second sum in Eq. (68) vanishes since one sums on all pairs (p, q) and $\partial\mathbf{K}^{pq}/\partial x_k = \partial\mathbf{K}^{qp}/\partial x_k$. Recalling that, for singular particles,

$$\frac{\partial K_l}{\partial x_k}=\frac{\partial}{\partial x_k}\left(-\frac{x_l}{4\pi\,|\mathbf{x}|^3}\right)=-\frac{\delta_{lk}}{4\pi\,|\mathbf{x}|^3}+3\frac{x_lx_k}{4\pi\,|\mathbf{x}|^5}, \quad (69)$$

one obtains

$$\begin{aligned}\frac{1}{2}\sum_p\left(\mathbf{x}^p\times\frac{d}{dt}\boldsymbol{\alpha}^p\right)_i &= \frac{1}{4}\sum_{p,q}\varepsilon_{ijk}\frac{(x_j^p-x_j^q)}{4\pi\,|\mathbf{x}^p-\mathbf{x}^q|^3}(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q)_k\\ &\quad -\frac{3}{4}\sum_{p,q}\varepsilon_{ijk}\frac{(x_j^p-x_j^q)(x_k^p-x_k^q)}{4\pi\,|\mathbf{x}^p-\mathbf{x}^q|^5}\\ &\quad \times((\mathbf{x}^p-\mathbf{x}^q)\cdot(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q))\\ &= \frac{1}{4}\sum_{p,q}\varepsilon_{ijk}\frac{(x_j^p-x_j^q)}{4\pi\,|\mathbf{x}^p-\mathbf{x}^q|^3}(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q)_k\\ &\quad (\text{since } \varepsilon_{ijk}x_jx_k=0)\\ &= -\frac{1}{4}\sum_{p,q}(\mathbf{K}^{pq}\times(\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q))_i\\ &= -\frac{1}{2}\sum_{p,q}(\boldsymbol{\alpha}^p\times(\mathbf{K}^{pq}\times\boldsymbol{\alpha}^q))_i, \quad (70)\end{aligned}$$

where the last equality has been obtained using the symmetry property $\mathbf{K}^{pq} = -\mathbf{K}^{qp}$ and the vector identity: $\mathbf{a}\times(\mathbf{b}\times\mathbf{c})+\mathbf{b}\times(\mathbf{c}\times\mathbf{a})+\mathbf{c}\times(\mathbf{a}\times\mathbf{b})=0$. For regularized particles, one obtains:

$$\begin{aligned}\frac{\partial K_l}{\partial x_k}&=\frac{\partial}{\partial x_k}\left(-\frac{q_\sigma(\mathbf{x})}{|\mathbf{x}|^3}x_l\right)\\ &= -\frac{q_\sigma(\mathbf{x})}{|\mathbf{x}|^3}\delta_{lk}+\left(3\frac{q_\sigma(\mathbf{x})}{|\mathbf{x}|^3}-\zeta_\sigma(\mathbf{x})\right)\frac{x_lx_k}{|\mathbf{x}|^2}, \quad (71)\end{aligned}$$

so that the same result as for singular particles, Eq. (70), is obtained. Finally, combining Eqs. (67) and (70), one obtains, for both singular or regularized particles,

$$\begin{aligned}\frac{d}{dt}\mathbf{I}&=\frac{d}{dt}\left(\frac{1}{2}\sum_p\mathbf{x}^p\times\boldsymbol{\alpha}^p\right)\\ &= -\sum_{p,q}\boldsymbol{\alpha}^p\times(\mathbf{K}^{pq}\times\boldsymbol{\alpha}^q). \quad (72)\end{aligned}$$

The right-hand side of Eq. (72) is essentially a particle discretization of $-\int\boldsymbol{\omega}\times\mathbf{u}\,d\mathbf{x}$ and will be small as long as the particle field remains a good representation of $\boldsymbol{\omega}$. Indeed, if Eq. (1) integrated over an unbounded volume, one obtains that $\int\boldsymbol{\omega}\times\mathbf{u}\,d\mathbf{x}=0$ for a physical flow. The linear impulse is thus nearly conserved by the transpose scheme as long as the particle vorticity field remains a good representation of a divergence-free field. Now, since all schemes for the stretching of the vorticity vector are identical when this condition is satisfied, it follows that linear impulse is nearly conserved by all schemes as long as the particle field remains a good representation of a divergence-free field. For singular particles, it was seen numerically that the transpose scheme is the only one that performs well on the conservation of linear impulse. Recall that it is also the only one which constitutes a weak solution of the "transpose vorticity equation." For regularized particles, all schemes appear to perform equally.

The conservation of the angular impulse, $\mathbf{A}$, was not investigated theoretically. Numerical experiments indicate that $\mathbf{A}$ is not generally conserved by the method but that it is conserved as long as the particle vorticity field remains a good representation of a divergence-free field.

One must now investigate the conservation of the linear invariants when the viscous method is used. First, it is easy to see that the viscous integral operator (49) is conservative (i.e., conserves total vorticity). Indeed,

$$\iint(\boldsymbol{\omega}(\mathbf{y})-\boldsymbol{\omega}(\mathbf{x}))\,\eta_\sigma(\mathbf{x}-\mathbf{y})\,d\mathbf{y}\,d\mathbf{x}=0. \quad (73)$$

The particle discretization (56) of the integral operator is also conservative since

$$\sum_{p,q}(vol^p\boldsymbol{\alpha}^q-vol^q\boldsymbol{\alpha}^p)\,\eta_\sigma(\mathbf{x}^p-\mathbf{x}^q)=0. \quad (74)$$

Thus, the total vorticity is not affected by the treatment of viscous diffusion. Second, as pointed out by Mas-Gallic (private communication, 1988), the linear impulse is also not affected by the viscous integral operator but is affected by the particle discretization of the integral operator. Indeed, since

$$0 = \int \mathbf{x}' \eta_\sigma(\mathbf{x}')\, d\mathbf{x}' = \int (\mathbf{x}-\mathbf{y})\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{x}, \qquad (75)$$

so that

$$\int \mathbf{x}\eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{x} = \int \mathbf{y}\eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{x}, \qquad (76)$$

one obtains

$$\begin{aligned}
\int \mathbf{x} \times \left[\int (\boldsymbol{\omega}(\mathbf{y}) - \boldsymbol{\omega}(\mathbf{x}))\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{y} \right] d\mathbf{x}
&= \int \left[\int \mathbf{x}\eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{x} \right] \times \boldsymbol{\omega}(\mathbf{y})\, d\mathbf{y} \\
&\quad - \iint \mathbf{x} \times \boldsymbol{\omega}(\mathbf{x})\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\
&= \int \left[\int \mathbf{y}\eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{x} \right] \times \boldsymbol{\omega}(\mathbf{y})\, d\mathbf{y} \\
&\quad - \iint \mathbf{x} \times \boldsymbol{\omega}(\mathbf{x})\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\
&= \iint \mathbf{y} \times \boldsymbol{\omega}(\mathbf{y})\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{x}\, d\mathbf{y} \\
&\quad - \iint \mathbf{x} \times \boldsymbol{\omega}(\mathbf{x})\, \eta_\sigma(\mathbf{x}-\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\
&= 0, \qquad (77)
\end{aligned}$$

by interchanging the role of $\mathbf{x}$ and $\mathbf{y}$ in the first integral. If one now considers the particle discretization of the integral operator, one obtains

$$\begin{aligned}
\sum_p \mathbf{x}^p \times \left[\sum_q (vol^p \boldsymbol{\alpha}^q - vol^q \boldsymbol{\alpha}^p)\, \eta_\sigma(\mathbf{x}^p - \mathbf{x}^q) \right]
&= \tfrac{1}{2} \sum_{p,q} (\mathbf{x}^p - \mathbf{x}^q) \times (vol^p \boldsymbol{\alpha}^q - vol^q \boldsymbol{\alpha}^p)\, \eta_\sigma(\mathbf{x}^p - \mathbf{x}^q) \qquad (78)
\end{aligned}$$

which does not vanish, in general. It is thus a matter of discretization to conserve linear impulse with the particle approximation of the integral operator.

