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A Higher Order Vorticity Redistribution Method for 3-D Diffusion in Free Space

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A Higher Order Vorticity Redistribution Method For 3-D Diffusion In Free Space

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ABSTRACT

The Vorticity Redistribution Method (VRM) for the simulation of 3-D diffusion is revisited. The method is demonstrated to maintain the solenoidality of an initially divergence-free vorticity field to an order of accuracy that is consistent with that of the solution. A novel strategy is developed for implementing the VRM with *third-order* theoretical accuracy in the diffusion length scale, while maintaining positivity. The super-cubic convergence rate of the high-order VRM and its superior accuracy compared to the lower order case are established using four (2-D and 3-D) test problems. The effects of cutoff circulation, core function and core radius on accuracy are studied as well. In all cases tested, the high-order VRM uses at least an order of magnitude larger time-step compared to the low-order method to achieve the same level of accuracy. This improvement in accuracy is associated with a factor of 3.5 ~ 8 drop in the number of particles and 1.5 ~ 3 reduction in the *total* CPU time. Finally, the formulation for the 3-D diffusion with *spatially varying* viscosity is derived as well.

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1 INTRODUCTION

The ability to simulate diffusion accurately by a *truly* grid-free method is essential to the success of Lagrangian vortex element methods as potentially powerful Direct Numerical (DNS) or Large Eddy (LES) Simulation tools. To this end, several deterministic diffusion schemes with various levels of accuracy and implementation complexity have been developed in recent years [6]:

The Corrected Core Expansion Method (CCEM) [20]: This is a truly grid-free approach as it requires no background grids and frequent regridding to maintain accuracy. In its basic form, the method is very inexpensive (per computational element) and quite simple to implement. Unfortunately, the basic implementation tends to increase the number of vortex elements indiscriminately. This is because, rather than adding new elements only at the boundaries of the vorticity field to account for its expansion, the algorithm replaces an old element with new ones irrespective of its position relative to the neighboring elements. As a result, as large as 70 percent of the elements add only to the computational cost but not to its accuracy [21]. To this end, frequent merging is necessary to maintain an acceptable number of elements [21], which undoubtedly contributes to loss of accuracy and increased computational cost. Additionally, a recent study suggests that the vorticity field is not necessarily preserved subsequent to core splitting [22].

The Diffusion Velocity Method [10]: This is a conceptually interesting approach but it is computationally difficult to justify implementing. To begin with, there is no rigorous proof of convergence for the method. Further, the accuracy of the method depends strongly on the accuracy with which the first and second derivatives of vorticity are evaluated [16]. Clearly, computationally induced perturbations in (small) values of vorticity; e.g., near the field boundaries, can lead to substantially large gradients. Additionally, the diffusion velocity involves the logarithm of the (magnitude of) vorticity; or, equivalently, division by the magnitude of vorticity [9], which can contribute to accuracy and stability problems for small values of vorticity. See [6] for more details.

The Particle Strength Exchange (PSE) Method [7]: The PSE method has been used in conjunction with DNS [11, 19] and LES [15] of "simple" flow topologies with relative success. For *uniformly distributed* particles the PSE method is quite accurate. However, since it uses the particle positions as quadrature points to evaluate the Laplacian integral, the accuracy of the integral evaluations deteriorates sharply as the vortex element distributions inevitably become more disordered [11, 16, 19]. The practiced remedy is to frequently project the vorticity field onto a uniform distribution of vortex elements and to discard the disordered ones [11, 15, 19]. However, regridding defeats the entire purpose of utilizing a "grid-free Lagrangian method" for at least two important reasons: (1) It introduces some level of numerical diffusion into the computations, and (2) it uses (background) grids to redistribute the particles, which demand special attention near the boundaries [11, 19]. Another disadvantage of the PSE scheme (as with other core function based methods) is that the diffusion length scale is resolved only in the order of the core radius, which must be asymptotically large compared to the inter-particle separation to maintain quadrature accuracy [7]. This implies that a comparatively larger number of vortex

elements will be required to resolve the flow field down to the diffusion length scale. Additionally, the requirement for solution positivity limits the choice for the PSE core functions to second-order in the core radius only [7].

The Vorticity Redistribution Method (VRM) [23, 26]: This is a new scheme with attractive attributes. VRM simulates diffusion by redistributing fractions of the circulation of each vortex element to the neighbors that lie within a radius in the order of the diffusion length scale, such that the positivity of the solution and the conservation properties of the system are preserved to *arbitrarily high order* [23, 26]. This is done without involving quadratures. VRM is *truly* grid-free, and it requires no background grids and frequent remeshing to maintain accuracy. Another advantage of VRM is that the solution of the diffusion equation turns out to be independent of the choice for a core function. Indeed, the method is capable of simulating diffusion of (singular) point vortices. Therefore, unlike PSE and other similar methods, VRM is not constrained by a necessary condition for core overlap, and its resolution is in the order of inter-particle spacing. At present, the main disadvantage of VRM is the absence of a robust method for determining the optimal size of the core radius for the core functions, which are used to recover the vorticity field during the post-processing stage (only).

To illustrate the relative merits of VRM, we note that VRM- [23] and PSE-based [11] DNS of the initial stages of impulsively started flow over a cylinder at $Re = 9,500$ required 60,000 and 350,000 vortex elements, respectively, to produce similar results. The latter applied frequent remeshing, whereas the former did not. Another example is the DNS of the same problem at $Re = 550$. In this case, VRM used 50,700 vortex elements [23, 25], whereas PSE used 70,000 [19]. Yet, the latter is not converged. In addition, the cutoff circulation values in the VRM [23] and PSE [19] simulations were set at 10^{-5} and 10^{-3} of the maximum circulation, respectively. Had the smaller cutoff value of 10^{-5} been used in [19] the number of PSE elements would have been significantly larger. In light of the examples above, and in the absence of similar benchmark tests for other methods, VRM is the clear choice for the accurate, truly grid-free simulation of diffusion.

In this report, a recently developed generalization of VRM for 1-D [24] is used to derive the formulation for the 3-D diffusion of the vorticity vector field. The method is demonstrated to maintain the solenoidality of an initially divergence-free vorticity field to arbitrarily high order, consistent with the order of accuracy of the solution. A *third-order* accurate VRM is then developed. The main difficulty with the latter is the development of a robust algorithm for inserting new elements to account for the expansion of the vorticity field, such that positivity is maintained. To this end, the 1-D analogue problem is analyzed to provide guidelines for possible element insertion strategies. The accuracy and convergence rate of the high-order VRM are examined using the diffusion of a 2-D point vortex. The effect of cutoff circulation on solution accuracy, and core function and its radius on post-processing accuracy are studied as well. The superiority of the high-order VRM over its low-order counterpart is demonstrated further using the diffusion of a 2-D vortex pair, a 3-D point vortex, and a 3-D vortex ring as examples. Finally, the formulation for 3-D diffusion with *spatially varying* viscosity is derived in Appendix A as a first step towards developing a VRM-based LES capability.

2 FORMULATION

The generalized VRM for the diffusion of a 1-D point source [24] is extended herein to develop the formulation for the diffusion of a 3-D vorticity vector field.

The equation for the diffusion of vorticity in 3-D free space is

$$\frac{\partial \vec{\omega}}{\partial t} = \nu \nabla^2 \vec{\omega} \quad (1a)$$

$$\vec{\omega}(\vec{x}, t = 0) = \vec{\omega}_0(\vec{x}) \quad (1b)$$

$$\vec{\nabla} \cdot \vec{\omega} = 0 \quad (1c)$$

where $\vec{\omega}(\vec{x}, t)$ is the vorticity vector at any point $\vec{x} = (x, y, z)$ and time t , $\vec{\omega}_0(\vec{x})$ is its value at an initial time t_0 , ν is the kinematic viscosity, and $\vec{\nabla} = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$.

Let's discretize the vorticity field by N_v point vortices, each with a vectorial circulation $\vec{\Gamma}_i(t)$ and an associated elemental volume ΔV_i centered at $\vec{x}_i$:

$$\vec{\omega}(\vec{x}, t) \equiv \sum_{i=1}^{N_v} \vec{\Gamma}_i(t) \delta(\vec{x} - \vec{x}_i) = \sum_{i=1}^{N_v} \vec{\omega}_i(t) \Delta V_i \delta(\vec{x} - \vec{x}_i) \quad (2)$$

where $\vec{\omega}_i(t)$ is the vorticity of the element at $\vec{x}_i$, and $\delta(\cdot)$ is the Dirac delta. Note that the choice for delta functions in this analysis is purely for simplicity of presentation; we have verified that smooth (symmetric) core functions yield an identical system of VRM equations. In what follows, the VRM for the diffusion of *one* vortex at $\vec{x}_i$ will be described. The diffusion of the whole field is evaluated by a linear superposition of the diffusion by all N_v particles.

Consider a point vortex at $\vec{x}_i$ and aim at diffusing its vorticity, to some order of accuracy, to the neighboring particles at $\vec{x}_j$ inside a (not necessarily) spherical neighborhood of influence. The latter is centered at $\vec{x}_i$ and has non-dimensional radius R_n , such that $|\vec{x}_i - \vec{x}_j|/h_v \leq R_n$. Here, $h_v = \sqrt{\nu \Delta t}$ is a diffusion length scale and Δt is the corresponding computational time-step.

The vorticity $\vec{\omega}^n$ of a point vortex at $\vec{x}_i$, at time level n is

$$\vec{\omega}^n = \vec{\Gamma}_i^n \delta(\vec{x} - \vec{x}_i) \quad (3)$$

where $\vec{\Gamma}_i^n$ is the corresponding vectorial circulation. At time level $n+1$, subsequent to diffusion from point i to its neighbors j , the vorticity $\vec{\omega}^{n+1}$ at $\vec{x}_i$ can be described as

$$\bar{\omega}^{n+1} = \sum_j f_{ij}^n \bar{\Gamma}_i^n \delta(\bar{x} - \bar{x}_j) \quad (4)$$

where f_{ij}^n are the fractions of the circulation that are diffused from point i to neighbors j during the computational time-step. In VRM, the objective is to find these fractions such that the vorticity moments of the diffusion equation are satisfied over the small neighborhood radius to a desired order of accuracy. In the following, the generalized VRM for the diffusion equation, which leads to a system of equations for the unknown fractions, is described.

Since the discrete vorticity field may not satisfy (1a) exactly, let's define a residual error function $\bar{R}(\bar{\omega})$, such that

$$\bar{R}(\bar{\omega}) = \frac{\partial \bar{\omega}}{\partial t} - \nu \nabla^2 \bar{\omega} \quad (5)$$

Let's also define an arbitrary smooth function $W(\bar{x})$. Then, a point source of vorticity will diffuse to points within its neighborhood to some accuracy if

$$\int W(\bar{x}) \bar{R}(\bar{\omega}) dV(\bar{x}) = 0 \quad (6)$$

where the integration is over the (not necessarily) spherical neighborhood with volume $V(\bar{x})$, outside of which $W(\bar{x})$ and, equivalently, $\bar{R}(\bar{\omega})$ vanish [24]. Expanding $W(\bar{x})$ around the point source at $\bar{x}_i = (x_i, y_i, z_i)$ and forcing the resulting moments to vanish for all positive integers (L, M, N) yields

$$\int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{R}(\bar{\omega}) dV(\bar{x}) = 0 \quad (7)$$

Substituting (5) in (7) yields

$$\frac{d}{dt} \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\omega} dV = \nu \int (x - x_i)^L (y - y_i)^M (z - z_i)^N (\nabla^2 \bar{\omega}) dV \quad (8)$$

where $V \equiv V(\bar{x})$. Now, let's re-express the right hand side of (8):

$$\begin{aligned} \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\nabla} \cdot \bar{\nabla} \bar{\omega} dV &= \int \bar{\nabla} \cdot \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\nabla} \bar{\omega} \right] dV \\ &\quad - \int \bar{\nabla} \cdot \left\{ \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} \right\} dV \\ &\quad + \int \bar{\nabla} \cdot \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dV \end{aligned} \quad (9)$$

