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CONVERGENCE OF A BOUNDARY INTEGRAL METHOD FOR 3-D WATER WAVES

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Abstract. We prove convergence of a modified point vortex method for time-dependent water waves in a three-dimensional, inviscid, irrotational and incompressible fluid. Our stability analysis has two important ingredients. First we derive a leading order approximation of the singular velocity integral. This leading order approximation captures all the leading order contributions of the original velocity integral to linear stability. Moreover, the leading order approximation can be expressed in terms of the Riesz transform, and can be approximated with spectral accuracy. Using this leading order approximation, we construct a near field correction to stabilize the point vortex method approximation. With the near field correction, our modified point vortex method is linearly stable and preserves all the spectral properties of the continuous velocity integral to the leading order. Nonlinear stability and convergence with 3rd order accuracy are obtained using Strang's technique by establishing an error expansion in the consistency error.

1. **Introduction.** We prove convergence of a modified point vortex method for time-dependent water waves in a three-dimensional, inviscid, irrotational and incompressible fluid. Boundary integral methods have been one of the commonly used numerical methods in studying fluid dynamical instabilities associated with free interface problems. They have the advantage of reducing the problem of the free surface flow to one defined on the interface only and thus allow higher order approximations of the interface. Computations using a boundary integral formulation in three space dimensions include [2, 6, 14, 20, 21, 25]. On the other hand, boundary integral methods often suffer from high frequency numerical instabilities [22, 11, 15]. Various stabilizing methods have been proposed in the literature to alleviate this difficulty [11, 3, 5]. Using a spectral discretization and certain Fourier filtering, Beale, Hou and Lowengrub [5] proved convergence of a spectrally accurate boundary integral method for two-dimensional water waves. A key idea is to enforce a compatibility between the quadrature rule of the singular velocity integral *and* that of the spatial derivative. This discrete compatibility is achieved by using a Fourier filtering. The amount of filtering is determined by the quadrature rule in approximating the velocity integral and the derivative rule being used.

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The stability of boundary integral methods for three-dimensional water waves is considerably more difficult than the corresponding two-dimensional problem. The two-dimensional interface problem has a special property, namely the singular kernel has a removable simple pole singularity. As a consequence, spectrally accurate approximations can be constructed for the velocity integral and certain compatibility between the quadrature for velocity integral and the quadrature for the derivative can be enforced. In a three-dimensional free surface, the singular kernel has a branch point singularity which is not removable. Straightforward approximations of the singular integrals do not preserve the spectral properties of these singular integral operators. By the spectral properties of a singular integral operator, we mean the high frequency information contained in the Fourier transform of a singular integral operator. The well-posedness of 3-D water waves is a consequence of the subtle balance of the spectral properties of various singular integral operators. Violation of this subtle balance makes it susceptible to numerical instability. This is why it is difficult to design a numerically stable boundary integral method for three-dimensional water waves.

In this paper, we propose a stable and convergent boundary integral method for three-dimensional water waves. The method is a variant of the point vortex approximation. Without any modification, the point vortex method approximation is numerically unstable for three-dimensional water waves. Our stability analysis has two important ingredients. First we derive a leading order approximation of the singular velocity integral. This leading order approximation captures all the leading order contributions of the original velocity integral to linear stability. Moreover, the leading order approximation can be expressed in terms of the Riesz transform, and can be approximated with spectral accuracy. Thus the spectral properties of the original velocity integral are preserved exactly at the discrete level by this leading order approximation. Secondly, the term consisting of the difference of the original velocity integral and the leading order approximation is less singular and does not contribute to linear stability. Thus it can be approximated by any consistent quadrature rule such as the point vortex method approximation. Since the leading order approximation in effect has desingularized the velocity integral, we obtain an improved 3rd order accuracy of the (modified) point vortex method approximation for 3-D water waves.

Our boundary integral method can be interpreted as a stabilizing method for the point vortex method. The difference between the spectral discretization and the point vortex discretization of the leading order approximation constitutes a near field correction to the original point vortex method. This nonlocal correction accounts for the near field contribution of the singular velocity integral. Although this correction term is small (of order $O(h)$), it contains the critical small scale information which is essential to the stability of the boundary integral method. With the near field correction, we can show that our modified point vortex method preserves all the spectral properties of the linearized operators at the continuum level. As a consequence, we prove that the modified point vortex method is stable and convergent with third order accuracy. Furthermore, using a generalized arclength frame (see section 6, and [16]), the near field correction becomes a convolution operator which can be computed by Fast Fourier Transform with $O(M \log M)$ operation count, here $M = N^2$ is the total number of discrete Lagrangian particles on the free surface.