The evaluation of the "once-regularized" quadratic diagnostics, energy E_σ, helicity $\mathscr{H}_\sigma$, and enstrophy $\mathscr{E}_\sigma$, is involved. The difficulty comes from the fact that the particle field, $\tilde{\boldsymbol{\omega}}_\sigma$ is not generally divergence-free. The derivation of the appropriate expressions is presented in detail in Appendix C. In particular, the high order algebraic smoothing (42) is a case for which closed form expressions for all quadratic diagnostics can be obtained.

The inviscid method of vortex particles, both singular and regularized, does not generally conserve kinetic energy and helicity exactly with any of the choices for the stretching term. These quantities are thus used as diagnostics to measure the performance of the method on a particular problem. With singular particles, it is found numerically that the transpose scheme again performs best. With regularized particles, it is found that all schemes perform equally.

In viscous computations, the decay of the kinetic energy is used as a diagnostic to check if Eq. (96) is satisfied.

6. SUMMARY AND CONCLUSIONS

- The method of 3D vortex particles was investigated, both theoretically and numerically. Both singular and regularized particles were considered. The method suffers from the fact that the particle representation of the vorticity field is not guaranteed to remain a good representation of a divergence-free field for long times. Different evolution equations for the strength vector were reviewed. With singular particles, the *transpose scheme* leads to a weak solution of the "transpose vorticity equation" and was also shown numerically to perform best on the conservation laws.

- For regularized particles, a relaxation scheme which forces the particle vorticity field to remain nearly divergence-free for all times was introduced.

- Addition and/or redistribution of computational elements is necessary wherever stretching is intense.

- In inviscid flows, vortex tubes retain their identity and move as material volumes. The vortex filament method which is based on these simple facts could, in some cases, be preferred to the vortex particle method when computing inviscid flows. Indeed, with vortex filaments, the filament vorticity field is divergence-free.

- For viscous flows, filament methods cannot generally be used. A viscous version of the method of regularized vortex particles was developed. The method proved successful in computing vortex tube interactions where viscosity plays an major role such as vortex reconnection.

- A new 3D regularization function was introduced: the *high order algebraic smoothing*. It is numerically convenient and has convergence properties equal to those of Gaussian smoothing. This smoothing is also a case for which closed form expressions for all global quadratic diagnostics (energy, helicity, and enstrophy) can be obtained.

- Linear and quadratic global diagnostics proved very useful in assessing the accuracy and consistency of numerical computations with respect to known conservation laws.

APPENDIX A: THE EVOLUTION EQUATIONS FOR A SET OF VORTEX PARTICLES

For $1 \leqslant p \leqslant N$,

$$\frac{d}{dt}\mathbf{x}^p = \mathbf{u}_\sigma(\mathbf{x}^p) = -\sum_q \frac{q_\sigma(\mathbf{x}^p - \mathbf{x}^q)}{|\mathbf{x}^p - \mathbf{x}^q|^3}(\mathbf{x}^p - \mathbf{x}^q) \times \boldsymbol{\alpha}^q. \quad (79)$$

For the classical scheme,

$$\frac{d}{dt}\alpha_i^p = \alpha_l^p \frac{\partial u_i}{\partial x_l} = \alpha_l^p \frac{\partial}{\partial x_l}\left[\sum_q \varepsilon_{ijk}\frac{\partial}{\partial x_j} G_\sigma(\mathbf{x} - \mathbf{x}^q)\,\alpha_k^q\right]_{\mathbf{x}=\mathbf{x}^p}$$
$$= \sum_q \varepsilon_{ijk}\alpha_l^p \alpha_k^q \left(\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_j} G_\sigma(\mathbf{x}-\mathbf{x}^q)\right)_{\mathbf{x}=\mathbf{x}^p}. \quad (80)$$

Recalling that $\rho = |\mathbf{x}|/\sigma = (x_m x_m)^{1/2}/\sigma$ with $\partial\rho/\partial x_i = x_i/\sigma^2\rho$ and that $-(1/\rho)(dG/d\rho) = q(\rho)/\rho^3$, one obtains

$$\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_j} G_\sigma(\mathbf{x}) = -\frac{1}{\sigma^3}\left[\frac{q(\rho)}{\rho^3}\delta_{lj} - \frac{x_j x_l}{\sigma^2} \times \left(-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right)\right)\right], \quad (81)$$

so that finally, for the classical scheme,

$$\frac{d}{dt}\alpha_i^p = \sum_q \frac{1}{\sigma^3}\varepsilon_{ijk}\alpha_l^p\alpha_k^q\left[-\frac{q(\rho)}{\rho^3}\delta_{jl} + \frac{1}{\sigma^2} \times \left(-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right)\right)(x_j^p - x_j^q)(x_l^p - x_l^q)\right],$$
$$\frac{d}{dt}\boldsymbol{\alpha}^p = \sum_q \frac{1}{\sigma^3}\left[-\frac{q(\rho)}{\rho^3}\boldsymbol{\alpha}^p \times \boldsymbol{\alpha}^q + \frac{1}{\sigma^2}\left(-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right)\right) \times (\boldsymbol{\alpha}^p\cdot(\mathbf{x}^p - \mathbf{x}^q))((\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q)\right], \quad (82)$$

with $\rho = |\mathbf{x}^p - \mathbf{x}^q|/\sigma$. In a similar way, the transpose scheme gives

$$\frac{d}{dt}\alpha_i^p = \alpha_l^p \frac{\partial u_l}{\partial x_i} = \alpha_l^p \frac{\partial}{\partial x_i}\left[\sum_q \varepsilon_{ljk}\frac{\partial}{\partial x_j} G_\sigma(\mathbf{x} - \mathbf{x}^q)\,\alpha_k^q\right]_{\mathbf{x}=\mathbf{x}^p}, \quad (83)$$

which leads to

$$\frac{d}{dt}\boldsymbol{\alpha}^p = \sum_q \frac{1}{\sigma^3}\left[\frac{q(\rho)}{\rho^3}\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q + \frac{1}{\sigma^2}\left(-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right)\right) \times (\boldsymbol{\alpha}^p\cdot((\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q))(\mathbf{x}^p - \mathbf{x}^q)\right]. \quad (84)$$

The combination of the above two schemes gives the mixed scheme

$$\frac{d}{dt}\boldsymbol{\alpha}^p = \sum_q \frac{1}{2}\frac{1}{\sigma^5}\left(-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right)\right) \times [(\boldsymbol{\alpha}^p\cdot(\mathbf{x}^p - \mathbf{x}^q))((\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q) + (\boldsymbol{\alpha}^p\cdot((\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q))(\mathbf{x}^p - \mathbf{x}^q)]. \quad (85)$$

In the above formulas, the term $-(1/\rho)(d/d\rho)(q(\rho)/\rho^3)$ can be evaluated directly or by recalling that

$$-\frac{1}{\rho}\frac{d}{d\rho}\left(\frac{q(\rho)}{\rho^3}\right) = \frac{1}{\rho^2}\left(3\frac{q(\rho)}{\rho^3} - \zeta(\rho)\right). \quad (86)$$

The case of singular vortex particles is obtained by setting $4\pi q(\rho) = 1$ with $4\pi(-(1/\rho)(d/d\rho)(q(\rho)/\rho^3)) = 3/\rho^5$ and by excluding the $q = p$ term from the above sums.