The first two terms on the right hand side of (9) can be expressed as surface integrals due to the Gauss' Theorem [17]

$$\begin{aligned}
\int (x - x_i)^L (y - y_i)^M (z - z_i)^N \vec{\nabla} \cdot \vec{\nabla} \bar{\omega} dV &= \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \vec{n} \cdot \vec{\nabla} \bar{\omega} dS \\
&\quad - \int \vec{n} \cdot \vec{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dS \\
&\quad + \int \vec{\nabla} \cdot \vec{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dV
\end{aligned} \tag{10}$$

where S is the bounding surface of V . Since the point vortex is inside the volume, the surface integrals do not contribute to the diffusion process and are no longer considered. As a result, substituting (10) into (8) yields the following compact form of the generalized VRM for the diffusion of a 3-D vorticity vector field for arbitrary (L, M, N) :

$$\frac{d\bar{G}_{LMN}}{dt} = \nu \left[L(L-1)\bar{G}_{(L-2)MN} + M(M-1)\bar{G}_{L(M-2)N} + N(N-1)\bar{G}_{LM(N-2)} \right] \tag{11a}$$

$$\bar{G}_{LMN} = \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\omega} dV \quad (L + M + N) = 0, 1, 2, \dots \tag{11b}$$

In essence the partial differential equation has been reduced to a system of ordinary differential equations (ODEs). Since $\bar{G}_{LMN}$ are polynomials in time, the moments of (11) can be conserved *exactly* up to order $(L + M + N)$ if a consistent time integration scheme is applied. This yields a solution that is $O(h_v^{L+M+N-1})$ accurate. To get the system of equations for the lowest order of consistency, we substitute $(L + M + N) = 0, 1, 2$ in (11)

$$\frac{d\bar{G}_{000}}{dt} = 0 \tag{12a}$$

$$\frac{d\bar{G}_{100}}{dt} = \frac{d\bar{G}_{010}}{dt} = \frac{d\bar{G}_{001}}{dt} = 0 \tag{12b}$$

$$\frac{d\bar{G}_{110}}{dt} = \frac{d\bar{G}_{101}}{dt} = \frac{d\bar{G}_{011}}{dt} = 0 \tag{12c}$$

$$\frac{d\bar{G}_{200}}{dt} = \frac{d\bar{G}_{020}}{dt} = \frac{d\bar{G}_{002}}{dt} = 2\nu\bar{G}_{000} \tag{12d}$$

For the system of equations (12), the local truncation error is $O(h_v) \approx O(\sqrt{\Delta t})$ and a first-order forward Euler time integration will be sufficient. In this case, $\bar{G}_{LMN}$ or, equivalently, $\bar{\omega}$ must be evaluated at time levels n and $n+1$. Thus, performing the forward Euler time integration of (12) and substituting (3), (4) and (11b) in (12) yields the desired system of equations for f_{ij}^n :

$$\sum_j f_{ij}^n = 1 \quad (13a)$$

$$\sum_j f_{ij}^n x_{ij} = 0 \quad (13b)$$

$$\sum_j f_{ij}^n y_{ij} = 0 \quad (13c)$$

$$\sum_j f_{ij}^n z_{ij} = 0 \quad (13d)$$

$$\sum_j f_{ij}^n x_{ij} y_{ij} = 0 \quad (13e)$$

$$\sum_j f_{ij}^n y_{ij} z_{ij} = 0 \quad (13f)$$

$$\sum_j f_{ij}^n z_{ij} x_{ij} = 0 \quad (13g)$$

$$\sum_j f_{ij}^n x_{ij}^2 = 2 \quad (13h)$$

$$\sum_j f_{ij}^n y_{ij}^2 = 2 \quad (13i)$$

$$\sum_j f_{ij}^n z_{ij}^2 = 2 \quad (13j)$$

where $\bar{x}_{ij} = (\bar{x}_j - \bar{x}_i)/h_v$ is the *scaled* difference in the position vectors of particles i and j .

Equations (13) are identical to the ones obtained by the original VRM formulation [26], based on the Fourier modes of the fundamental solution. Therefore, VRM is a methodology that seeks to obtain the fractions of a conserved quantity (circulation), which are redistributed from a point to its neighbors due to diffusion, such that the discretization error is minimized in an integral sense up to a desired order of accuracy or, equivalently, moment condition. Note that, for positive fractions, if the diffusing and six other particles are placed on a seven-point finite-difference stencil, and the remaining (minimum) three particles are placed randomly anywhere on a sphere that is defined by the stencil, the fractions obtained by the solution of Eqns. (13) will recover a finite-difference scheme that uses second-order central differencing to discretize the Laplacian and a first-order forward Euler method for time integration. That is, particles that are not part of the seven-point stencil will have *zero* fraction.

In [23, 26], while a general formulation for obtaining arbitrarily high order equations for the fractions was derived, only the $O(h_v)$ discretization; i.e., the system represented by Eqns.

(13), was implemented and tested for accuracy. In this report, an $O(h_v^3)$ VRM is developed and its accuracy compared to that of the $O(h_v)$ method. To get the $O(h_v^3)$ system of equations, we substitute $(L + M + N) = 0, 1, \dots, 4$ in (11), and perform a second-order Runge-Kutta (modified Euler) time integration of the resulting set of ODEs, which is *exact* for the $O(h_v^3) \approx O(\Delta t^{3/2})$ system. We then substitute (3), (4) and (11b) in the latter to yield the system of equations for f_{ij}^n :

$$O(1): \quad \sum_j f_{ij}^n = 1 \quad (14a)$$

$$O(\sqrt{\Delta t}): \quad \sum_j f_{ij}^n x_{ij} = \sum_j f_{ij}^n y_{ij} = \sum_j f_{ij}^n z_{ij} = 0 \quad (14b)$$

$$O(\Delta t): \quad \sum_j f_{ij}^n x_{ij} y_{ij} = \sum_j f_{ij}^n y_{ij} z_{ij} = \sum_j f_{ij}^n z_{ij} x_{ij} = 0 \quad (14c)$$

$$O(\Delta t): \quad \sum_j f_{ij}^n x_{ij}^2 = \sum_j f_{ij}^n y_{ij}^2 = \sum_j f_{ij}^n z_{ij}^2 = 2 \quad (14d)$$

$$O(\Delta t^{3/2}): \quad \sum_j f_{ij}^n x_{ij} y_{ij}^2 = \sum_j f_{ij}^n y_{ij} z_{ij}^2 = \sum_j f_{ij}^n z_{ij} x_{ij}^2 = 0 \quad (14e)$$

$$O(\Delta t^{3/2}): \quad \sum_j f_{ij}^n x_{ij} z_{ij}^2 = \sum_j f_{ij}^n z_{ij} y_{ij}^2 = \sum_j f_{ij}^n y_{ij} x_{ij}^2 = 0 \quad (14f)$$

$$O(\Delta t^{3/2}): \quad \sum_j f_{ij}^n x_{ij}^3 = \sum_j f_{ij}^n y_{ij}^3 = \sum_j f_{ij}^n z_{ij}^3 = \sum_j f_{ij}^n x_{ij} y_{ij} z_{ij} = 0 \quad (14g)$$

$$O(\Delta t^2): \quad \sum_j f_{ij}^n x_{ij} y_{ij}^3 = \sum_j f_{ij}^n y_{ij} z_{ij}^3 = \sum_j f_{ij}^n z_{ij} x_{ij}^3 = 0 \quad (14h)$$

$$O(\Delta t^2): \quad \sum_j f_{ij}^n x_{ij} z_{ij}^3 = \sum_j f_{ij}^n z_{ij} y_{ij}^3 = \sum_j f_{ij}^n y_{ij} x_{ij}^3 = 0 \quad (14i)$$

$$O(\Delta t^2): \quad \sum_j f_{ij}^n x_{ij} y_{ij} z_{ij}^2 = \sum_j f_{ij}^n y_{ij} z_{ij} x_{ij}^2 = \sum_j f_{ij}^n z_{ij} x_{ij} y_{ij}^2 = 0 \quad (14j)$$

$$O(\Delta t^2): \quad \sum_j f_{ij}^n x_{ij}^2 y_{ij}^2 = \sum_j f_{ij}^n y_{ij}^2 z_{ij}^2 = \sum_j f_{ij}^n z_{ij}^2 x_{ij}^2 = 4 \quad (14k)$$

$$O(\Delta t^2): \quad \sum_j f_{ij}^n x_{ij}^4 = \sum_j f_{ij}^n y_{ij}^4 = \sum_j f_{ij}^n z_{ij}^4 = 12 \quad (14l)$$

The methodology for solving the system of equations (13) and (14) will be discussed in Section 4. Additionally, the formulation for 3-D diffusion with spatially varying viscosity is presented in Appendix A.

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3 SOLENOIDALITY CONDITION

The redistribution equations (13) and (14) are purely geometric in nature and do not involve the circulation vectors of the points. The fractions are simply multiplied by the three components of the circulation vector of the diffusing point to evaluate the amount of circulation (in each coordinate direction) that must be given off to the neighboring points. That is, the diffusion of a circulation vector is predicted as the diffusion of three *independent* scalar functions in x , y and z directions, without regard to the solenoidality constraint (1c). Naturally, the question arises whether such an approach will maintain the solenoidality of the vorticity field in the (arbitrarily high-order) *discrete* formulation.

It turns out that VRM does preserve the solenoidality of an initially divergence-free vorticity field to an order that is consistent with the order of accuracy of the solution. To demonstrate this, we discretize the diffusion equation for the divergence of vorticity using the generalized VRM:

$$\int (x - x_i)^L (y - y_i)^M (z - z_i)^N \left\{ \frac{\partial \vec{\nabla} \cdot \vec{\omega}}{\partial t} = \nu \nabla^2 (\vec{\nabla} \cdot \vec{\omega}) \right\} dV \quad (15)$$

Performing successive integration-by-parts, similar to the process demonstrated in Section 2, yields the compact form of the generalized VRM for the diffusion of the divergence of the vorticity field for arbitrary (L, M, N) :

$$\begin{aligned} L \frac{dG_{(L-1)MN}^x}{dt} + M \frac{dG_{L(M-1)N}^y}{dt} + N \frac{dG_{LM(N-1)}^z}{dt} = \\ \nu \left\{ \begin{aligned} &L(L-1) \left[(L-2)G_{(L-3)MN}^x + MG_{(L-2)(M-1)N}^y + NG_{(L-2)M(N-1)}^z \right] + \\ &M(M-1) \left[LG_{(L-1)(M-2)N}^x + (M-2)G_{L(M-3)N}^y + NG_{L(M-2)(N-1)}^z \right] + \\ &N(N-1) \left[LG_{(L-1)M(N-2)}^x + MG_{L(M-1)(N-2)}^y + (N-2)G_{LM(N-3)}^z \right] \end{aligned} \right\} \quad (16a) \end{aligned}$$

$$G_{LMN}^\alpha = \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \omega_\alpha dV \quad (L + M + N) = 0, 1, 2, \dots \quad (16b)$$

where ω_α is the vorticity in the α direction.

It is now a simple matter to verify, by substituting the (x, y, z) components of (11a) into (16a), that a VRM solution based on Eqn. (11) with arbitrary order $(L + M + N)$ satisfies (16a) identically up to order $(L + M + N - 1)$. That is, if a solution of (11) exists, then the *discrete* diffusion of the (x, y, z) components of the circulation vector as three independent processes will be solenoidal up to one order lower than the order of accuracy of the solution.

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4 SOLUTION METHODOLOGY

The main contribution in this report is the development of a methodology to obtain a positive solution of the system of equations (14), which represent the $O(h_v^3)$ VRM. In particular, issues such as the optimal choice for the radius of neighborhood of the diffusing element, as well as the appropriate particle distribution within the neighborhood are addressed.

The systems of equations (13) and (14) are linear, but generally under-determined. This is because the number of rows corresponds to the (fixed) order $(L + M + N)$ of the system, whereas the number of columns equals the number of particles that are present within the sphere of radius R_n . The latter can range from as few as one column, corresponding to the diffusing element, to more columns than there are rows. If a solution of the systems exists it is obtained using linear programming techniques [1, 2, 4, 8, 18, 23]. However, if a solution does not exist, new vortices are inserted within the neighborhood until a solution becomes possible. The linear programming and particle insertion techniques used in our VRM are presented in the subsequent sections.