As in the convergence study for a boundary integral method for 2-D water waves in [5], it is important to separate the treatment of linear stability from that of nonlinear stability. It is linear stability that plays the most important role in obtaining convergence of a boundary integral method, as long as the solution is sufficiently smooth. As observed by Strang [24], if there exists an error expansion for the consistency error and the problem is linearly stable, then nonlinear stability can be obtained by the smallness of the error. In conventional convergence analysis, we usually compare our numerical solution with the exact solution. Strang's trick is not to use the "exact" solution in studying convergence, but to construct a "smooth approximate solution" that is $O(h^p)$ perturbation of the "exact" solution (p is the order of the numerical scheme being considered). This smooth approximate solution satisfies the discrete equations more accurately: $R(t) = O(h^r)$ for arbitrarily large r as long as the continuous solution is sufficiently smooth. Existence of such smooth particles is guaranteed by the existence of the error expansion for the consistency error. Then, in the stability step, one can bound $e(t)$, the difference between the smooth approximate solution and the numerical solution. If the numerical method is linearly stable, nonlinear stability can be obtained by using the smallness of the error $e(t)$. This greatly simplifies the nonlinear stability analysis. In our modified point vortex method, the order of accuracy is $p = 3$. This is not accurate enough and Strang's trick has to be applied to obtain nonlinear stability. In section 5, we prove the existence of the error expansion in terms of the odd powers of h. We then use this error expansion to construct a smooth particle solution which satisfies the modified point vortex method with 5th order accuracy. Thus application of Strang's technique proves nonlinear stability and convergence.

We remark that Beale [4] has recently analyzed convergence of a boundary integral method for three-dimensional water waves. The method analyzed in [4] is based on a different boundary formulation and uses a desingularization in the integral formulation. Another important ingredient in his analysis is the use of a special cut-off function in regularizing the singular kernel. One advantage of using desingularization in the boundary integral formulation is that it does not require smoothing to control the aliasing error. In this paper, we also use a similar desingularization technique to avoid the need of using Fourier smoothing.

The organization of the rest of the paper is as follows. In section 2, we present a boundary integral formulation for three-dimensional water waves. In section 3, we demonstrate the instability of the classical point vortex method. In section 4, we introduce our new stabilizing technique and present our modified point vortex method. Section 5 is devoted to the consistency analysis. Section 6 is devoted to studying properties of some singular integral operators which are closely related to our stability analysis. In section 7, we present our stability and convergence analysis. The proof of several technical lemmas is deferred to the Appendix.

2. **A Boundary Integral Formulation for 3-D Water Waves.** We first review the boundary integral formulation for the 3-D water wave problem. Throughout the paper, we will use bold face letters to denote vector variables. We assume that the flow is inviscid, incompressible, irrotational, and is separated by a free interface. We assume that the fluid has infinite depth. The state of the system at a time t is specified by the interface $\mathbf{x}(\alpha, t)$ and the velocity potential $\phi(\alpha, t)$ on the interface, where $\alpha = (\alpha_1, \alpha_2)$. To simplify the notations, we often drop the time variable from now on, but all the quantities, $\mathbf{x}, \phi$ and μ will be time-dependent. To

express the evolution, we need to write the velocity on the surface in terms of these variables. Following [1, 14], we begin with a double layer or dipole representation for the potential in terms of the dipole strength $\mu(\alpha)$, to be determined from ϕ. We write the potential in the fluid domain as

$$\phi(\mathbf{x}) = \int\int \mu(\alpha')\mathbf{N}(\alpha') \cdot \nabla_{x'} G(\mathbf{x} - \mathbf{x}(\alpha'))d\alpha', \tag{1}$$

where $\mathbf{N}(\alpha') = \mathbf{x}_{\alpha_1}(\alpha') \times \mathbf{x}_{\alpha_2}(\alpha')$ is the unnormalized outward normal to the surface,

$$G(\mathbf{x} - \mathbf{x}') = -\frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|},$$

is the free space Green function for the Laplace equation, and

$$\nabla_{x'} G(\mathbf{x} - \mathbf{x}') = -\frac{\mathbf{x} - \mathbf{x}'}{4\pi|\mathbf{x} - \mathbf{x}'|^3}.$$