The equations obtained with the high order algebraic smoothing (42) and with viscous diffusion are

$$\frac{d}{dt}\mathbf{x}^p = -\frac{1}{4\pi}\sum_q \frac{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \frac{5}{2}\sigma^2)}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{5/2}}(\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q, \quad (87)$$

$$\frac{d}{dt}\boldsymbol{\alpha}^p = \frac{1}{4\pi}\sum_q\left[-\frac{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \frac{5}{2}\sigma^2)}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{5/2}}\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q + 3\frac{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \frac{7}{2}\sigma^2)}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{7/2}} \times (\boldsymbol{\alpha}^p\cdot(\mathbf{x}^p - \mathbf{x}^q))((\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q) + 105\nu\frac{\sigma^4}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{9/2}} \times (vol^p\boldsymbol{\alpha}^q - vol^q\boldsymbol{\alpha}^p)\right] \quad \text{(classical scheme)}$$

$$\frac{d}{dt}\boldsymbol{\alpha}^p = \frac{1}{4\pi}\sum_q\left[\frac{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \frac{5}{2}\sigma^2)}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{5/2}}\boldsymbol{\alpha}^p\times\boldsymbol{\alpha}^q + 3\frac{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \frac{7}{2}\sigma^2)}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{7/2}} \times (\boldsymbol{\alpha}^p\cdot((\mathbf{x}^p - \mathbf{x}^q)\times\boldsymbol{\alpha}^q))(\mathbf{x}^p - \mathbf{x}^q) + 105\nu\frac{\sigma^4}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{9/2}} \times (vol^p\boldsymbol{\alpha}^q - vol^q\boldsymbol{\alpha}^p)\right] \quad \text{(transpose scheme)} \quad (88)$$

$$\frac{d}{dt}\boldsymbol{\alpha}^p = \frac{1}{4\pi}\sum_q \left[\frac{3}{2}\frac{(|\mathbf{x}^p-\mathbf{x}^q|^2+\frac{7}{2}\sigma^2)}{(|\mathbf{x}^p-\mathbf{x}^q|^2+\sigma^2)^{7/2}} \times ((\boldsymbol{\alpha}^p\cdot(\mathbf{x}^p-\mathbf{x}^q))((\mathbf{x}^p-\mathbf{x}^q)\times\boldsymbol{\alpha}^q) + (\boldsymbol{\alpha}^p\cdot((\mathbf{x}^p-\mathbf{x}^q)\times\boldsymbol{\alpha}^q))(\mathbf{x}^p-\mathbf{x}^q)) + 105\nu\frac{\sigma^4}{(|\mathbf{x}^p-\mathbf{x}^q|^2+\sigma^2)^{9/2}} \times (vol^p\boldsymbol{\alpha}^q - vol^q\boldsymbol{\alpha}^p)\right] \quad \text{(mixed scheme).}$$

APPENDIX B: CONSERVATION LAWS FOR THREE-DIMENSIONAL INCOMPRESSIBLE UNBOUNDED FLOWS

In what follows, the density is taken as unity. Only 3D unbounded flows with zero vorticity at infinity are considered. The total vorticity is therefore zero.

In inviscid flows, there are three linear invariants associated with conservation of total vorticity, linear impulse and angular impulse (Batchelor [4]):

$$\boldsymbol{\Omega} = \int \boldsymbol{\omega}\, d\mathbf{x} = 0, \tag{89}$$

$$\mathbf{I} = \int \mathbf{u}\, d\mathbf{x} = \tfrac{1}{2}\int \mathbf{x}\times\boldsymbol{\omega}\, d\mathbf{x}, \tag{90}$$

$$\mathbf{A} = \int \mathbf{x}\times\mathbf{u}\, d\mathbf{x} = \tfrac{1}{3}\int \mathbf{x}\times(\mathbf{x}\times\boldsymbol{\omega})\, d\mathbf{x}. \tag{91}$$

There are also two quadratic invariants associated with conservation of kinetic energy and helicity

$$E = \tfrac{1}{2}\int \mathbf{u}\cdot\mathbf{u}\, d\mathbf{x} = \tfrac{1}{2}\int \boldsymbol{\psi}\cdot\boldsymbol{\omega}\, d\mathbf{x}, \tag{92}$$

$$\mathscr{H} = \int \boldsymbol{\omega}\cdot\mathbf{u}\, d\mathbf{x}. \tag{93}$$

In viscous unbounded flows, $\boldsymbol{\Omega}=0$, $\mathbf{I}$ and $\mathbf{A}$ are also conserved. The kinetic energy, E, is not conserved. Indeed, taking the dot product of $\mathbf{u}$ with the momentum equation and integrating over an unbounded volume (Lamb [29] and Batchelor [4]),

$$\frac{d}{dt}E = -2\nu\int e_{ij}e_{ij}\, d\mathbf{x} = -\int \boldsymbol{\Phi}\, d\mathbf{x}, \tag{94}$$

where $\boldsymbol{\Phi}$ is the dissipation function. From kinematics [29],

$$\boldsymbol{\Phi} = \nu\boldsymbol{\omega}\cdot\boldsymbol{\omega} + 2\nu\,\nabla\cdot((\mathbf{u}\cdot\nabla)\,\mathbf{u}), \tag{95}$$

so that one obtains

$$\frac{d}{dt}E = -\nu\mathscr{E}, \tag{96}$$

where

$$\mathscr{E} = \int \boldsymbol{\omega}\cdot\boldsymbol{\omega}\, d\mathbf{x} \tag{97}$$

is the enstrophy. Moffatt [33] showed that the helicity, $\mathscr{H}$, measures the net linkage of vortex lines. Thus, it is not conserved in viscous flows because of the reconnection of vortex lines. The enstrophy in not conserved in both inviscid or viscous flows because of the stretching of vortex lines. Taking the dot product of ω with the vorticity equation, one obtains (Batchelor [4])

$$\frac{\partial}{\partial t}\left(\frac{\omega_i\omega_i}{2}\right) + \frac{\partial}{\partial x_j}\left(\frac{\omega_i\omega_i}{2}u_j\right) = \omega_i\omega_j e_{ij} + \nu\omega_i\frac{\partial}{\partial x_j}\frac{\partial\omega_i}{\partial x_j} = \omega_i\omega_i e_{ij} + \nu\left[\frac{\partial}{\partial x_j}\frac{\partial}{\partial x_j}\left(\frac{\omega_i\omega_i}{2}\right) - \frac{\partial\omega_i}{\partial x_j}\frac{\partial\omega_i}{\partial x_j}\right] \tag{98}$$

so that, integrating over an unbounded volume,

$$\frac{d}{dt}\mathscr{E} = 2\int \omega_i\omega_j e_{ij}\, d\mathbf{x} - 2\nu\int \frac{\partial\omega_i}{\partial x_j}\frac{\partial\omega_i}{\partial x_j}\, d\mathbf{x}. \tag{99}$$