It should be noted here that in order to limit the proliferation of vortex elements, the vorticity of particles with circulation below a small user-specified cutoff value is not allowed to diffuse. This is generally the case near the edges of the vorticity field, where the magnitude of vorticity is exponentially small. Disallowing diffusion below a cutoff limit still conserves the (global) zeroth and first moments, but it does not conserve the (global) second moment as accurately. That is, the rate of expansion of the diffusing region is smaller than it should be for the obvious reason that the leading edges may not diffuse, depending on the circulation value of the particles there. As demonstrated in [23] and in Section 5, the correct choice of the cutoff circulation is crucial to the accuracy of the simulations. Two clarifications are in order here: (1) *All* moment conditions of individual *diffusing elements* are satisfied up to machine precision subsequent to the solution of the linear system of equations for the fractions; it is only the global second moment that may not be conserved because of the *non-diffusing elements* at the outer edges. (2) With the selection of smaller cutoff values, the global second moment may be conserved to machine precision as well; however, this is accomplished at the expense of an unnecessarily large number of particles. Note that the PSE method suffers from the same shortcoming [11, 19].

4.1 The Linear Programming Procedure

A procedure is presented for obtaining a positive solution for the fractions f_{ij}^n , assuming one exists. The requirement that the fractions be positive is imposed as a stability condition, as it ensures that the l_1 norm $|\vec{\Gamma}^n| = \sum_{i=1}^{N_v} |\vec{\Gamma}_i^n|$ of the circulation will not grow [23, 26, 27]. To obtain a positive solution of the (generally) under-determined system of equations (13) or (14), following [23, 26, 27], we note that $0 \leq f_{ij}^n \leq 1$ and shift the origin to the center of the range, using

$$w_j = f_{ij}^n - \frac{1}{2} \quad (17)$$

where the dependence of w_j on vortex i and time level n is implicitly understood. Substituting (17) into (13) or (14), and rearranging coefficient terms yields a linear system of equations in terms of the new unknown vector $\vec{w}$

$$A\vec{w} = \vec{b} \quad (18)$$

Any solution of system (18) is then acceptable if $-1/2 \leq w_j \leq 1/2$ for all j ; or, equivalently, if the maximum norm of the solution vector $\|\vec{w}\|_\infty \equiv \max_j \{|w_j|\}$ is less than or equal to $1/2$. The approach here, following [23, 26, 27], is to find the solution vector $\vec{w}$ with the least maximum norm. If the latter is less than or equal to $1/2$, an acceptable solution exists. Otherwise, an acceptable solution cannot be found; new particles have to be inserted and the system solved again until an acceptable solution is obtained. Note that the existence/non-existence of a solution of the system equips VRM with a mathematically-based intelligent mechanism to automatically detect when and where a new element must be added.

The problem of finding the least maximum solution of the linear system of equations (18) is one of linear programming, which may be obtained by the simplex method [4, 8, 18]. This is done by considering the maximum norm $\|\vec{w}\|_\infty$ as an additional unknown, and by converting the equality in (18) into two inequalities $\leq$ and $\geq$

$$\begin{pmatrix} A & \vec{0} \\ I & \vec{1} \\ -A & \vec{0} \\ -I & \vec{1} \end{pmatrix} \begin{pmatrix} \vec{w} \\ \|\vec{w}\|_\infty \end{pmatrix} \geq \begin{pmatrix} \vec{b} \\ \vec{0} \\ -\vec{b} \\ \vec{0} \end{pmatrix} \quad (19)$$

where I is the identity matrix, and $\vec{0}$ and $\vec{1}$ are vectors of zeros and ones, respectively. The objective function to minimize is the maximum norm $\|\vec{w}\|_\infty$. It turns out that solving the dual problem of (19), which maximizes

$$z = (\vec{b}^T \quad \vec{0}^T \quad -\vec{b}^T \quad \vec{0}^T) \vec{y} \quad (20a)$$

subject to the constraints

$$\begin{pmatrix} A^T & I & -A^T & -I \\ \vec{0}^T & \vec{1}^T & \vec{0}^T & \vec{1}^T \end{pmatrix} \vec{y} = \begin{pmatrix} \vec{0} \\ 1 \end{pmatrix} \quad (20b)$$

$$\vec{y} \geq 0 \quad (20c)$$

is more efficient, since an initial feasible solution can readily be found without requiring slack variables [1]. Further, the structure of the matrix is such that only the original matrix and a few extra vectors need be stored, and that the work required to find the optimal solution is reduced.

The theoretical background and the corresponding algorithm for solving (20) is detailed in [1] and is beyond the scope of this paper. Suffice it to say that the sought optimum (minimized) objective function $\|\bar{w}\|_\infty$ for the primal problem (19) is identical to the optimum (maximized) objective function z^* for the dual problem (20) [1]. A FORTRAN program listing of this method is available in [2], and was implemented for this project. The standard simplex method was used for this purpose; however, the revised simplex method [4, 8, 18] may prove to be more efficient when dealing with the larger matrices of higher order VRM. We have to caution potential users of the program in [2] that we found several serious logical bugs in the code. Further, the simplex method in [2] does not utilize a tolerance control mechanism, which is generally necessary for algorithmic stability and improved convergence [4, 8, 18]. To this end, certain automatic tolerance control techniques [5] were utilized in the code, as recommended in [23].

4.2 The Particle Insertion Strategy

As mentioned earlier, a positive solution of the system of equations (13) or (14) may not necessarily exist. For example, there may be fewer particles within R_n than the minimum 10 or 35 required to solve equations (13) or (14), respectively. Also, a positive solution will always require the addition of new vortices at the outer edge of the vorticity field to account for its expansion by an order of the diffusion length scale. There are additional minimum conditions for the existence of a solution, which were estimated due to an analysis conducted in [23]: a) there must be at least one neighborhood vortex at a scaled distance of more than 2 from the diffusing particle; b) the maximum scaled distances should be at least $\sqrt{2}$ in the x , y and z directions and at least $(\sqrt{R_n^2 + 8} - R_n)/2$ in any direction; c) for third-order accuracy or higher, there should be at least one vortex within a scaled distance $\sqrt{8}$; and d) for a desired order of accuracy $(L + M + N)$, the scaled neighborhood radius R_n must be at least $\sqrt{2M_e}$, where M_e is the even integer $(L + M + N)$ or $(L + M + N) + 1$.

Naturally, the question arises *where* to insert the new elements. For the lower order VRM in 2-D [23], the new elements were inserted on a circle of scaled radius $R_i < R_n$. The angular location of an inserted vortex was determined by maximizing the minimum distances between the existing vortices within the neighborhood of radius R_n and 12 possible positions on R_i , spaced 30 degrees apart. This procedure is certainly not unique; however, as discussed in [23], it will always succeed as it tends to fill up the "holes" in the distribution of the particles. The values for R_i and R_n were set in [23] to $\sqrt{6}$ and $\sqrt{12}$, respectively. This was based on a 1-D argument that if a point vortex is diffused by inserting new elements at every $R_i = \sqrt{6}$, the distribution of the particles and their circulation recover a fourth-order accurate finite-difference scheme [23].

In our implementation, we use 24 checkpoints spaced 15 degrees apart. The larger number of checkpoints generally improves the chances that the newly inserted vortex element will be at the optimal position to yield a solution of the linear system of equations. The penalty for this is a marginal increase in the cost of computing. We also note that, depending on the particle distribution, multiple (yet equal) minmax solutions may exist for more than one choice out of the 24 possible positions on R_i . Therefore, we accept that minmax solution, which corresponds to a position that minimizes the sum of the absolute values of the three components of the first moments in the x , y and z directions, assuming equal circulation for the particles. This step tends to distribute the particles more uniformly and attempts to maintain geometric symmetry. Finally, we assign $\sqrt{8}$ and $\sqrt{16}$ to R_i and R_n , respectively. These choices relax the linear system of equations considerably, and obtaining an optimal solution of the system becomes less sensitive to the particle distribution within the neighborhood as well as the exact/optimal positioning of the inserted elements. In addition, the total number of particles during a simulation is reduced due to the increase in the nominal inter-particle separation.

The particle insertion strategy is the same for diffusion in 3-D; however, R_i and R_n refer to insertion and neighborhood radii, respectively, of *spheres* instead of circles. In 3-D, the assignment of a constellation of checkpoints that will improve the chances for finding an optimal position, and will thus yield a solution of the system at first pass, is tricky. For example, using the vertices of an icosahedron (that discretize the insertion sphere) as checkpoints usually leads to a larger-than-nominal number of particles, in spite of the attractive symmetries of icosahedrons. The approach used in [23] is as follows: (a) apply a 2-D checkpoint assignment to the equator of the sphere in, for example, the zx plane, and (b) apply 2-D checkpoint assignments to the meridians of the sphere, which pass through the checkpoints on the equator and are on planes parallel to, for example, the xy plane [25]. This is quite a robust method and worked well in a number of test cases. However, there is clearly a preferred direction along the normal to the equator in this approach, which we would like to avoid.

In our implementation of the 3-D checkpoint assignment, we (a) apply the 2-D checkpoint assignment rule to the equators of the sphere in the xy , yz and zx planes, using 16 equidistant points on each equator, and (b) apply the 2-D checkpoint assignment rule to meridians on the sphere, which pass through the checkpoints on the equators and whose axes of symmetry are coincident with the z , x and y coordinates, respectively. We adjust the number of checkpoints on the meridians so that the respective arc-lengths are as close to the equatorial arc-lengths as possible. Therefore, the number of checkpoints on the meridians can be less than or equal to 16.

For the $O(h_v^3)$ case, numerical experiments with various choices for R_i revealed that the particle distributions obtained by the insertion strategy used in the low-order case lead to systems of equations that generally do not have optimal solutions. Indeed, only the case with $R_i = \sqrt{8}$ could be used to predict the diffusion of a 2-D point vortex. The failure of the previous insertion strategy may be explained by recognizing that diffusing a 2-D point vortex with $O(h_v^3)$ accuracy will necessitate placing 14 particles on the perimeter of the insertion circle, because there are 15 equations in the 2-D $O(h_v^3)$ system. Clearly, the distance between neighboring inserted elements

is quite smaller than R_i , which is the distance between the diffusing and the inserted elements. Such disparity in the inter-particle separations stiffens the system of equations.

In order to devise a particle insertion mechanism for the $O(h_v^3)$ case, we concentrated on the 1-D simplification of the system of equations (14), as detailed in Appendix B. For a positive solution of such a system to exist in 1-D, a minimum of five particles are necessary. Further, for a uniform distribution of particles, the symmetry condition dictates that two particles be placed on each side of the diffusing element. It then follows immediately, by deduction, that *two* particle insertion radii are necessary for the higher order 2-D and 3-D cases. What remains is to determine $R_{i,i}$ and $R_{i,o}$, the inner and outer insertion radii, respectively, as well as R_n . The 1-D analysis suggests that the uniform scaled grid spacing, or equivalently $R_{i,i}$, must be less than or equal to $\sqrt{6}$. Further, recall from the analysis in [23] that the scaled inter-particle spacing can at most be $\sqrt{8}$ for third or higher order accuracy, and that R_n must be at least $\sqrt{8}$ since $M_e = 4$. Using these conditions as guidelines, we performed a series of tests with the diffusion of a 2-D point vortex to determine the values of $R_{i,i}$, $R_{i,o}$ and R_n that produce the most (visually) homogenous particle distribution. In this report, we use $R_{i,i} = 2$, $R_{i,o} = 4$ and $R_n = 5$.

Figure 1 depicts a comparison between the length scales involved in the low- and high-order VRM, for a fixed time-step. Clearly, the particle density and the corresponding computational cost of the higher order solution are larger than those of the lower order method. However, as verified in Section 5, for a *fixed* level of accuracy, the number of particles and the computational cost of the higher order solution are actually *lower* than those of the lower order method. This reduction in cost per accuracy level was the motivation behind implementing the higher order VRM.

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5 RESULTS

The $O(h_v)$ and $O(h_v^3)$ Vorticity Redistribution Methods are examined parametrically in this section. The diffusion of a 2-D point vortex is used to analyze the accuracy and convergence rate of the low- and high-order methods as functions of the computational time-step and the cutoff circulation value. The accuracy of the post-processed smooth vorticity field is also examined as a function of the smoothing core function and its core radius. Further comparisons of the accuracy of the low- and high-order methods are provided using examples of the diffusion of a 2-D vortex pair, a 3-D point vortex, and a 3-D vortex ring. A comparison of the computational cost for the two methods is presented as well. In all cases, $\nu = 1/\text{Re} = 1$, which is simply equivalent to simulating diffusion in a viscosity-weighted time-scale. All computations were performed in double precision on a 64-bit SGI Octane with a 195 MHz CPU.