We define the corresponding unit outward normal vector as $\mathbf{n}(\alpha) = \mathbf{N}(\alpha)/|\mathbf{N}(\alpha)|$. It follows from the properties of the double layer potential that the value of ϕ on the interface is given by

$$\phi(\alpha) = \frac{1}{2}\mu(\alpha) + K\mu(\alpha), \tag{2}$$

where $\phi(\alpha) = \phi(\mathbf{x}(\alpha))$ and

$$K\mu(\alpha) = \int\int \mu(\alpha')\mathbf{N}(\alpha') \cdot \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha'. \tag{3}$$

Differentiating both sides of equation (1) with respect to $\mathbf{x}$ and integrating by parts, we obtain

$$\nabla\phi(\mathbf{x}) = \int\int \eta(\alpha') \times \nabla_{x'} G(\mathbf{x} - \mathbf{x}(\alpha'))d\alpha', \tag{4}$$

where $\eta(\alpha) = (\gamma_1 \mathbf{x}_{\alpha_2} - \gamma_2 \mathbf{x}_{\alpha_1})(\alpha)$, and $\gamma_i = \frac{\partial \mu}{\partial \alpha_i}, \quad i = 1, 2$. Since the tangential velocity of the interface is not unique, we need to specify an interface velocity. For water waves, it is customary to evolve the interface with the interface velocity from the fluid domain. Thus, to obtain the interface velocity, we need to compute the limiting value of $\nabla\phi(\mathbf{x})$ as $\mathbf{x}$ approaches to the interface from below. By combining the stream function formulation with the double layer potential formulation, Haroldsen and Meiron in [14] have shown that the interface velocity is given by

$$\mathbf{w}(\alpha, t) = \int\int \eta(\alpha') \times \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha' + \frac{1}{2}\eta(\alpha) \times \frac{\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|^2}. \tag{5}$$

To make it easier for our presentation, we denote by $\mathbf{w}_0$ the integral part of the interface velocity,

$$\mathbf{w}_0(\alpha) = \int\int \eta(\alpha') \times \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha', \tag{6}$$

and by $\mathbf{w}_{loc}$ the local velocity field

$$\mathbf{w}_{loc}(\alpha) = \frac{1}{2}\eta(\alpha) \times \frac{\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|^2}. \tag{7}$$

In Lagrangian formulation, we evolve the free surface by the interface velocity derived above, i.e.

$$\frac{\partial \mathbf{x}}{\partial t}(\alpha, t) = \mathbf{w}(\alpha, t), \qquad \mathbf{x}(\alpha, 0) = \mathbf{x}_0(\alpha). \tag{8}$$

For the evolution of $\phi(\alpha, t)$, we use Bernoulli's equation. If we neglect surface tension, Bernoulli's equation in the Lagrangian frame is

$$\phi_t - \frac{1}{2}|\mathbf{w}|^2 + \mathbf{g}\cdot\mathbf{x} = 0, \tag{9}$$

where $\mathbf{g} = (0, 0, g)$, g is the gravity acceleration coefficient. The evolution equations (8) and (9), together with the relations (2)-(5) completely specify the motion of the system.

Using equation (2) directly in numerical approximations is more sensitive to numerical instability. To alleviate this difficulty, we first derive an equivalent formulation for equation (2) which gives better numerical stability property than (2). To this end, we differentiate equation (2) with respect to α_l. Using (4)-(5), we obtain

$$\phi_{\alpha_l} \quad = \quad \frac{\gamma_l}{2} + \mathbf{x}_{\alpha_l}\cdot\mathbf{w}_0, \qquad l = 1, 2. \tag{10}$$

Note that γ_1 and γ_2 are not independent. Thus equation (10) as it stands is not invertible in general. To solve for γ_1 and γ_2, one has to supplement equation (10) by the constraint $\gamma_l = \mu_{\alpha_l}, l = 1, 2$. Instead of solving (10) subject to the above constraint, we will use an equivalent formulation of (10) for γ in our numerical discretization:

$$\phi_{\alpha_l} = \frac{\gamma_l}{2} + P_{l1}(\mathbf{x}_{\alpha_1}\cdot\mathbf{w}_0) + P_{l2}(\mathbf{x}_{\alpha_2}\cdot\mathbf{w}_0), \qquad l = 1, 2. \tag{11}$$