APPENDIX C: THE EVALUATION OF QUADRATIC DIAGNOSTICS

C.1. *The Singular Case*

The kinetic energy is given by

$$E = \tfrac{1}{2}\int \mathbf{u}\cdot\mathbf{u}\, d\mathbf{x} = \tfrac{1}{2}\int (\nabla\times\tilde{\boldsymbol{\psi}})\cdot(\nabla\times\tilde{\boldsymbol{\psi}})\, d\mathbf{x} = \tfrac{1}{2}\int \tilde{\boldsymbol{\psi}}\cdot(\nabla\times(\nabla\times\tilde{\boldsymbol{\psi}}))\, d\mathbf{x} = \tfrac{1}{2}\int \tilde{\boldsymbol{\psi}}\cdot(-\nabla^2\tilde{\boldsymbol{\psi}} + \nabla(\nabla\cdot\tilde{\boldsymbol{\psi}}))\, d\mathbf{x} = \tfrac{1}{2}\int \tilde{\boldsymbol{\psi}}\cdot\tilde{\boldsymbol{\omega}}\, d\mathbf{x} + \tfrac{1}{2}\int \tilde{\boldsymbol{\psi}}\cdot\nabla(\nabla\cdot\tilde{\boldsymbol{\psi}})\, d\mathbf{x}, \tag{100}$$

where integration by parts has been used. Due to the nonzero divergence of $\tilde{\boldsymbol{\psi}}$, the kinetic energy cannot be simply written as

$$\tilde{E} = \frac{1}{2}\int \tilde{\boldsymbol{\psi}}\cdot\tilde{\boldsymbol{\omega}}\, d\mathbf{x} = \left(\frac{1}{8\pi}\right)\sum_{\substack{p,q\\ p\neq q}} \frac{\boldsymbol{\alpha}^p\cdot\boldsymbol{\alpha}^q}{|\mathbf{x}^p-\mathbf{x}^q|}, \tag{101}$$

where the $q = p$ term has been removed to avoid an infinity in the evaluation of $\tilde{E}$. Aksman, Novikov, and Orszag [1] obtained the correct expression for the kinetic energy by considering the Fourier transform of the velocity field (7) and by integrating Eq. (100) in Fourier space:

$$E = \frac{1}{16\pi} \sum_{\substack{p,q \\ p \neq q}} \frac{1}{|\mathbf{x}^p - \mathbf{x}^q|} \left(\boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q + \frac{((\mathbf{x}^p - \mathbf{x}^q) \cdot \boldsymbol{\alpha}^p)}{|\mathbf{x}^p - \mathbf{x}^q|} \frac{((\mathbf{x}^p - \mathbf{x}^q) \cdot \boldsymbol{\alpha}^q)}{|\mathbf{x}^p - \mathbf{x}^q|} \right). \quad (102)$$

Direct integration of Eq. (100) in physical space can be done and leads to the same result.. The advantage of integrating directly in physical space is that the procedure can be extended to regularized particles. Going back to Eq. (100), one obtains, using suffix notation,

$$\begin{aligned} E &= \frac{1}{2} \left(\frac{1}{4\pi} \right)^2 \sum_{\substack{p,q \\ p \neq q}} \varepsilon_{ijk} \varepsilon_{iln} \alpha_k^p \alpha_n^q \times \int \frac{\partial}{\partial x_j} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right) \frac{\partial}{\partial x_l} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^q|} \right) d\mathbf{x} \\ &= \frac{1}{2} \left(\frac{1}{4\pi} \right)^2 \sum_{\substack{p,q \\ p \neq q}} (\delta_{jl} \delta_{kn} - \delta_{jn} \delta_{kl}) \alpha_k^p \alpha_n^q \frac{\partial}{\partial x_j^p} \frac{\partial}{\partial x_l^q} \times \left(\int \frac{1}{|\mathbf{x} - \mathbf{x}^p|} \frac{1}{|\mathbf{x} - \mathbf{x}^q|} d\mathbf{x} \right), \end{aligned} \quad (103)$$

where use of the symmetry relation $(\partial/\partial x_i)(1/|\mathbf{x} - \mathbf{x}^p|) = -(\partial/\partial x_i^p)(1/|\mathbf{x} - \mathbf{x}^p|)$ has been made. Considering a local spherical coordinate system centered at $\mathbf{x}^p$ and defining $\mathbf{x} - \mathbf{x}^p = \mathbf{x}'$, $\mathbf{x} - \mathbf{x}^q = \mathbf{x}' + (\mathbf{x}^p - \mathbf{x}^q)$, $d\mathbf{x} = d\mathbf{x}' = dr\, r d\theta\, r \sin\theta\, d\phi = -r^2\, dr\, d\mu\, d\phi$ with $\mu = \cos\theta$ and $z = |\mathbf{x}^p - \mathbf{x}^q|$, one obtains

$$\int \frac{1}{|\mathbf{x} - \mathbf{x}^p|} \frac{1}{|\mathbf{x} - \mathbf{x}^q|} d\mathbf{x} = \int_0^{2\pi} d\phi \int_0^\infty dr \int_{-1}^1 d\mu \frac{r}{(r^2 + 2rz\mu + z^2)^{1/2}}. \quad (104)$$

This integral does not converge. However, since only derivatives of this integral with respect to z are of interest $((\partial/\partial x_j^p) \int \cdots d\mathbf{x} = (\partial z/\partial x_j^p)(d/dz) \int \cdots d\mathbf{x})$, a converging factor that is independent of z can be added to the integral:

$$\begin{aligned} I &= 2\pi \int_0^\infty dr \int_{-1}^1 d\mu \left(\frac{r}{(r^2 + 2rz\mu + z^2)^{1/2}} - 1 \right) \\ &= 2\pi \int_0^\infty \left[\frac{(r^2 + 2rz\mu + z^2)^{1/2}}{z} - \mu \right]_{-1}^1 dr \\ &= 2\pi \int_0^\infty \left(\frac{|r+z| - |r-z|}{z} - 2 \right) dr \\ &= 2\pi z \int_0^\infty (|t+1| - |t-1| - 2)\, dt \\ &= 2\pi z \int_0^1 (2t - 2)\, dt = -(2\pi) z. \end{aligned} \quad (105)$$