5.1 2-D Point Vortex Diffusion

For the aforementioned parametric studies, the diffusion of a 2-D point vortex centered at $(x = 0, y = 0)$ and with circulation $\Gamma_{\text{max}} = 1$ is considered. For the purpose of post-processing, the diffused vorticity profiles are obtained along $(-3 \leq x \leq 3, y = 0)$ using 241 equi-spaced evaluation points. Unless specified otherwise, the "smoothed" vorticity is evaluated using the infinite-order core function

$$J_1(|\vec{x}|/\sigma)/(2\pi\sigma|\vec{x}|) \quad (21)$$

where $J_1(\cdot)$ is the Bessel function of the first kind of order one and σ is the corresponding core radius [13, 23]. In what follows, references to σ imply the core radius scaled by h_v . As will be demonstrated in this section, assigning an optimum value for the core radius is a difficult task in VRM, and presently the main challenge. In this report, unless noted otherwise, the optimal core radius σ_{opt} is obtained by trial and error, varying σ in scaled increments of 0.01 until the L_2 norm of the difference between the exact and the predicted vorticity profiles is a minimum. This is done to retrieve correct information about the true accuracy and convergence properties of VRM; the fact that a robust method for identifying σ_{opt} (and thus extracting maximum information from the solution) is unavailable *at present* is irrelevant to such analyses!

Figure 2 shows a typical particle distribution due to the diffusion of the point vortex by the $O(h_v^3)$ method during the early stages of the process. The three concentric circles at $T = 0.1$ depict the insertion and neighborhood radii, and demonstrate the relative length scales involved in the computation. Note that the particle distribution is fairly homogeneous, which is a first evidence of the efficacy of the particle insertion strategy as well as the choices in this report for the insertion and neighborhood radii. Lower values of R_n , for example, cause a small percentage of the particles to be packed closely together in pairs and triplets (not shown here), which may lead to instability when used in conjunction with convection.

Figures 3a and 3b depict the diffused vorticity of the point vortex at times $T = 0.25$ and $T = 0.5$, respectively; obtained analytically and predicted by the low- and high-order VRM using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Table 1 lists the corresponding L_2 norm of the errors, the number of particles N_v , and the optimal core radii σ_{opt} . The cutoff circulation in this case is $\varepsilon = 10^{-8}$. Note in Figs. 3 and Table 1 that the prediction errors follow similar trends at $T = 0.25$ and $T = 0.5$; however, the magnitudes of the errors are larger at $T = 0.25$. Indeed, for a fixed Δt in Table 1, the L_2 error at $T = 0.25$ is about three times the L_2 error at $T = 0.5$ for the low-order prediction, and about five times for the high-order case. This is to be expected, since vorticity tends toward a point singularity at earlier times and becomes increasingly more challenging to approximate. A smooth initial condition will likely subdue this discrepancy in the errors at different times.

In Table 1, the L_2 errors versus $\sqrt{\Delta t}$ reveal that, at $T = 0.5$, the low- and high-order methods are actually $O(h_v^{1.83})$ and $O(h_v^{3.55})$, respectively, which are superior to the theoretical convergence rates of $O(h_v)$ and $O(h_v^3)$, respectively. At $T = 0.25$, the corresponding rates are $O(h_v^{2.10})$ and $O(h_v^{3.56})$, respectively. The observed super-linear and -cubic rates are attributed to the fairly homogenous/uniform particle distributions that the particle insertion strategies in this report yield. This claim is based on the 1-D analysis for VRM, which shows that for *uniform* grid distributions the low- and high-order methods are $O(h_v^2)$ and $O(h_v^4)$, respectively. In the following, we will focus our attention mainly on the results at $T = 0.25$, where vorticity is still close to its initial (singular) profile and thus represents a fairly severe test of the robustness of VRM.

In Fig. 3a the lower resolution $O(h_v)$ prediction, using $\Delta t = 10^{-2}$, deviates considerably from the exact solution near the peak. Furthermore, the predicted vorticity is not perfectly symmetric. The asymmetry is caused by the non-uniform particle distribution, the choice of core radius for smoothing, and/or insufficient grid resolution. We have verified (not shown here) that applying VRM on a uniform mesh reproduces a perfectly symmetric vorticity field. We have also observed that core radii larger than σ_{opt} yield more symmetric vorticity profiles, but with lower peaks. As for the effect of spatial resolution, we note in Fig. 3a that the better converged $O(h_v^3)$ prediction, using $\Delta t = 10^{-3}$, is more symmetric. The improvement in the vorticity profile symmetry in the latter case and an order of magnitude drop in the L_2 error are achieved at the expense of an eight-fold increase in the number of particles, as seen in Table 1. By extension, accurate predictions of more complex 3-D flow topologies by the low-order method will require (unrealistically) large numbers of particles. This was the primary incentive for us to develop the higher order VRM, which we expected to be more cost effective by providing sufficiently accurate results at relatively coarser resolutions.

As shown in Fig. 3a, the $O(h_v^3)$ prediction using the coarse $\Delta t = 10^{-2}$ is slightly more accurate than the $O(h_v)$ prediction using the finer $\Delta t = 10^{-3}$. Table 1 verifies that the coarse $O(h_v^3)$ prediction has, on average, 2.4 times smaller L_2 error and requires 3.73 times fewer elements than the fine $O(h_v)$ prediction. As will be demonstrated later, the reduction in the required number of elements for the high-order method (to achieve a level of accuracy that is

comparable to that of the low-order prediction) corresponds to a respectable drop in the *total* computational time, in spite of the increased cost *per particle* to evaluate larger systems of equations.

Note that at the finer resolution level, with $\Delta t = 10^{-3}$, the $O(h_v^3)$ prediction, with an L_2 error of $O(10^{-5})$, becomes indistinguishable from the exact solution. To achieve this level of accuracy with the $O(h_v)$ method, say at $T = 0.5$, assuming the trends in Table 1 are valid for all resolutions, we would need to set the time-step to $\Delta t = 6 \times 10^{-6}$. This would lead to about 10^6 particles compared to the 20,000 required for the higher order method!

To reduce the number of particles and the corresponding computational cost further, one may propose to increase the cutoff circulation ε . However, assigning an arbitrarily large ε without carefully considering its physical and mathematical implications may be a futile exercise. To demonstrate the significance of ε to the convergence rate and accuracy of the simulations, the 2-D point vortex diffusion problem was repeated for $\varepsilon = 10^{-6}$ and $\varepsilon = 10^{-4}$. Table 2 is a list of the L_2 errors, N_v , and σ_{opt} for the low- and high-order VRM predictions using $\varepsilon = 10^{-6}$ versus $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$, at times $T = 0.25$ and $T = 0.5$. Table 3 is the corresponding list for $\varepsilon = 10^{-4}$. Figure 4 is the accompanying $\varepsilon - N_v$ plot of the low- and high-order VRM predictions at $T = 0.25$, using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. The plots at $T = 0.5$ are not shown here as they are simply parallel to the plots at $T = 0.25$, reflecting the increase in the number of particles in time. Figure 5 is the corresponding L_2 errors versus $\sqrt{\Delta t}$ and depicts the effect of ε on the convergence rate and accuracy of the low- and high-order VRM.

Figure 4 concurs that for both low- and high-order methods, using $\Delta t = 10^{-2}$ or $\Delta t = 10^{-3}$, the increase in ε leads to a sizable reduction in N_v . However, as verified in Fig. 5, the latter is associated with diminished solution accuracy, sub-optimal rates of convergence and even non-convergence! Specifically, note in Fig. 5 and Tables 1-3 that as the value of cutoff circulation is increased from $\varepsilon = 10^{-8}$ to $\varepsilon = 10^{-4}$ the L_2 errors for the low- and high-order predictions using the larger time-step $\Delta t = 10^{-2}$ remain fairly unchanged in the order of 10^{-2} and 10^{-3} , respectively. Further, the errors decrease with increasing T . However, the accuracy of the predictions do not necessarily improve with the smaller time-step $\Delta t = 10^{-3}$. With the *low-order* method, the convergence rates for the $\varepsilon = 10^{-8}$ and $\varepsilon = 10^{-6}$ cases are nearly equal and optimal at approximately $O(h_v^2)$; and for the $\varepsilon = 10^{-4}$ case, the rate drops significantly to $O(h_v)$ at $T = 0.25$ and even to $O(1)$ at $T = 0.5$. In contrast, the rates for the *high-order* method are nearly optimal at $O(h_v^{3.6})$ for $\varepsilon = 10^{-8}$, sub-optimal at $O(h_v^{1.2})$ for $\varepsilon = 10^{-6}$, and non-convergent at $O(h_v^{-1.8})$ for $\varepsilon = 10^{-4}$.

Interestingly, Figs. 4 and 5 reveal that the high-order method using $\Delta t = 10^{-2}$ and $\varepsilon = 10^{-8}$ requires fewer particles and is an order of magnitude more accurate than the low-order method using $\Delta t = 10^{-3}$ and $\varepsilon = 10^{-4}$. Clearly, the best price-performance is achieved by the high-order method using relatively large Δt of $O(10^{-2})$ and moderate ε of $O(10^{-6})$.

To summarize Fig. 5, optimal accuracy and convergence rates for the low- and high-order methods are attainable with sufficiently small ε values only. For relatively large ε values, reasonably accurate solutions may be obtained with the high-order method using *large* time-steps; however, the accuracy deteriorates sharply when smaller time-steps are used, especially with the high-order method. The reason that the computations do not converge for small Δt and large ε combination is discussed in [23] for the low-order VRM: As the time-step is reduced, the number of particles increases in an inversely proportional manner. Since the total circulation is fixed, this increase in the number of particles implies that the average circulation of individual vortex particles is reduced. Consequently, a given ε neglects relatively more circulation at smaller time-steps, and thus chops off more of the vorticity field. Of course, this argument applies to the high-order VRM as well, since the latter is essentially equivalent to the low-order method using smaller time-steps.

Note that the problem of losing circulation/vorticity due to a large ε assignment is one of numerical resolution only, and it is not unique to VRM. In, say, finite-difference methods this is similar to specifying a computational domain that is smaller than the actual physical domain and applying zero-vorticity boundary condition. In the Diffusion Velocity Method, since the velocity at the outer edge of the expanding field is infinite, a vorticity cutoff value must be imposed at the outer region to avoid numerical complications associated with infinity. Also, the PSE method applies the same cutoff assignment strategy as VRM.

As has already been demonstrated, solutions based on the high-order method are generally more accurate and generate fewer elements than solutions by the low-order method using an order of magnitude smaller time-step. However, the linear system for the high-order method is represented by 2.5 times as many equations as for the low-order method, and the corresponding computational cost per diffusing element is expected to be at least 6.25 times higher. Figure 6a compares the CPU times as a function of N_v for the low- and high-order methods using $\Delta t = 10^{-3}$ and $\Delta t = 10^{-2}$, respectively. The simulation was extended to $T = 1.0$, and $\varepsilon = 10^{-6}$ was used to obtain moderate accuracy and particle density. Figure 6b depicts the corresponding *cumulative* CPU times as a function of N_v . The symbols and their indices $i = 1, 2, \dots, 10$ in Fig. 6b represent different time levels $T = i/10$ during the simulation. For the larger number of particles, a visual inspection of Fig. 6a reveals that the CPU times for both methods grow linearly with N_v . Furthermore, for fixed values of N_v , the high-order method is about thirteen times more expensive than the low-order method. However, as verified in Fig. 6b, the *total* cost of computing with the high-order method is lower than with the low-order method at all times T during the simulation. Indeed, the low-order method is consistently more costly than its high-order counterpart by a factor of three.

We turn our attention now to post-processing. The selection process for the core radius σ for post-processing purposes is currently a matter of art, and a robust mathematically reliable strategy to extract σ_{opt} from the particle distribution remains to be developed. The range of values used in [23] is $R_i \leq \sigma \leq R_n$. However, notice in Table 1-3 that σ_{opt} is a function of T and Δt , and it even falls outside the range used in [23]. Then the obvious question to address is how sensitive the accuracy of post-processed vorticity is to the variations in σ as a function of T , Δt and even VRM order.