where P_{ij} $(i, j = 1, 2)$ are projection operators with zero constant mode. More precisely we define P_{ij} in Fourier transform space as follows: $(\widehat{P_{ij}})_{\mathbf{k}} = \frac{k_i k_j}{|\mathbf{k}|^2}$ for $\mathbf{k} \neq \mathbf{0}$, where $\mathbf{k} = (k_1, k_2)$, and $(\widehat{P_{ij}})_{\mathbf{k}} = \mathbf{0}$ for $\mathbf{k} = \mathbf{0}$. Here $(\widehat{P_{ij}})_{\mathbf{k}}$ stands for the Fourier transform of P_{ij}. Using the definition of operator P_{ij}, we have

$$D_2P_{11} = D_1P_{12}, \quad D_1P_{22} = D_2P_{12}, \quad P_{12} = P_{21}, \quad P_{11} + P_{22} = I, \tag{12}$$

for functions with zero modes, i.e. $\hat{f}_{\mathbf{0}} = 0$. Here $D_l = \frac{\partial}{\partial\alpha_l}$ is a partial derivative operator with respect to $\partial\alpha_l$, $l = 1, 2$. The reason that equation (11) has a better stability property than equation (2) at the discrete level is because in deriving equation (11) we have performed one integration by parts to cancel the leading order singular terms.

We now show that (2) and (11) are equivalent formulations at the continuum level. We assume that $\hat{\phi}_{\mathbf{0}} = \hat{\mu}_{\mathbf{0}}/2$. As we mentioned earlier, γ_1 and γ_2 are not independent. Using (11) and (12), we can prove $(\gamma_1)_{\alpha_2} = (\gamma_2)_{\alpha_1}$. Thus there exists μ, such that $\gamma_l = \mu_{\alpha_l}, l = 1, 2$. To solve for γ_l from (11), we differentiate (11) with respect to α_l and add the resulting equations. This gives

$$\triangle\phi = \frac{\triangle\mu}{2} + (\mathbf{x}_{\alpha_1}\cdot\mathbf{w}_0)_{\alpha_1} + (\mathbf{x}_{\alpha_2}\cdot\mathbf{w}_0)_{\alpha_2}, \tag{13}$$

where we have used the identities:

$$\begin{aligned} D_1P_{11} + D_2P_{21} &= D_1P_{11} + D_1P_{22} = D_1(P_{11} + P_{22}) = D_1, \\ D_1P_{12} + D_2P_{22} &= D_2P_{11} + D_2P_{22} = D_2(P_{11} + P_{22}) = D_2, \end{aligned}$$

which follows from (12).

Define $\triangle^{-1}$ as follows:

$$\left(\widehat{\triangle^{-1}}\right)_{\mathbf{k}} = -\frac{1}{|\mathbf{k}|^{\mathbf{2}}}, \text{if} \quad \mathbf{k} \neq \mathbf{0}, \qquad \left(\widehat{\triangle^{-1}}\right)_{\mathbf{0}} = 0.$$

Applying the $\triangle^{-1}$ operator to the both sides of the above equation, we get the equation for μ

$$\phi = \frac{\mu}{2} + \triangle^{-1}\left((\mathbf{x}_{\alpha_1} \cdot \mathbf{w}_0)_{\alpha_1} + (\mathbf{x}_{\alpha_2} \cdot \mathbf{w}_0)_{\alpha_2}\right), \tag{14}$$

where we have used the fact that $\hat{\phi}_{\mathbf{0}} = \hat{\mu}_{\mathbf{0}}/2$. Using integration by parts and equation (4), we can show that $\frac{\partial K}{\partial \alpha_j} = \mathbf{x}_{\alpha_j} \cdot \mathbf{w}_0$, which implies

$$(\mathbf{x}_{\alpha_1} \cdot \mathbf{w}_0)_{\alpha_1} + (\mathbf{x}_{\alpha_2} \cdot \mathbf{w}_0)_{\alpha_2} = \triangle K(\mu).$$

Therefore, equation (11) is equivalent to equation (2) up to a constant. Since $\hat{\phi}_{\mathbf{0}} = \hat{\mu}_{\mathbf{0}}/2$, the constant must be zero. Thus the solvability of (2) for μ [1] implies solvability of (11) for γ.