Differentiating I gives

$$\begin{aligned} \frac{\partial}{\partial x_j^p} \frac{\partial}{\partial x_l^q} (-(2\pi) z) &= \frac{\partial}{\partial x_j^p} \left(\frac{\partial z}{\partial x_l^q} \frac{d}{dz} (-2\pi z) \right) \\ &= -2\pi \frac{\partial}{\partial x_j^p} \left(\frac{\partial z}{\partial x_l^q} \right) = 2\pi \frac{\partial}{\partial x_j^p} \left(\frac{(x_l^p - x_l^q)}{z} \right) \\ &= 2\pi \left(\frac{\delta_{jl}}{z} - \frac{(x_j^p - x_j^q)(x_l^p - x_l^q)}{z^3} \right) \end{aligned} \quad (106)$$

so that the kinetic energy is finally obtained as

$$\begin{aligned} E &= \frac{1}{16\pi} \sum_{\substack{p,q \\ p \neq q}} (\delta_{jl} \delta_{kn} - \delta_{jn} \delta_{kl}) \alpha_k^p \alpha_n^q \times \left(\frac{\delta_{jl}}{|\mathbf{x}^p - \mathbf{x}^q|} - \frac{(x_l^p - x_l^q)(x_j^p - x_j^q)}{|\mathbf{x}^p - \mathbf{x}^q|^3} \right) \\ &= \frac{1}{16\pi} \sum_{\substack{p,q \\ p \neq q}} \frac{1}{|\mathbf{x}^p - \mathbf{x}^q|} \left(\boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q + \frac{((\mathbf{x}^p - \mathbf{x}^q) \cdot \boldsymbol{\alpha}^p)}{|\mathbf{x}^p - \mathbf{x}^q|} \frac{((\mathbf{x}^p - \mathbf{x}^q) \cdot \boldsymbol{\alpha}^q)}{|\mathbf{x}^p - \mathbf{x}^q|} \right). \end{aligned} \quad (107)$$

The result of Aksman, Novikov, and Orszag [1] has thus been recovered using a different method. Equation (107) can be written as

$$E = \frac{1}{16\pi} \sum_{\substack{p,q \\ p \neq q}} \frac{1}{|\mathbf{x}^p - \mathbf{x}^q|} \left[2\boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q + \left(\frac{((\mathbf{x}^p - \mathbf{x}^q) \cdot \boldsymbol{\alpha}^p)}{|\mathbf{x}^p - \mathbf{x}^q|} \times \frac{((\mathbf{x}^p - \mathbf{x}^q) \cdot \boldsymbol{\alpha}^q)}{|\mathbf{x}^p - \mathbf{x}^q|} - \boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q \right) \right]. \quad (108)$$

In this form, the correct expression for the kinetic energy can easily be compared with Eq. (101). The first term in Eq. (108) is equal to $\frac{1}{2} \int \tilde{\boldsymbol{\psi}} \cdot \tilde{\boldsymbol{\omega}}\, d\mathbf{x}$. The second term is equal to $\frac{1}{2} \int \tilde{\boldsymbol{\psi}} \cdot \nabla(\nabla \cdot \tilde{\boldsymbol{\psi}})\, d\mathbf{x}$. This term remains negligible as long as $\tilde{\boldsymbol{\omega}}$ remains a good representation of $\boldsymbol{\omega}$. In fact, the difference between the two expressions can be used as a diagnostic to check the consistency of numerical computations.

Proceeding now with the evaluation of the helicity,

$$\mathscr{H} = \int \boldsymbol{\omega} \cdot \mathbf{u}\, d\mathbf{x}, \tag{109}$$

one obtains

$$\begin{aligned}\mathscr{H} &= \int \left(\sum_p \boldsymbol{\alpha}^p\, \delta(\mathbf{x}-\mathbf{x}^p) + \nabla \left(\boldsymbol{\alpha}^p \cdot \nabla \left(\frac{1}{4\pi\, |\mathbf{x}-\mathbf{x}^p|} \right)\right)\right) \\ &\quad \cdot \left(\sum_q \nabla \left(\frac{1}{4\pi\, |\mathbf{x}-\mathbf{x}^q|} \right) \times \boldsymbol{\alpha}^q \right) d\mathbf{x} \\ &= -\frac{1}{4\pi} \sum_{p,q} \boldsymbol{\alpha}^p \cdot \left(\frac{(\mathbf{x}^p-\mathbf{x}^q)}{|\mathbf{x}^p-\mathbf{x}^q|^3} \times \boldsymbol{\alpha}^q \right) \\ &\quad + \left(\frac{1}{4\pi}\right)^2 \sum_{p,q} \varepsilon_{ijk} \alpha_l^p \alpha_k^q \int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_l} \\ &\quad \times \left(\frac{1}{|\mathbf{x}-\mathbf{x}^p|} \right) \frac{\partial}{\partial x_j} \left(\frac{1}{|\mathbf{x}-\mathbf{x}^q|} \right) d\mathbf{x}. \end{aligned} \tag{110}$$

The second term in (110) vanishes. Indeed,

$$\begin{aligned} &\varepsilon_{ijk} \alpha_l^p \alpha_k^q \int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_l} \left(\frac{1}{|\mathbf{x}-\mathbf{x}^p|} \right) \frac{\partial}{\partial x_j} \left(\frac{1}{|\mathbf{x}-\mathbf{x}^q|} \right) d\mathbf{x} \\ &= -\varepsilon_{ijk} \alpha_l^p \alpha_k^q \frac{\partial}{\partial x_i^p} \frac{\partial}{\partial x_l^p} \frac{\partial}{\partial x_j^q} \int \frac{1}{|\mathbf{x}-\mathbf{x}^p|} \frac{1}{|\mathbf{x}-\mathbf{x}^q|} d\mathbf{x} \\ &= 2\pi \varepsilon_{ijk} \alpha_l^p \alpha_k^q \frac{\partial}{\partial x_i^p} \frac{\partial}{\partial x_l^p} \left(\frac{\partial z}{\partial x_j^q} \right) \\ &= 2\pi \varepsilon_{ijk} \alpha_l^p \alpha_k^q \frac{\partial}{\partial x_i^p} \frac{\partial}{\partial x_l^p} \left(-\frac{\partial z}{\partial x_j^p} \right) = 0, \end{aligned} \tag{111}$$

since $\varepsilon_{ijk}(\partial/\partial x_i)(\partial/\partial x_j) = 0$. Thus,

$$\mathscr{H} = \frac{1}{4\pi} \sum_{p,q} \frac{(\mathbf{x}^p-\mathbf{x}^q)}{|\mathbf{x}^p-\mathbf{x}^q|^3} \cdot (\boldsymbol{\alpha}^p \times \boldsymbol{\alpha}^q). \tag{112}$$

The case $q = p$ is a removable singularity since $\boldsymbol{\alpha}^p \times \boldsymbol{\alpha}^p = 0$.

Finally, the enstrophy is not defined since the evaluation of

$$\mathscr{E} = \int \boldsymbol{\omega} \cdot \boldsymbol{\omega}\, d\mathbf{x} \tag{113}$$

amounts to integrating the square of the δ-function.

C.2. *The Regularized Case*

We refer to Chorin [11] for previous work on the evaluation of quadratic diagnostics when using a vortex model made of regularized straight-line segments: the "vortex lattice model."

"Twice-regularized" quadratic diagnostics are difficult to evaluate when considering regularized methods, filaments, or particles. For instance, the integral,

$$E_{\sigma\sigma} = \tfrac{1}{2} \int \mathbf{u}_\sigma \cdot \mathbf{u}_\sigma\, d\mathbf{x}, \tag{114}$$

cannot, in general, be evaluated in closed form. If "once-regularized" quadratic diagnostics are considered instead,

$$E_\sigma = \tfrac{1}{2} \int \mathbf{u} \cdot \mathbf{u}_\sigma\, d\mathbf{x}, \tag{115}$$

integrals of that form are easily evaluated in closed form in the case of vortex filaments. For vortex particles, they can only be evaluated in closed form with certain choices for the regularization function $\zeta(\rho)$.