Figure 7 depicts the L_2 errors versus σ for the low- and high-order predictions using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$, at times $T = 0.25$ and $T = 0.5$. A cutoff value of $\varepsilon = 10^{-8}$ was used in all cases. The solid vertical lines denote $R_{i,i}$, $R_{i,o}$ and R_n for the high-order VRM as reference. The dashed vertical line denotes R_i for the low-order VRM; R_n in this case is equal to $R_{i,o}$. Figure 7 shows that the σ - L_2 -error curves are V-shaped and that $\sigma \approx \sigma_{opt}$ within only very narrow ranges. Further, for fixed T and/or Δt , the range is narrower for the high-order method. Also, for both low- and high-order methods, the range becomes narrower at earlier times T and as Δt is increased. The fact that σ_{opt} is confined to a narrow range is not, by itself, a source of difficulty. Complications arise because σ_{opt} and the associated (narrow) range shift as a function of Δt and/or T . For example, for the low-order method, σ_{opt} is proximal to R_i when $\Delta t = 10^{-2}$ and it is closer to $R_{i,o}$ (the low-order R_n) when $\Delta t = 10^{-3}$. Similarly, for the high-order method, σ_{opt} is closer to $R_{i,i}$ when $\Delta t = 10^{-2}$ and closer to R_n when $\Delta t = 10^{-3}$. And in both cases σ_{opt} increases in time. It is interesting to note that for simulations using $\Delta t = 10^{-2}$, σ_{opt} may actually be smaller than the smallest length scale; i.e., R_i for low-order and $R_{i,i}$ for high-order VRM! This is counter-intuitive, and we do not have an explanation at present.

We were able to derive empirically obtained scaling rules that practically fit the apparently disassociated curves in Fig. 7 into one. We found that

$$\sigma_{opt}^2 \sim \left(T^{\sqrt{3}/2}, (\Delta t)^{-1/\sqrt{2}} \right) \quad (22)$$

with acceptable accuracy. The correlation does not account for the order of accuracy of the method in use explicitly, and the scaled curves for the low- and high-order methods are slightly separated from each other. However, the impact of this discrepancy on solution accuracy is minor. We note here that the above scaling rules cannot be utilized without knowing σ_{opt} at some Δt and T . Moreover, the presented results are based on a very limited number of tests and may not be accurate or general enough to be applicable to all flow conditions. Nevertheless, the fact that we were able to find scaling laws at all gives us reason to believe that it is possible to formulate a generalized theory for obtaining σ_{opt} . In lieu of such a theory, we propose a heuristic method for assigning σ_{opt} . According to Fig. 7, for both low- and high-order methods using $\Delta t = 10^{-3}$, assigning $R_{i,o}$ to the core radius σ yields accurate vorticity fields for all T with L_2 errors that are acceptably close to their corresponding optimal condition. Similarly, for the low- and high-order methods using $\Delta t = 10^{-2}$, $\sigma \approx R_i$ and $\sigma \approx R_{i,i}$, respectively, yield acceptably accurate vorticity fields for all T . More tests will be necessary to obtain similar heuristics for various time-steps.

We now examine the effect of lower order (and less expensive) core functions on the accuracy of post-processed data. To this end, we consider second-, fourth- and eighth-order Gaussian cores;

$$G_2(\bar{x}, \sigma) = \exp\left(-(|\bar{x}|/\sigma)^2\right) / \pi\sigma^2 \quad (23a)$$

$$G_4(\bar{x}, \sigma) = 2G_2(\bar{x}, \sigma) - G_2(\bar{x}/\sqrt{2}, \sigma)/2 \quad (23b)$$

$$G_8(\bar{x}, \sigma) = 64G_2(\bar{x}, \sigma)/21 - 4G_2(\bar{x}/\sqrt{2}, \sigma)/3 + G_2(\bar{x}/2, \sigma)/6 - G_2(\bar{x}/\sqrt{8}, \sigma)/168 \quad (23c)$$

respectively [3]. Figure 8a compares the effectiveness of G_2 , G_4 and G_8 in extracting the vorticity from the low-order VRM prediction at $T = 0.5$, using $\Delta t = 10^{-2}$ and $\varepsilon = 10^{-8}$. Figures 8b and 8c show similar comparisons for the low-order VRM using $\Delta t = 10^{-3}$ and the high-order VRM using $\Delta t = 10^{-2}$, respectively. In Fig. 8a, the vorticity using the infinite-order core function is displayed as a reference. Figure 8a suggests that for low-resolution simulations; e.g., low-order VRM using $\Delta t = 10^{-2}$, higher than eighth-order Gaussian or infinite-order core functions are necessary to capture the available information effectively. For moderate-resolution simulations, Figs. 8b and 8c reveal that G_4 or G_8 would be sufficient, but G_2 is too inaccurate to consider. However, for the high-resolution simulation in this report; i.e., the high-order VRM using $\Delta t = 10^{-3}$, G_2 smoothing provides quite accurate results (not shown,) as expected and verified by the trends in Figs. 8. Therefore, except in low-resolution simulations, for which the infinite-order core function must be used, G_4 smoothing is recommended for fast post-processing with acceptable accuracy.

In Figs. 8a and 8b, the core radii that were used are larger than the radii that minimize the respective L_2 errors. This is because with G_4 and G_8 smoothing σ_{opt} yields asymmetric vorticity profiles similar to the one observed and discussed earlier. The larger cores used in the figures tend to shift the profiles in the correct direction, while simultaneously diffusing the vorticity out; i.e., the peaks of the more symmetric profiles are smaller. This asymmetry gets corrected in the finer simulations as it did with infinite-order smoothing. For the case with G_2 smoothing, σ_{opt} is smaller than the nominal inter-particle separation R_i and it yields an asymmetric bi-Gaussian! Clearly, in this case, the L_2 norm is not a good measure for the accuracy of post-processed data. Indeed, the L_∞ norm of the errors, which corresponds to a larger core than that for the L_2 norm is a better measure, and it does not produce a bi-Gaussian. The cores in Figs. 8a and 8b are assigned even larger values to produce the desired level of symmetry. We must point out here that for high-resolution simulations utilizing *any* order smoothing, as well as low-resolution simulations utilizing high-order smoothing, the core radii corresponding to L_2 and L_∞ norms converge to a single value. Otherwise, cores that minimize the L_2 norm are smaller than cores that minimize the L_∞ norm.

5.2 2-D Vortex Pair Diffusion

The diffusion of a pair of 2-D point vortices at $(x = \pm 0.5, y = 0)$, with respective circulations $\Gamma_{max} = \pm 1$, is considered in this section. The objective is to demonstrate how well the symmetry of the vorticity field is preserved, especially near the symmetry axis where vorticity is negligible and more susceptible to errors. This is true despite the fact that the particle distribution in VRM is non-uniform and completely blind to the symmetry condition in the field. For this

case, $\varepsilon = 10^{-6}$ is used because of its acceptable level of accuracy. For the purpose of post-processing, the diffused vorticity profiles are obtained along $(-6 \leq x \leq 6, y = 0)$ using 241 equi-spaced evaluation points. The "smoothed" vorticity is evaluated using the previously defined infinite-order core function. The optimal core radius σ_{opt} is obtained by trial and error, as before, to minimize the L_2 norm of the errors.

Figure 9 shows the early stages of the evolution of the particle distribution for the $O(h_v^3)$ VRM. The three concentric circles at $T = 0.1$ depict the insertion and neighborhood radii to denote the relative length scales involved in the computation. Note that no special treatment was introduced to accommodate the "fusing" of the particles as the edges of the oppositely signed vorticity fields begin to contact (and diffuse into) each other at the centerline.

Figure 10 shows the diffused vorticity at time-slices $T = 0.1, 0.2, 0.5$ and 1.0 , obtained analytically and by the $O(h_v^3)$ VRM using $\Delta t = 10^{-2}$. At $T = 0.1$, the L_2 norm of the error is 9.4×10^{-3} , which, considering the singularities in the initial condition, is quite acceptable at the earlier stages of the simulation. Beyond $T = 0.2$, where the L_2 error is already 1.5×10^{-3} , the exact and the numerical results are in excellent agreement; the corresponding plots are indistinguishable even when they are normalized by their respective maxima at each T .

Figure 11a shows the diffused vorticity at $T = 0.1$, obtained analytically and by the $O(h_v)$ VRM using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Figure 11b shows the corresponding results at $T = 0.5$ and $T = 1.0$. Note that the scales in Figs. 11a and 11b are different. As expected, the low-resolution predictions by the low-order method are quite inaccurate at earlier times but improve considerably when the time-step is reduced by an order of magnitude. Indeed, as listed in Figs. 10 and 11a, the L_2 errors of the predictions by the low-order method using $\Delta t = 10^{-3}$ and the high-order method using $\Delta t = 10^{-2}$ are equal at $T = 0.1$. Interestingly, however, Figs. 10 and 11b indicate that the results by the high-order method are increasingly more accurate than their high-resolution low-order VRM counterparts at later times. For example, the L_2 error of the former is about four times smaller than that of the latter at $T = 0.5$, and about eight times smaller at $T = 1.0$.

At $T = 1.0$, 3,752 particles were necessary to represent the diffusion of vorticity by the high-order VRM using $\Delta t = 10^{-2}$ and $\varepsilon = 10^{-6}$. The corresponding numbers for the low-order VRM using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$ were 1,789 and 13,181, respectively. Therefore, for the same level of accuracy, the high-order method required 3.5 times fewer particles and correspondingly less cumulative CPU time.

5.3 3-D Point Vortex Diffusion

The diffusion of a 3-D point vortex centered at $(x = 0, y = 0, z = 0)$ and with vectorial circulation $\vec{\Gamma}_{max} = (1, 0, 0)$ is considered in this section. For the purpose of post-processing, the diffused vorticity profiles are obtained along $(-3 \leq x \leq 3, y = 0, z = 0)$ using 60 equi-spaced evaluation points. The "smoothed" vorticity is evaluated using the infinite-order core function

$$J_{3/2}(|\bar{x}|/\sigma)/(2\pi\sigma|\bar{x}|)^{3/2} \quad (24)$$

where $J_{3/2}(\cdot)$ is the fractional order Bessel function of the first kind of order $3/2$ and σ is the core radius [23]. The optimal core size corresponds to the minimum L_2 norm of the difference between the exact and the predicted vorticity profiles and is obtained by trial and error, as explained in Section 5.1. Note that the choice of this core function is not ideal for post-processing since, as will be demonstrated shortly, it decays too slowly and leads to oscillations at large distances. The slow decay is caused (or explained) by the Fourier transform of the function, which has a discontinuity at the highest (resolved) wave-number of the solution [23].

Figure 12 depicts the diffused vorticity of the 3-D point vortex at $T = 0.22$ as predicted by the $O(h_v^3)$ VRM using $\Delta t = 10^{-2}$, and the $O(h_v)$ VRM using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. The cutoff circulation was set conservatively to $\varepsilon = 10^{-6}$. The high-order prediction is in excellent agreement with the exact solution; however, the low-order method is far from converged, even with the higher resolution case using $\Delta t = 10^{-3}$. Again, this is mainly because the vorticity is evaluated at a relatively early time near the initial singularity. Lower resolution predictions by the low-order method will probably suffice at much later times.

For the above test problem, the high-order method used up to 11,472 particles, whereas the low-order method required 5,040 and 80,482 particles for the $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$ cases, respectively. The large number of particles used in the high-resolution low-order case did not warrant the continuation of the run for simply the sake of conducting a parametric study at longer times. For this purpose, we can refer to the results of the previous parametric studies in 2-D. Note that for about the same level of accuracy at $T = 0.22$, the high-order method requires *seven* times fewer particles than does the low-order method using $\Delta t = 10^{-3}$. On the other hand, the linear system for the high-order method is represented by 3.5 times as many equations as for the low-order method, and the corresponding computational cost per diffusing element is expected to be at least 12.25 times higher. Indeed, as demonstrated in Fig. 13a, for fixed values of N_v the high-order method is about *sixty* times more expensive than the low-order method! Furthermore, a visual inspection of Fig. 13a reveals that the CPU times for both methods grow linearly with N_v , similar to the 2-D case. These lead to a 44 percent reduction in the *total* computing cost with the high-order method, as verified in Fig. 13b. The computational saving in 3-D is not as impressive as in 2-D, primarily because of the high cost of computing incurred by the high-order method *per* diffusing element. This can be improved substantially by implementing advanced linear programming techniques, which are generally effective when applied to linear systems of equations that are as large as (or larger than) the system representing the high-order 3-D VRM. Nevertheless, the significance of using the high-order VRM becomes more clear when the cost of evaluating the particle velocities for the convection sub-process is included in the total as well. In this case, at least a factor of seven cost reduction in the particle velocity evaluations may be realized (per time-step) because of a factor of seven drop in the number of particles.