In the filament method where points on a filament are convected with the local regularized velocity $\mathbf{u}_\sigma$, E_σ is of interest because it is an invariant of the motion. Also, with the inviscid particle method, it is found numerically that E_σ remains nearly conserved as long as $\tilde{\boldsymbol{\omega}}_\sigma$ remains a good representation of $\boldsymbol{\omega}_\sigma$. This indicates that once-regularized diagnostics are indeed of interest for both filament and particle methods.

If one uses instead the local averaged-velocity $\mathbf{u}_\sigma * \zeta_\sigma$ to compute the dynamics of vortex filaments, then $E_{\sigma\sigma}$ becomes an invariant of the motion (Leonard [30]).

The once-regularized integral E_σ can also be understood as a twice-regularized integral with the regularization function $\zeta(\rho) = \hat{\zeta}(\rho) * \hat{\zeta}(\rho)$. This is easily seen if one recalls the associativity property of the convolution product:

$$\begin{aligned} E_\sigma &= \tfrac{1}{2} \int \mathbf{u} \cdot (\mathbf{u} * (\hat{\zeta}_\sigma * \hat{\zeta}_\sigma))\, d\mathbf{x} \\ &= \tfrac{1}{2} \int (\mathbf{u} \cdot \hat{\zeta}_\sigma) \cdot (\mathbf{u} \cdot \hat{\zeta}_\sigma)\, d\mathbf{x}. \end{aligned} \tag{116}$$

Note that this property also suggests a method for evaluating (if needed) $E_{\sigma\sigma}$ with vortex filaments or particles: Given $\zeta(\rho)$, find $\bar{\zeta}(\rho) = \zeta(\rho) * \zeta(\rho)$. Then

$$E_{\sigma\sigma} = \tfrac{1}{2} \int \mathbf{u} \cdot (\mathbf{u} * \bar{\zeta}_\sigma)\, d\mathbf{x}. \tag{117}$$

Unfortunately, finding analytically $\bar{\zeta}(\rho)$ from $\zeta(\rho)$ is usually not possible. One exception is the Gaussian smoothing (40) for which the use of the Fourier transform and the convolution theorem leads to $\bar{\zeta}(\rho) = \zeta(\rho/\sqrt{2})$. This smoothing can be useful for vortex filament methods. With vortex particles, however, the Gaussian smoothing is unfortunately a case for which Eq. (117) (or Eq. (115)) cannot be integrated in closed form.

In what follows, all quadratic diagnostics are once-regularized. As mentioned above, with vortex particles these can only be integrated in closed form for certain regularization functions. The high order algebraic smoothing (42) is a case for which all necessary integrals (energy, helicity, and enstrophy) can be evaluated in closed form.

The evaluation of the kinetic energy is first considered,

$$\begin{aligned} E_\sigma &= \tfrac{1}{2}\int \mathbf{u}_\sigma \cdot \mathbf{u}\, d\mathbf{x} = \tfrac{1}{2}\int (\nabla\times\tilde{\boldsymbol\psi}_\sigma)\cdot(\nabla\times\tilde{\boldsymbol\psi})\, d\mathbf{x} \\ &= \tfrac{1}{2}\int \tilde{\boldsymbol\psi}_\sigma\cdot(\nabla\times(\nabla\times\tilde{\boldsymbol\psi}))\, d\mathbf{x} \\ &= \tfrac{1}{2}\int \tilde{\boldsymbol\psi}_\sigma\cdot(-\nabla^2\tilde{\boldsymbol\psi}+\nabla(\nabla\cdot\tilde{\boldsymbol\psi}))\, d\mathbf{x} \\ &= \tfrac{1}{2}\int \tilde{\boldsymbol\psi}_\sigma\cdot\tilde{\boldsymbol\omega}\, d\mathbf{x} + \tfrac{1}{2}\int \tilde{\boldsymbol\psi}_\sigma\cdot\nabla(\nabla\cdot\tilde{\boldsymbol\psi})\, d\mathbf{x}, \end{aligned} \tag{118}$$

where integration by parts has been used. Due to the nonzero divergence of $\tilde{\boldsymbol\psi}_\sigma$, the energy cannot be simply written as

$$\begin{aligned} \tilde{E}_\sigma &= \frac{1}{2}\int \tilde{\boldsymbol\psi}_\sigma\cdot\tilde{\boldsymbol\omega}\, d\mathbf{x} = \frac{1}{2}\sum_{p,q} G_\sigma(\mathbf{x}^p-\mathbf{x}^q)\,\boldsymbol\alpha^p\cdot\boldsymbol\alpha^q \\ &= \frac{1}{8\pi}\sum_{p,q}\frac{(|\mathbf{x}^p-\mathbf{x}^q|^2+\frac{3}{2}\sigma^2)}{(|\mathbf{x}^p-\mathbf{x}^q|^2+\sigma^2)^{3/2}}\,\boldsymbol\alpha^p\cdot\boldsymbol\alpha^q. \end{aligned} \tag{119}$$

Instead, Eq. (115) must be integrated in closed form. Following the same procedure as in Section C.1, one obtains

$$\begin{aligned} E_\sigma &= \frac{1}{2}\left(\frac{1}{4\pi}\right)^2\sum_{p,q}(\delta_{jl}\,\delta_{kn}-\delta_{jn}\,\delta_{kl}\alpha_k^p\alpha_n^q\frac{\partial}{\partial x_j^p}\frac{\partial}{\partial x_l^q} \\ &\quad\times\left(\int\frac{(|\mathbf{x}-\mathbf{x}^p|^2+\frac{3}{2}\sigma^2)}{(|\mathbf{x}-\mathbf{x}^p|^2+\sigma^2)^{3/2}}\frac{1}{|\mathbf{x}-\mathbf{x}^q|}\,d\mathbf{x}\right). \end{aligned} \tag{120}$$

The evaluation of the integral in Eq. (120) is done as in Section C.1. It leads us to consider

$$\begin{aligned} I &= 2\pi\int_0^\infty dr\,\frac{r(r^2+\frac{3}{2}\sigma^2)}{(r^2+\sigma^2)^{3/2}}\int_{-1}^1 d\mu\left(\frac{r}{(r^2+2rz\mu+z^2)^{1/2}}-1\right) \\ &= 2\pi\int_0^\infty\frac{r(r^2+\frac{3}{2}\sigma^2)}{(r^2+\sigma^2)^{3/2}}\left[\frac{(r^2+2rz\mu+z^2)^{1/2}}{z}-\mu\right]_{-1}^1 dr \\ &= 2\pi z\int_0^\infty\frac{t(t^2+\frac{3}{2}a^2)}{(t^2+a^2)^{3/2}}(|t+1|-|t-1|-2)\,dt \\ &= 2\pi z\int_0^1\frac{t(t^2+\frac{3}{2}a^2)}{(t^2+a^2)^{3/2}}(2t-2)\,dt, \end{aligned} \tag{121}$$