We experimented with $\varepsilon = 10^{-5}$ to entertain the idea of reducing the number of particles to manageable values by increasing the cutoff circulation. At $T = 0.22$, the number of particles dropped by 30 percent to 7,988 in the high-order method, and 48 percent to 41,813 in the low-

order method using $\Delta t = 10^{-3}$. We now refer to Fig. 14 to evaluate the impact of using $\varepsilon = 10^{-5}$ on the accuracy of the diffused vorticity at $T = 0.25$, as predicted by the high-order VRM using $\Delta t = 10^{-2}$ and the low-order VRM using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. The prediction by the high-order method is in excellent agreement with the exact solution - the L_2 norm of the error being 4.4×10^{-4} . On the other hand, the solution by the low-order method using $\Delta t = 10^{-2}$ underpredicts the peak vorticity and oscillates at the tails, as seen in the zoomed window. The higher resolution low-order method using $\Delta t = 10^{-3}$ agrees quite well with the exact solution, except near the tail ends. Note that the dashed line beyond $|x| > 1$ is short and is part of the higher resolution profile. The oscillations near the tail ends exist partially because the infinite-order core function in 3-D does not damp out as quickly [23], and partially because a larger cutoff circulation is being used. The latter claim is supported by the results shown in Fig. 12, where $\varepsilon = 10^{-6}$ is used. The former claim has been verified by using second- and fourth-order core functions (not shown) and obtaining benign oscillations at the tails. It may at first appear peculiar that the predictions by the low-order method agree with the exact solution better when $\varepsilon = 10^{-5}$ is used (Fig. 14) than when $\varepsilon = 10^{-6}$ is used (Fig. 12). However, recall that the case with $\varepsilon = 10^{-6}$ corresponds to $T = 0.22$, whereas the case with $\varepsilon = 10^{-5}$ corresponds to a later time $T = 0.25$. Within this time differential the peak vorticity drops by as much as 18 percent. Therefore, in agreement with earlier observations, we note that the accuracy of the predictions improves in time as the vorticity departs from its initial singular character.

5.4 3-D Vortex Ring Diffusion

The final example considered in this report is the diffusion of a 3-D vortex ring, initially centered at $(x = 0, y = 0, z = 0)$ with radius $(R_r = 1, z = 0)$ and circulation $|\vec{\Gamma}_{\max}| = 2\pi$. The ring is discretized using 32 equi-spaced particles, which is the minimum required to satisfy the inter-particle separation criterion for the high-order VRM with $\Delta t = 10^{-2}$. The cutoff circulation is set to $\varepsilon = 10^{-5}$. For the purpose of post-processing, the "smoothed" vorticity is evaluated using the infinite-order core function of the previous sub-section. The optimal core size corresponds to the minimum L_2 norm of the error, as explained in Section 5.1.

Figure 15a depicts the time evolution of the diffusion of the vortex ring in its plane of symmetry along $(-3 \leq x \leq 3, y = 0, z = 0)$, as obtained analytically [24] and by the high-order VRM using $\Delta t = 10^{-2}$. Figure 15b shows the time evolution along $(x = 1, y = 0, -3 \leq z \leq 3)$. 81 equally separated evaluation points are used in each case. Note, by $T = 0.25$ the vorticity is diffused substantially and the simulation was stopped. A total of 24,474 particles were created in the process. Figures 15 show that except for the minor differences at $T = 0.05$, the VRM predictions are in excellent agreement with the exact solution. In particular, notice that the curvatures and slopes of the profiles around the origin are captured quite accurately. This is an indication that the high-order VRM particle insertion strategy is robust in 3-D as well. That is, the method can accommodate the geometric transitions from a thin vortex at $T = 0.0$, to a fat vortex ring at $T = 0.05$, and eventually to a (thick) pancake shape at $T > 0.05$ effortlessly, without requiring any special adjustments and/or regridding.

Figures 16a and 16b show the vorticity at $T = 0.05$ along $(-3 \leq x \leq 3, y = 0, z = 0)$ and $(x = 1, y = 0, -2 \leq z \leq 2)$, respectively, obtained analytically and by the low-order VRM using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Figures 17a and 17b are the corresponding profiles for $T = 0.1$. The lower resolution results tend to under-predict the peaks and oscillate at the tail ends - as was the case with the diffusion of a 3-D point vortex. Further, the oscillations from the positive and negative "eddies" super-impose to produce an inaccurate prediction of the slopes around the origin, as seen in Figs. 16a and 17a. On the other hand, the accuracy of the higher resolution predictions using $\Delta t = 10^{-3}$ is superb, as expected. The price for this is the generation of a large number of particles; by $T = 0.1$, 79,699 particles were in use and the simulation was stopped. In contrast, the high-order VRM used only 10,044 particles, producing similarly accurate results at 51 percent of the *total* CPU time spent by the low-order VRM. Further, an estimated 190,000 particles would be necessary for the low-order VRM to simulate the diffusion of the vortex ring through $T = 0.25$. Recall that the high-order VRM used only 24,474 particles at $T = 0.25$.

Figure 18 depicts the maximum error in the divergence of the vorticity field versus $\sqrt{\Delta t}$ at $T = 0.05$ and $T = 0.1$, using low-order VRM and $\varepsilon = 10^{-5}$. Divergence is evaluated on the particles using

$$\bar{\nabla} \cdot \bar{\omega}(\bar{x}, t) \approx \sum_{i=1}^{N_v} \bar{\Gamma}_i(t) \cdot \bar{\nabla} g_\sigma(\bar{x} - \bar{x}_i) \quad (25a)$$

$$g_\sigma(\bar{x}) = J_{3/2}(|\bar{x}|/\sigma) / (2\pi\sigma|\bar{x}|)^{3/2} \quad (25b)$$

We note that solenoidality is maintained quite accurately for this problem, even with the low-order VRM. At present, we do not have an explanation for the $O(h_v^3)$ convergence rate, which is higher than the convergence rate of the vorticity field itself!

Figure 19 is a representative 3-D image of the vorticity field at $T = 0.2$ as predicted by the high-order VRM using $\Delta t = 10^{-2}$. For this purpose, $61 \times 61 \times 41$ uniformly distributed nodes were used to grid a box of dimensions $6 \times 6 \times 4$, centered at the origin. The colors represent the magnitude of vorticity normalized by the maximum in the field. The shaded contours represent the vorticity in the $y = 0$ plane. The protrusions are selected vortex lines, which are shown as tubes to allow for the visual inspection of the divergence of the field; i.e., if the field "cross-flow" expands or compresses, the tube will enlarge or shrink accordingly. All vortex tubes that we tried in this example close onto themselves, into a circle, and maintain uniform tube "core" radii. The vortex tubes and the contours, supported by the comparisons with the exact solution in Fig. 15 (as well as the convergence study for the low-order VRM) demonstrate that the high-order VRM maintains the symmetry and the solenoidality of the vorticity field quite well, despite the fact that the particles are not distributed uniformly.

SUMMARY

In this report, an algorithm for the implementation of the Vorticity Redistribution Method with *third-order* theoretical accuracy in the diffusion length scale is developed for the simulation of 3-D diffusion. The formulation for 3-D diffusion with spatially varying viscosity is derived as well. Analysis and (limited) numerical experiments show that VRM maintains the solenoidality of an initially divergence-free vorticity field. It is shown that, unlike the first-order case [23, 26], the system of equations that represent diffusion from a point to its neighbors with third-order accuracy cannot generally have a positive solution if the neighboring points lie *nominally* on one circle of radius equal to some diffusion length scale. That is, as one may suspect, the support bases for the first- and third-order diffusion are different. An analysis of the 1-D analogue problem suggests that *two* concentric circles are necessary for the third-order case, and it provides the guidelines for selecting the corresponding radii.

The accuracy and convergence rate of the first- and third-order VRM are established parametrically as a function of the time-step and the cutoff circulation using the test problem of the diffusion of a 2-D point vortex in free space. Additionally, the effects of the core function order and core radius size on the accuracy of post-processed vorticity are examined. Further demonstrations of the accuracy and salient features of the high-order method are provided using the 2-D vortex pair, 3-D point vortex, and 3-D vortex ring examples.

It is shown that while large cutoff circulation values reduce the total number of particles and CPU time, optimal accuracy and convergence rates for both low- and high-order methods are attainable only with sufficiently small cutoff values. For relatively large cutoff values, reasonably accurate solutions may be obtained with the high-order method using *large* time-steps; however, the accuracy deteriorates sharply when smaller time-steps are used.

When a small cutoff circulation is used, the linear-order method converges (almost) quadratically in the diffusion length scale, and the third-order method converges with better than order 3.5. However, the convergence rates drop significantly for large cutoff values. In all cases tested, similar levels of solution accuracy are achieved by the high-order method using $\Delta t = 10^{-2}$ and its low-order counterpart using $\Delta t = 10^{-3}$. The time-step ratio increases further for more accurate solutions because of the difference in convergence rates between the two methods. As a result, for the same level of accuracy, the high-order method requires substantially fewer particles and is, thus, more cost effective than the low-order approach.

At the post-processing stage, the infinite-order core function is found to be the most effective for extracting the vorticity field from solutions with low resolution; at higher resolutions a fourth- or eighth-order Gaussian is shown to suffice. The post-processing error is found to be controlled by the core radius size. The criteria for selecting the *optimal* core size remain largely unknown, since the latter seems to depend at least on the core function order, the time-step, and the time level at which the data is analyzed.

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RECOMMENDATIONS

The development of a *truly grid-free third-order* VRM has provided the unprecedented capability to predict 3-D diffusion in free space accurately, at reduced computational cost, using considerably larger time-steps than would be necessary with the low-order method. Nevertheless, there are issues with (not necessarily third-order) VRM that call for further development effort.

First, although the CPU times for both low- and high-order methods vary linearly with the number of particles, the constants of proportionality may be large depending on the methodology used for solving the under-determined linear system of equations. In this report, the system is solved using the standard simplex method [1, 2, 4, 8, 18], which works quite well in the low-order method; especially in 2-D, because of the very small number of equations. However, the revised simplex method [4, 8, 18] or more advanced linear programming techniques may prove to be more cost effective for solving the larger set of equations that represent the high-order VRM in 3-D. Additionally, in this report, once the simplex vertex interchange is complete and a solution has been found, the system matrix is inverted one last time, as a purely precautionary measure, using a standard Gaussian elimination technique. The latter is cubic with respect to the number of particles in the neighborhood of the diffusing element, whereas the simplex method is only quadratic. Eliminating the final matrix inversion step is expected to reduce the computational cost noticeably.

Second, despite the tremendous advantages that VRM offers over the more established methods, such as truly grid-free and higher than second-order computing, there is a real need to formulate the criteria for selecting optimal core radii for post-processing purposes. This may be done either based on a sound mathematical derivation or by means of a heuristic approach that has been verified by a comprehensive set of test problems.

Third, VRM is formulated in this report for diffusion in free-space. To account for boundary effects, the method of images was used in [23], which, judging from the presented results, works well. However, for complex 3-D geometries, such an approach is not so appealing. The extension of the method to wall-bounded problems, perhaps by coupling the Boundary Element Method with Eqn. (6) and following, will have a wide range of applications and it needs to be taken into serious consideration.

Fourth, without an LES capability the application of VRM will remain limited to the simulation of flow at low Reynolds numbers. The basic framework for VRM-based LES; i.e., the VRM formulation for diffusion with spatially varying viscosity is provided in this report. The next obvious step is to develop a methodology for obtaining positive solutions of the system.

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TABLES

- Table 1: Diffusion of a 2-D point vortex using cutoff circulation $\varepsilon = 10^{-8}$. The matrix lists the L_2 norm of the errors, the number of particles N_v , and the optimal scaled core radii σ_{opt} (used with the infinite-order core function) at times $T = 0.25$ and $T = 0.5$, for low- and high-order VRM using time-steps $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$.
- Table 2: Diffusion of a 2-D point vortex using cutoff circulation $\varepsilon = 10^{-6}$. The matrix lists the L_2 norm of the errors, the number of particles N_v , and the optimal scaled core radii σ_{opt} (used with the infinite-order core function) at times $T = 0.25$ and $T = 0.5$, for low- and high-order VRM using time-steps $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$.
- Table 3: Diffusion of a 2-D point vortex using cutoff circulation $\varepsilon = 10^{-4}$. The matrix lists the L_2 norm of the errors, the number of particles N_v , and the optimal scaled core radii σ_{opt} (used with the infinite-order core function) at times $T = 0.25$ and $T = 0.5$, for low- and high-order VRM using time-steps $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$.