with $t=r/z$ and $a=\sigma/z$. Now, since

$$\begin{aligned} \int\frac{t(t^2+\frac{3}{2}a^2)}{(t^2+a^2)^{3/2}}\,dt &= \frac{(t^2+\frac{1}{2}a^2)}{(t^2+a^2)^{1/2}}, \\ \int\frac{t^2(t^2+\frac{3}{2}a^2)}{(t^2+a^2)^{3/2}}\,dt &= \frac{t(t^2+\frac{1}{2}a^2)}{(t^2+a^2)^{1/2}}-\frac{1}{2}\,t(t^2+a^2)^{1/2}, \end{aligned} \tag{122}$$

one obtains

$$\begin{aligned} I &= 2\pi z(a-(1+a^2)^{1/2}) \\ &= (2\pi)\,z\left(\frac{\sigma}{z}-\left(1+\left(\frac{\sigma}{z}\right)^2\right)^{1/2}\right) \\ &= 2\pi\sigma(1-(\rho^2+1)^{1/2}), \end{aligned} \tag{123}$$

with $\rho=z/\sigma=|\mathbf{x}^p-\mathbf{x}^q|/\sigma$. Differentiating I gives

$$\begin{aligned} \frac{\partial}{\partial x_j^p}\frac{\partial}{\partial x_l^q}(I) &= \frac{\partial}{\partial x_j^p}\left(\frac{\partial\rho}{\partial x_l^q}\frac{dI}{d\rho}\right) \\ &= \frac{\partial^2\rho}{\partial x_j^p\,\partial x_l^q}\frac{dI}{d\rho}+\frac{\partial\rho}{\partial x_j^p}\frac{\partial\rho}{\partial x_l^q}\frac{d^2I}{d\rho^2} \\ &= 2\pi\left(\frac{\rho}{(\rho^2+1)^{1/2}}\frac{\delta_{jl}}{z}-\frac{\rho^3}{(\rho^2+1)^{3/2}}\right. \\ &\quad\left.\times\frac{(x_j^p-x_j^q)(x_l^p-x_l^q)}{z^3}\right), \end{aligned} \tag{124}$$

Use of Eq. (120) and Eq. (124) finally leads to the following expression for the energy:

$$\begin{aligned} E_\sigma &= \frac{1}{16\pi}\sum_{p,q}\frac{1}{|\mathbf{x}^p-\mathbf{x}^q|}\left[2\frac{\rho}{(\rho^2+1)^{1/2}}\boldsymbol\alpha^p\cdot\boldsymbol\alpha^q+\frac{\rho^3}{(\rho^2+1)^{3/2}}\right. \\ &\quad\left.\times\left(\frac{((\mathbf{x}^p-\mathbf{x}^q)\cdot\boldsymbol\alpha^p)}{|\mathbf{x}^p-\mathbf{x}^q|}\frac{((\mathbf{x}^p-\mathbf{x}^q)\cdot\boldsymbol\alpha^q)}{|\mathbf{x}^p-\mathbf{x}^q|}-\boldsymbol\alpha^p\cdot\boldsymbol\alpha^q\right)\right]. \end{aligned} \tag{125}$$

The first term in Eq. (125) is not equal to $\frac{1}{2}\int\tilde{\boldsymbol\psi}_\sigma\cdot\tilde{\boldsymbol\omega}\,d\mathbf{x}$, Eq. (119), as was the case with singular particles. The two expressions give identical results as long as $\tilde{\boldsymbol\omega}_\sigma$ remains a good representation of $\boldsymbol\omega_\sigma$. Their difference provides a way of checking the global consistency of computations.

Another smoothing that leads to a closed form expression for the energy is the low order algebraic smoothing (41):

$$\begin{aligned} E_\sigma &= \frac{1}{16\pi}\sum_{p,q}\frac{1}{|\mathbf{x}^p-\mathbf{x}^q|}\left[2\frac{1}{\rho}\left((\rho^2+1)^{1/2}-\frac{\operatorname{arc\,sinh}\rho}{\rho}\right)\boldsymbol\alpha^p\cdot\boldsymbol\alpha^q\right. \\ &\quad+\frac{1}{\rho}\left((\rho^2+1)^{1/2}+2\frac{1}{(\rho^2+1)^{1/2}}-3\frac{\operatorname{arc\,sinh}\rho}{\rho}\right) \\ &\quad\left.\times\left(\frac{((\mathbf{x}^p-\mathbf{x}^q)\cdot\boldsymbol\alpha^p)}{|\mathbf{x}^p-\mathbf{x}^q|}\frac{((\mathbf{x}^p-\mathbf{x}^q)\cdot{}_\alpha{}^q)}{|\mathbf{x}^p-\mathbf{x}^q|}-\boldsymbol\alpha^p\cdot\boldsymbol\alpha^q\right)\right]. \end{aligned} \tag{126}$$

Proceeding with the evaluation of the helicity, one obtains

$$\mathscr{H}_\sigma = \int \boldsymbol{\omega} \cdot \mathbf{u}_\sigma \, d\mathbf{x}$$
$$= \int \left(\sum_p \boldsymbol{\alpha}^p \, \delta(\mathbf{x} - \mathbf{x}^p) + \nabla \left(\boldsymbol{\alpha}^p \cdot \nabla \left(\frac{1}{4\pi \, |\mathbf{x} - \mathbf{x}^p|} \right) \right) \right)$$
$$\cdot \left(\sum_q \nabla G_\sigma(\mathbf{x} - \mathbf{x}^q) \times \boldsymbol{\alpha}^q \right) d\mathbf{x}$$
$$= \sum_{p,q} \boldsymbol{\alpha}^p \cdot (\nabla G_\sigma(\mathbf{x} - \mathbf{x}^q) \times \boldsymbol{\alpha}^q)$$
$$+ \frac{1}{4\pi} \sum_{p,q} \varepsilon_{ijk} \alpha_l^p \alpha_k^q \int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_l} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right)$$
$$\times \frac{\partial}{\partial x_j} G_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}. \tag{127}$$

As was the case for singular vortex particles, Eq. (111), it is easy to show that the second term in Eq. (127) vanishes, so that the simple formula

$$\mathscr{H}_\sigma = -\sum_{p,q} \boldsymbol{\alpha}^p \cdot \left(\frac{q_\sigma(\mathbf{x}^p - \mathbf{x}^q)}{|\mathbf{x}^p - \mathbf{x}^q|^3} \left((\mathbf{x}^p - \mathbf{x}^q) \times \boldsymbol{\alpha}^q \right) \right)$$
$$= \sum_{p,q} \frac{q_\sigma(\mathbf{x}^p - \mathbf{x}^q)}{|\mathbf{x}^p - \mathbf{x}^q|} \left((\mathbf{x}^p - \mathbf{x}^q) \cdot (\boldsymbol{\alpha}^p \times \boldsymbol{\alpha}^q) \right) \tag{128}$$

is obtained. Equation (128) is applicable to any smoothing. With the high order algebraic smoothing (42), one obtains

$$\mathscr{H}_\sigma = \frac{1}{4\pi} \sum_{p,q} \frac{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \frac{5}{2}\sigma^2)}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{5/2}}$$
$$\times \left((\mathbf{x}^p - \mathbf{x}^q) \cdot (\boldsymbol{\alpha}^p \times \boldsymbol{\alpha}^q) \right) \tag{129}$$

and, with the low order algebraic smoothing (41),

$$\mathscr{H}_\sigma = \frac{1}{4\pi} \sum_{p,q} \frac{1}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{3/2}}$$
$$\times \left((\mathbf{x}^p - \mathbf{x}^q) \cdot (\boldsymbol{\alpha}^p \times \boldsymbol{\alpha}^q) \right). \tag{130}$$