Table 1

		$T = 0.25$		$T = 0.5$	
$\varepsilon = 10^{-8}$		$\Delta t = 10^{-2}$	$\Delta t = 10^{-3}$	$\Delta t = 10^{-2}$	$\Delta t = 10^{-3}$
L_2 Error	$O(h_v)$	2.905×10^{-2}	2.569×10^{-3}	8.553×10^{-3}	1.035×10^{-3}
	$O(h_v^3)$	1.552×10^{-3}	2.588×10^{-5}	3.283×10^{-4}	5.525×10^{-6}
N_v	$O(h_v)$	687	5,558	1,306	10,440
	$O(h_v^3)$	1,492	12,059	2,799	22,690
σ_{opt}	$O(h_v)$	2.228	5.568	2.928	7.688
	$O(h_v^3)$	1.730	4.560	2.330	6.130

Table 2

		$T = 0.25$		$T = 0.5$	
$\varepsilon = 10^{-6}$		$\Delta t = 10^{-2}$	$\Delta t = 10^{-3}$	$\Delta t = 10^{-2}$	$\Delta t = 10^{-3}$
L_2 Error	$O(h_v)$	2.929×10^{-2}	2.459×10^{-3}	8.054×10^{-3}	6.684×10^{-4}
	$O(h_v^3)$	1.663×10^{-3}	4.109×10^{-4}	3.231×10^{-4}	1.379×10^{-4}
N_v	$O(h_v)$	491	3,677	900	6,748
	$O(h_v^3)$	1,022	7,769	1,900	14,177
σ_{opt}	$O(h_v)$	2.240	5.618	2.928	7.578
	$O(h_v^3)$	1.740	2.710	2.320	3.030

Table 3

		$T = 0.25$		$T = 0.5$	
$\varepsilon = 10^{-4}$		$\Delta t = 10^{-2}$	$\Delta t = 10^{-3}$	$\Delta t = 10^{-2}$	$\Delta t = 10^{-3}$
L_2 Error	$O(h_v)$	3.239×10^{-2}	1.042×10^{-2}	1.006×10^{-2}	1.017×10^{-2}
	$O(h_v^3)$	3.745×10^{-3}	2.992×10^{-2}	2.966×10^{-3}	5.468×10^{-2}
N_v	$O(h_v)$	296	1,836	519	3,062
	$O(h_v^3)$	595	3,520	1,064	5,695
σ_{opt}	$O(h_v)$	2.248	6.728	2.968	10.018
	$O(h_v^3)$	1.590	5.310	2.830	5.080

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FIGURES

- Figure 1: Schematic diagram of the "stencils" for the low- and high-order VRM.
- Figure 2: Typical particle distribution due to the diffusion of a 2-D point vortex by the high-order VRM during the early stages of the process. $\Delta t = 10^{-2}$ and $\varepsilon = 10^{-4}$.
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- Figure 4: The number of particles N_v versus the cutoff circulation ε for the low- (LO) and high-order (HO) predictions at $T = 0.25$, using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$.
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- Figure 7: The L_2 error versus the core radius σ , at times $T = 0.25$ and $T = 0.5$, for the low- (LO) and high-order (HO) predictions using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Cutoff circulation is $\varepsilon = 10^{-8}$.
- Figure 8: An analysis of post-processing accuracy using second-, fourth, and eighth-order Gaussian core functions - G_2 , G_4 and G_8 , respectively. $T = 0.5$ and $\varepsilon = 10^{-8}$ in all cases. (a) Low-order VRM (LO) using $\Delta t = 10^{-2}$, (b) low-order VRM (LO) using $\Delta t = 10^{-3}$, and (c) high-order VRM (HO) using $\Delta t = 10^{-2}$.
- Figure 9: Typical particle distribution due to the diffusion of a 2-D point vortex pair by the high-order VRM during the early stages of the process. $\Delta t = 5 \times 10^{-3}$ and $\varepsilon = 10^{-4}$.
- Figure 10: The diffused vorticity of a 2-D vortex pair at time-slices $T = 0.1, 0.2, 0.5$ and 1.0 , obtained analytically and by the high-order VRM (HO) using $\Delta t = 10^{-2}$. Cutoff circulation is $\varepsilon = 10^{-6}$.
- Figure 11: The diffused vorticity of a 2-D vortex pair, obtained analytically and by the low-order VRM (LO), using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Cutoff circulation is $\varepsilon = 10^{-6}$. (a) Time level $T = 0.1$, and (b) time levels $T = 0.5$ and $T = 1.0$.

- Figure 12: The diffused vorticity of a 3-D point vortex at $T = 0.22$, predicted by the high-order VRM (HO) using $\Delta t = 10^{-2}$, and the low-order VRM (LO) using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Cutoff circulation is $\varepsilon = 10^{-6}$.
- Figure 13: The diffusion of a 3-D point vortex. (a) CPU time, and (b) cumulative CPU time, as a function of the number of particles N_v for the low-order VRM (LO) using $\Delta t = 10^{-3}$, and the high-order VRM (HO) using $\Delta t = 10^{-2}$. Cutoff circulation is $\varepsilon = 10^{-6}$.
- Figure 14: The diffused vorticity of a 3-D point vortex at $T = 0.25$ as predicted by the high-order VRM (HO) using $\Delta t = 10^{-2}$, and the low-order VRM (LO) using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Cutoff circulation is $\varepsilon = 10^{-5}$.
- Figure 15: The time evolution of the diffusion of a 3-D vortex ring obtained analytically and by the high-order VRM (HO) using $\Delta t = 10^{-2}$ and $\varepsilon = 10^{-5}$. The vorticity profiles are along (a) $(-3 \leq x \leq 3, y = 0, z = 0)$, and (b) $(x = 1, y = 0, -3 \leq z \leq 3)$.
- Figure 16: The diffused vorticity of a 3-D vortex ring at $T = 0.05$, obtained analytically and by the low-order VRM (LO) using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Cutoff circulation is $\varepsilon = 10^{-5}$. The vorticity profiles are along (a) $(-3 \leq x \leq 3, y = 0, z = 0)$, and (b) $(x = 1, y = 0, -2 \leq z \leq 2)$.
- Figure 17: The diffused vorticity of a 3-D vortex ring at $T = 0.1$, obtained analytically and by the low-order VRM (LO) using $\Delta t = 10^{-2}$ and $\Delta t = 10^{-3}$. Cutoff circulation is $\varepsilon = 10^{-5}$. The vorticity profiles are along (a) $(-3 \leq x \leq 3, y = 0, z = 0)$, and (b) $(x = 1, y = 0, -2 \leq z \leq 2)$.
- Figure 18: The maximum error in the divergence of the vorticity field of a 3-D vortex ring versus the diffusion length scale $\sqrt{\Delta t}$ at $T = 0.05$ and $T = 0.1$, using low-order VRM and cutoff circulation $\varepsilon = 10^{-5}$.
- Figure 19: A representative 3-D image of the vorticity of a vortex ring at $T = 0.2$, as predicted by the high-order VRM using $\Delta t = 10^{-2}$ and $\varepsilon = 10^{-5}$. The colors represent the magnitude of vorticity normalized by the maximum in the field - blue through red being zero through one, respectively. The shaded contours represent the vorticity in the $y = 0$ plane.
- Figure B-1: Schematic diagram of the 1-D stencil for the high-order VRM.

Figure 1

$T = 0.0$

$T = 0.01$

$T = 0.1$

$T = 0.2$

Figure 2

Figure 3

Figure 4

Figure 5

(a)

(b)

Figure 6

Figure 7

Effect Of Core Function On Vorticity In Low-Order VRM

$dt=10^{-2}$, $T=0.50$, $\varepsilon=10^{-8}$

(a)

Effect Of Core Function On Vorticity In Low-Order VRM

$dt=10^{-3}$, $T=0.50$, $\varepsilon=10^{-8}$

(b)

Figure 8

Figure 8 - Continued

$T = 0.0$

$T = 0.005$

$T = 0.01$

$T = 0.015$

$T = 0.035$

$T = 0.1$

Figure 9

Figure 10

Figure 11

Figure 12

(a)

(b)

Figure 13

Figure 14

(a)

(b)

Figure 15

(a)

(b)

Figure 16

(a)

(b)

Figure 17

Figure 18

Figure 19

Figure B-1

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APPENDIX A

The generalized VRM for the anisotropic diffusion of a 1-D point source [24] is extended to develop the formulation for the diffusion of a 3-D vorticity vector field with variable viscosity.

The equation for the diffusion of vorticity in 3-D free space with variable viscosity is

$$\frac{\partial \bar{\omega}}{\partial t} = \bar{\nabla} \cdot (\nu \bar{\nabla} \bar{\omega}) \quad (\text{A.1})$$

where Eqns. (1b) and (1c) still apply, and $\nu = \nu(\bar{x})$.

Similar to the analysis in Section 2, we seek to minimize the discretization error in (A.1), in an integral sense, to arbitrary order $(L + M + N) \geq 2$

$$\frac{d}{dt} \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\omega} dV = \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\nabla} \cdot (\nu \bar{\nabla} \bar{\omega}) dV \quad (\text{A.2})$$

Now, let's integrate the right hand side of (A.2) by parts

$$\begin{aligned} \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\nabla} \cdot (\nu \bar{\nabla} \bar{\omega}) dV &= \int \bar{\nabla} \cdot \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \nu \bar{\nabla} \bar{\omega} \right] dV \\ &\quad - \int \bar{\nabla} \cdot \left\{ \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \nu \bar{\omega} \right\} dV \\ &\quad + \int \nu \bar{\nabla} \cdot \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dV \\ &\quad + \int \bar{\nabla} \nu \cdot \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dV \end{aligned} \quad (\text{A.3})$$

The first two terms on the right hand side of (A.3) are surface integrals due to the Gauss' Theorem [17]

$$\begin{aligned} \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\nabla} \cdot (\nu \bar{\nabla} \bar{\omega}) dV &= \int \nu (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{n} \cdot \bar{\nabla} \bar{\omega} dS \\ &\quad - \int \nu \bar{n} \cdot \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dS \\ &\quad + \int \nu \bar{\nabla} \cdot \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dV \\ &\quad + \int \bar{\nabla} \nu \cdot \bar{\nabla} \left[(x - x_i)^L (y - y_i)^M (z - z_i)^N \right] \bar{\omega} dV \end{aligned} \quad (\text{A.4})$$

The surface integrals do not contribute to the diffusion process in free space. As a result, substituting (A.4) into (A.2) yields the following compact form of the generalized VRM for the diffusion of a 3-D vorticity vector field with spatially varying viscosity for arbitrary (L, M, N) :

$$\begin{aligned} \frac{d\bar{E}_{LMN}}{dt} = & \left[L(L-1)\bar{F}_{(L-2)MN} + M(M-1)\bar{F}_{L(M-2)N} + N(N-1)\bar{F}_{LM(N-2)} \right] \\ & + \left[L\bar{G}_{(L-1)MN}^x + M\bar{G}_{L(M-1)N}^y + N\bar{G}_{LM(N-1)}^z \right] \end{aligned} \quad (\text{A.5a})$$

$$\bar{E}_{LMN} = \int (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\omega} dV \quad (\text{A.5b})$$

$$\bar{F}_{LMN} = \int v (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\omega} dV \quad (L + M + N) = 0, 1, 2, \dots \quad (\text{A.5c})$$

$$\bar{G}_{LMN}^\alpha = \int (\bar{\nabla}_\alpha v) (x - x_i)^L (y - y_i)^M (z - z_i)^N \bar{\omega} dV \quad (\text{A.5d})$$

where $\bar{\nabla}_\alpha$ is the gradient in the α direction. Note the appearance of a viscosity gradient term in the equations, which is absent in the constant-viscosity case.

Since $\bar{E}_{LMN}$, $\bar{F}_{LMN}$ and $\bar{G}_{LMN}^\alpha$ are polynomials in time, the moments of (A.5a) can be conserved *exactly* up to order $(L + M + N)$ if a consistent time integration scheme is applied. To get the system of equations for the lowest order of consistency we substitute $(L + M + N) = 0, 1, 2$ in (A.5a)

$$\frac{d\bar{E}_{000}}{dt} = 0 \quad (\text{A.6a})$$

$$\frac{d\bar{E}_{100}}{dt} = \bar{G}_{000}^x \quad (\text{A.6b})$$

$$\frac{d\bar{E}_{010}}{dt} = \bar{G}_{000}^y \quad (\text{A.6c})$$

$$\frac{d\bar{E}_{001}}{dt} = \bar{G}_{000}^z \quad (\text{A.6d})$$

$$\frac{d\bar{E}_{110}}{dt} = \frac{d\bar{E}_{101}}{dt} = \frac{d\bar{E}_{011}}{dt} = 0 \quad (\text{A.6e})$$

$$\frac{d\bar{E}_{200}}{dt} = \frac{d\bar{E}_{020}}{dt} = \frac{d\bar{E}_{002}}{dt} = 2\bar{F}_{000} \quad (\text{A.6f})$$

where $\bar{G}_{100}^\alpha \equiv \bar{G}_{010}^\alpha \equiv \bar{G}_{001}^\alpha \equiv 0$ is used in (A.6e) and (A.6f). Performing a forward Euler time integration of (A.6) and substituting Eqns. (3) and (4) yields the desired system of equations for f_{ij}^n :

$$\sum_j f_{ij}^n = 1 \quad (\text{A.7a})$$

$$\sum_j f_{ij}^n x_{ij} = v_{,x} \Delta t / h_v \quad (\text{A.7b})$$

$$\sum_j f_{ij}^n y_{ij} = v_{,y} \Delta t / h_v \quad (\text{A.7c})$$

$$\sum_j f_{ij}^n z_{ij} = v_{,z} \Delta t / h_v \quad (\text{A.7d})$$

$$\sum_j f_{ij}^n x_{ij} y_{ij} = 0 \quad (\text{A.7e})$$

$$\sum_j f_{ij}^n y_{ij} z_{ij} = 0 \quad (\text{A.7f})$$

$$\sum_j f_{ij}^n z_{ij} x_{ij} = 0 \quad (\text{A.7g})$$

$$\sum_j f_{ij}^n x_{ij}^2 = 2 \quad (\text{A.7h})$$

$$\sum_j f_{ij}^n y_{ij}^2 = 2 \quad (\text{A.7i})$$

$$\sum_j f_{ij}^n z_{ij}^2 = 2 \quad (\text{A.7j})$$

where i and j refer to the diffusing element and its neighbors, respectively, $\bar{x}_{ij} = (\bar{x}_j - \bar{x}_i) / h_v$, $h_v = \sqrt{v_i \Delta t}$, $v_i \equiv v(\bar{x}_i)$, $v_{,\alpha} \equiv \partial v_i / \partial \alpha$ and $\alpha = (x, y, z)$. Note that Eqns. (A.7) reduce to Eqns. (13) for constant viscosity.

Equations (A.7) are more complicated to solve than Eqns. (13). This is because $v_{,\alpha} \Delta t / h_v$ may be much larger than $O(1)$ and, thus, a positive solution of the system may not exist. To this end, alternative particle insertion strategies and/or other choices for neighborhoods of influence may be necessary to guarantee positive solutions. A successful solution of this system is a must for VRM-based LES.

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APPENDIX B

The linear system of equations for the $O(h_v^3)$ VRM is solved herein for the 1-D case in an attempt to identify the range of scaled inter-particle separations that yield positive solutions. The system of equations is obtained by reducing (14) to the 1-D case, as follows:

$$O(1): \quad \sum_j f_{ij}^n = 1 \quad (\text{B.1a})$$

$$O(\sqrt{\Delta t}): \quad \sum_j f_{ij}^n x_{ij} = 0 \quad (\text{B.1b})$$

$$O(\Delta t): \quad \sum_j f_{ij}^n x_{ij}^2 = 2 \quad (\text{B.1c})$$

$$O(\Delta t^{3/2}): \quad \sum_j f_{ij}^n x_{ij}^3 = 0 \quad (\text{B.1d})$$

$$O(\Delta t^2): \quad \sum_j f_{ij}^n x_{ij}^4 = 12 \quad (\text{B.1e})$$

A minimum of five particles will suffice to solve (B.1). Let's assign a uniform distribution of particles positioned symmetrically about the diffusing particle. The coordinate and the (circulation) fraction of the particles are then indexed consecutively for $-2 \leq j \leq 2$, so that $i = j = 0$ corresponds to the diffusing element, as depicted in Fig. B-1. Consequently, the system of equations (B.1) reduces to the following set:

$$f_{-2} + f_{-1} + f_0 + f_1 + f_2 = 1 \quad (\text{B.2a})$$

$$-2f_{-2} - f_{-1} + f_1 + 2f_2 = 0 \quad (\text{B.2b})$$

$$4f_{-2} + f_{-1} + f_1 + 4f_2 = 2\alpha^2 \quad (\text{B.2c})$$

$$-8f_{-2} - f_{-1} + f_1 + 8f_2 = 0 \quad (\text{B.2d})$$

$$16f_{-2} + f_{-1} + f_1 + 16f_2 = 12\alpha^4 \quad (\text{B.2e})$$

where $\alpha \equiv h_v/\Delta x$, $\Delta x \equiv (x_1 - x_0)$, and $f_j \equiv f_{ij}^n$ is to be understood. The solution of (B.2) yields

$$f_0 = 1 - (-6\alpha^4 + 5\alpha^2)/2 \quad (\text{B.3})$$

$$f_{-1} = f_1 = (-6\alpha^4 + 4\alpha^2)/3 \quad (\text{B.4})$$

$$f_{-2} = f_2 = (6\alpha^4 - \alpha^2)/12 \quad (\text{B.5})$$

We are interested in fractions that yield positive solutions. From (B.3) it is clear that $f_0 > 0$ for all values of α . The positivity of the remaining fractions is enforced via (B.4) and (B.5), which yield $1/6 < \alpha^2 < 2/3$. In addition to positivity, we insist the fractions to be at their maximum at x_0 , and to drop monotonically in the outward direction; i.e., $f_0 > f_1 > f_2 > 0$. It is then a simple matter to demonstrate that $f_0 > f_1$ for all values of α , and that $f_1 > f_2$ for $\alpha^2 < 17/30$. Therefore, positive and monotonically decreasing solutions of (B.1) are possible if

$$1/6 < \alpha^2 < 17/30 \quad (\text{B.6})$$

We are now interested in determining what finite-difference scheme a VRM solution represented by fractions (B.3)-(B.5) is equivalent to. We note that for the configuration analyzed in this section, and depicted in Fig. B-1, the fraction that is used to diffuse the circulation of an element to a neighbor is identical to the fraction used by that neighbor to diffuse its circulation to the element in consideration; i.e., $f_{ij}^n = f_{ji}^n$. Using this identity in conjunction with Eqn. (4), we formulate the vorticity ω_0^{n+1} at x_0 and at time level $n+1$ in terms of the vorticity at time level n :

$$\omega_0^{n+1} = \sum_{j=-2}^2 f_j \omega_j^n \quad (\text{B.7})$$

Substituting (B.3)-(B.5) into (B.7) and rearranging terms yields

$$\omega_0^{n+1} = \omega_0^n + \alpha^2 \left[\frac{-\omega_{\pm 2}^n + 16\omega_{\pm 1}^n - 30\omega_0^n}{12} \right] + \frac{\alpha^4}{2} [\omega_{\pm 2}^n - 4\omega_{\pm 1}^n + 6\omega_0^n] \quad (\text{B.8})$$

where $\omega_{\pm j}^n = \omega_{+j}^n + \omega_{-j}^n$ has been used for compactness.

The task now is to describe (B.8) in terms of a finite-difference discretization. Recall that the system of equations for the $O(h_v^3)$ VRM was obtained using a second-order Runge-Kutta time integration, which is of the form

$$\frac{d\omega}{dt} = g(\omega) \quad \Rightarrow \quad \omega^{n+1} = \omega^n + \Delta t g \left[t_n + \frac{\Delta t}{2}, \omega^n + \frac{\Delta t}{2} g(t_n, \omega^n) \right] + O((\Delta t)^3) \quad (\text{B.9})$$

where t_n is the time at time level n . $g(\omega) \equiv \nu d^2 \omega / dx^2$ in the current context, which upon substitution in (B.9) yields

$$\omega^{n+1} = \omega^n + h_v^2 \frac{d^2 \omega^n}{dx^2} + \frac{h_v^4}{2} \frac{d^4 \omega^n}{dx^4} + O((\Delta t)^3) \quad (\text{B.10})$$

Let's now consider the diffusion of vorticity at x_0 according to (B.10), and let's apply Taylor series expansion to approximate the corresponding spatial derivatives:

$$\omega_1 = \omega_0 + (\Delta x)\omega'_0 + \frac{(\Delta x)^2}{2}\omega''_0 + \frac{(\Delta x)^3}{3!}\omega'''_0 + \frac{(\Delta x)^4}{4!}\omega_0^{(IV)} + \frac{(\Delta x)^5}{5!}\omega_0^{(V)} + O((\Delta x)^6) \quad (\text{B.11a})$$

$$\omega_{-1} = \omega_0 - (\Delta x)\omega'_0 + \frac{(\Delta x)^2}{2}\omega''_0 - \frac{(\Delta x)^3}{3!}\omega'''_0 + \frac{(\Delta x)^4}{4!}\omega_0^{(IV)} - \frac{(\Delta x)^5}{5!}\omega_0^{(V)} + O((\Delta x)^6) \quad (\text{B.11b})$$

$$\omega_2 = \omega_0 + (2\Delta x)\omega'_0 + \frac{(2\Delta x)^2}{2}\omega''_0 + \frac{(2\Delta x)^3}{3!}\omega'''_0 + \frac{(2\Delta x)^4}{4!}\omega_0^{(IV)} + \frac{(2\Delta x)^5}{5!}\omega_0^{(V)} + O((\Delta x)^6) \quad (\text{B.12a})$$

$$\omega_{-2} = \omega_0 - (2\Delta x)\omega'_0 + \frac{(2\Delta x)^2}{2}\omega''_0 - \frac{(2\Delta x)^3}{3!}\omega'''_0 + \frac{(2\Delta x)^4}{4!}\omega_0^{(IV)} - \frac{(2\Delta x)^5}{5!}\omega_0^{(V)} + O((\Delta x)^6) \quad (\text{B.12b})$$

where vorticity is understood to be at time level n and the superscripts on vorticity imply spatial derivatives. Adding (B.11a) to (B.11b) and (B.12a) to (B.12b) yields, respectively,

$$\omega_{\pm 1} - 2\omega_0 = (\Delta x)^2\omega''_0 + \frac{(\Delta x)^4}{12}\omega_0^{(IV)} + O((\Delta x)^6) \quad (\text{B.13})$$

$$\omega_{\pm 2} - 2\omega_0 = 4(\Delta x)^2\omega''_0 + \frac{16(\Delta x)^4}{12}\omega_0^{(IV)} + O((\Delta x)^6) \quad (\text{B.14})$$

which can now be used to approximate the spatial derivatives:

$$\omega''_0 = \frac{-\omega_{\pm 2} + 16\omega_{\pm 1} - 30\omega_0}{12(\Delta x)^2} + O((\Delta x)^4) \quad (\text{B.15})$$

$$\omega_0^{(IV)} = \frac{\omega_{\pm 2} - 4\omega_{\pm 1} + 6\omega_0}{(\Delta x)^4} + O((\Delta x)^2) \quad (\text{B.16})$$

Substituting (B.15) and (B.16) into (B.10), and recalling that $\alpha \equiv h_v/\Delta x$ yields

$$\omega_0^{n+1} = \omega_0^n + \alpha^2 \left[\frac{-\omega_{\pm 2}^n + 16\omega_{\pm 1}^n - 30\omega_0^n}{12} \right] + \frac{\alpha^4}{2} [\omega_{\pm 2}^n - 4\omega_{\pm 1}^n + 6\omega_0^n] + O((\Delta t)^3) \quad (\text{B.17})$$

which is identical to (B.8), the equation derived from the solution of $O(h_v^3)$ VRM. Therefore, the higher order VRM is equivalent to a finite-difference scheme that uses central-differencing to approximate the Laplacian and a second-order Runge-Kutta method for time integration. Note, however, that the above finite-difference solution for the *uniform* distribution of particles reveals that the method is actually $O((\Delta t)^2) \approx O(h_v^4)$, which is one order higher than the VRM estimate of $O(h_v^3)$. This explains why the convergence rate of the higher order method has been found in this report to be super-cubic. A similar analysis shows the $O(h_v)$ VRM to actually be $O(\Delta t) \approx O(h_v^2)$ for a uniform distribution of particles, which is also verified numerically in this report.

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