Finally, the evaluation of the enstrophy is examined:

$$\mathscr{E}_\sigma = \int \boldsymbol{\omega} \cdot \boldsymbol{\omega}_\sigma \, d\mathbf{x}. \tag{131}$$

Due to the nonzero divergence of $\tilde{\boldsymbol{\omega}}_\sigma$, the enstrophy cannot simply be written as

$$\tilde{\mathscr{E}}_\sigma = \int \tilde{\boldsymbol{\omega}} \cdot \tilde{\boldsymbol{\omega}}_\sigma \, d\mathbf{x} = \sum_{p,q} \zeta_\sigma(\mathbf{x}^p - \mathbf{x}^q) \, \boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q$$
$$= \frac{1}{4\pi} \sum_{p,q} \frac{15}{2} \frac{\sigma^4}{(|\mathbf{x}^p - \mathbf{x}^q|^2 + \sigma^2)^{7/2}} \boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q. \tag{132}$$

Instead, Eq. (131) must be integrated in closed form. This leads to

$$\mathscr{E}_\sigma = \int \left(\sum_p \boldsymbol{\alpha}^p \, \delta(\mathbf{x} - \mathbf{x}^p) + \nabla \left(\boldsymbol{\alpha}^p \cdot \left(\frac{1}{4\pi \, |\mathbf{x} - \mathbf{x}^p|} \right) \right) \right)$$
$$\cdot \left(\sum_q \boldsymbol{\alpha}^q \zeta_\sigma(\mathbf{x} - \mathbf{x}^q) + \nabla(\boldsymbol{\alpha}^q \cdot \nabla G_\sigma(\mathbf{x} - \mathbf{x}^q)) \right)$$
$$= \sum_{p,q} \Bigg[\boldsymbol{\alpha}^p \cdot \boldsymbol{\alpha}^q \zeta_\sigma(\mathbf{x}^p - \mathbf{x}^q) + \boldsymbol{\alpha}^p \cdot \nabla(\boldsymbol{\alpha}^q \cdot \nabla G_\sigma(\mathbf{x} - \mathbf{x}^q)_{\mathbf{x} = \mathbf{x}^p})$$
$$+ \frac{1}{4\pi} \alpha_k^p \alpha_i^q \int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_k} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right) \zeta_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}$$
$$+ \frac{1}{4\pi} \alpha_k^p \alpha_l^q \int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_k} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right)$$
$$\times \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_l} G_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x} \Bigg]. \tag{133}$$

The integrals in Eq. (133) are evaluated using the same procedure as for the kinetic energy evaluation, together with

$$\int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_k} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right) \zeta_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}$$
$$= -\int \frac{\partial}{\partial x_k} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right) \frac{\partial}{\partial x_i} \zeta_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}$$
$$= -\frac{\partial}{\partial x_k^p} \frac{\partial}{\partial x_i^q} \int \frac{1}{|\mathbf{x} - \mathbf{x}^p|} \zeta_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}, \tag{134}$$
$$\int \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_k} \left(\frac{1}{|\mathbf{x} - \mathbf{x}^p|} \right) \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_l} G_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}$$
$$= \frac{\partial}{\partial x_i^p} \frac{\partial}{\partial x_k^p} \frac{\partial}{\partial x_i^q} \frac{\partial}{\partial x_l^q} \int \frac{1}{|\mathbf{x} - \mathbf{x}^p|} G_\sigma(\mathbf{x} - \mathbf{x}^q) \, d\mathbf{x}.$$

The first integral in Eq. (134) leads us to consider

$$I_1 = (2\pi) \left(\frac{15}{8\pi\sigma^3} \right) \int_0^\infty dr \frac{r}{(r^2 + \sigma^2)^{7/2}}$$
$$\times \int_{-1}^{1} d\mu \left(\frac{r}{(r^2 + 2rz\mu + z^2)^{1/2}} - 1 \right)$$
$$= \left(\frac{15}{4} \right) \frac{a^4}{z} \int_0^1 \frac{t}{(t^2 + a^2)^{7/2}} (2t - 2) \, dt, \tag{135}$$

with $t = r/z$ and $a = \sigma/z$. Now, since

$$\int \frac{t}{(t^2 + a^2)^{7/2}} \, dt = -\frac{1}{5} \frac{1}{(t^2 + a^2)^{5/2}},$$
$$\int \frac{t^2}{(t^2 + a^2)^{7/2}} \, dt = \frac{2}{15a^2} \frac{t^3(t^2 + \frac{5}{2}a^2)}{(t^2 + a^2)^{5/2}}, \tag{136}$$

one finally obtains

$$I_1 = \frac{1}{\sigma}\left(\frac{\rho^2(\rho^2+\frac{5}{2})}{(\rho^2+1)^{5/2}} + \frac{3}{2}\left(\frac{1}{(\rho^2+1)^{5/2}} - 1\right)\right), \qquad (137)$$

where $\rho = z/\sigma = |\mathbf{x}^p - \mathbf{x}^q|/\sigma$. The second integral in Eq. (134) leads us to consider the same integral I as in the energy evaluation, Eq. (121). Differentiation of I and I_1 gives

$$-\frac{\partial}{\partial x_k^p}\frac{\partial}{\partial x_i^q}(I_1) = \frac{1}{\sigma^3}\left(\left(\frac{\rho^2(\rho^2+\frac{7}{2})+\frac{5}{2}}{(\rho^2+1)^{7/2}}\right)\delta_{ik} - \frac{3}{\sigma^2}\left(\frac{\rho^2(\rho^2+\frac{9}{2})+\frac{7}{2}}{(\rho^2+1)^{9/2}}\right) \times (x_i^p - x_i^q)(x_k^p - x_k^q)\right),$$

$$\frac{\partial}{\partial x_i^p}\frac{\partial}{\partial x_k^p}\frac{\partial}{\partial x_i^q}\frac{\partial}{\partial x_l^q}(I) = \frac{1}{\sigma^3}\left(\frac{(\rho^2+\frac{5}{2})}{(\rho^2+1)^{5/2}}\delta_{kl} - \frac{3}{\sigma^2}\frac{(\rho^2+\frac{7}{2})}{(\rho^2+1)^{7/2}} \times (x_k^p - x_k^q)(x_l^p - x_l^q)\right). \qquad (138)$$

All the necessary terms have been obtained. The final result is

$$\mathscr{E}_\sigma = \frac{1}{4\pi}\sum_{p,q}\frac{1}{\sigma^3}\left[\frac{(5-\rho^2(\rho^2+\frac{7}{2}))}{(\rho^2+1)^{7/2}}\boldsymbol{\alpha}^p\cdot\boldsymbol{\alpha}^q + 3\,\frac{(\rho^2(\rho^2+\frac{9}{2})+\frac{7}{2})}{(\rho^2+1)^{9/2}} \times ((\mathbf{x}^p-\mathbf{x}^q)\cdot\boldsymbol{\alpha}^p)((\mathbf{x}^p-\mathbf{x}^q)\cdot\boldsymbol{\alpha}^q)\right]. \qquad (139)$$

Again, the succes of the above derivation strongly depends on the integration properties of the high order algebraic smoothing (42). No attempt was made to obtain the expression for the enstrophy when using the low order algebraic smoothing (41).

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