Next we express (11) as follows:

$$(\frac{1}{2}I + A)\gamma = \bigtriangledown_\alpha \phi, \tag{15}$$

where A is two by two matrix, $A = (a_{ij})$, with

$$a_{11} = P_{11}K_1 + P_{12}K_3, \qquad a_{12} = P_{11}K_2 + P_{12}K_4,$$
$$a_{21} = P_{21}K_1 + P_{22}K_3, \qquad a_{22} = P_{21}K_2 + P_{22}K_4,$$

and

$$\begin{aligned}
K_1 f(\alpha) &= \mathbf{x}_{\alpha_1}(\alpha) \cdot \int f(\alpha')\mathbf{x}_{\alpha_2}(\alpha') \times \bigtriangledown_{\mathbf{x}'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha', \\
K_2 f(\alpha) &= -\mathbf{x}_{\alpha_1}(\alpha) \cdot \int f(\alpha')\mathbf{x}_{\alpha_1}(\alpha') \times \bigtriangledown_{\mathbf{x}'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha', \\
K_3 f(\alpha) &= \mathbf{x}_{\alpha_2}(\alpha) \cdot \int f(\alpha')\mathbf{x}_{\alpha_2}(\alpha') \times \bigtriangledown_{\mathbf{x}'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha', \\
K_4 f(\alpha) &= -\mathbf{x}_{\alpha_2}(\alpha) \cdot \int f(\alpha')\mathbf{x}_{\alpha_1}(\alpha') \times \bigtriangledown_{\mathbf{x}'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))d\alpha'.
\end{aligned}$$

Recall that an integral kernel $K(x, y)$ is called weakly singular (see e.g. page 6 of [7]) if there exists a positive constant M and $\alpha \in (0, 2]$ such that for all $x, y \in G$, $x \neq y$, we have

$$|K(x, y)| \leq M|x - y|^{\alpha - 2}.$$

It is easy to prove that the kernels $K_i, i = 1, 2, 3, 4$ defined above are integral operators with weakly singular kernels. It follows from Theorem 1.11 in page 6 of [7] that $K_i, i = 1, 2, 3, 4$ are compact operators. Moreover, $P_{ij}K_l$ is a compact operator since P_{ij} is a bounded operator (see Definition 1.1 in page 2 of [7]). Consequently A is a compact operator (see Theorem 1.4 in page 2 of [7]).

By the solvability of (11) for γ, we have

$$(\frac{1}{2}I + A)\gamma = 0 \Longrightarrow \gamma = 0. \tag{16}$$

Using (16) and the fact that A is a compact operator, we can apply Theorem 1.16 in Colton and Kress [7] (page 13) to show that $(\frac{1}{2}I + A)^{-1}$ exists and is bounded.

Moreover, we define a set of complementary tangent vectors $\mathbf{x}^*_{\alpha_l}$ and $\mathbf{x}^*_{\alpha_2}$ as follows:

$$\mathbf{x}^*_{\alpha_1} = \frac{1}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|}(\mathbf{x}_{\alpha_2} \times \mathbf{n}), \qquad \mathbf{x}^*_{\alpha_2} = \frac{1}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|}(\mathbf{n} \times \mathbf{x}_{\alpha_1}).$$

It is easy to verify that

$$\mathbf{x}^*_{\alpha_l} \cdot \mathbf{x}_{\alpha_k} = \delta_{lk}, \qquad l,k = 1,2, \tag{17}$$

where δ_{lk} are the Kronecker delta functions. By projecting the interface velocity $\mathbf{w}(\alpha)$ into $\mathbf{x}^*_{\alpha_1}$, $\mathbf{x}^*_{\alpha_2}$ and $\mathbf{n}$ vectors respectively, we obtain using (17) that

$$\begin{aligned} \mathbf{w}(\alpha) &= \mathbf{w}_0 + \mathbf{w}_{loc} \\ &= (\mathbf{w}\cdot\mathbf{x}_{\alpha_1})\mathbf{x}^*_{\alpha_1} + (\mathbf{w}\cdot\mathbf{x}_{\alpha_2})\mathbf{x}^*_{\alpha_2} + (\mathbf{w}\cdot\mathbf{n})\mathbf{n} \\ &= (\phi_{\alpha_1})\mathbf{x}^*_{\alpha_1} + (\phi_{\alpha_2})\mathbf{x}^*_{\alpha_2} + (\mathbf{w}_0\cdot\mathbf{n})\mathbf{n}\ , \end{aligned} \tag{18}$$

where we have used

$$\frac{d}{d\alpha_l}\phi(\mathbf{x}(\alpha)) = \nabla\phi\cdot\mathbf{x}_{\alpha_l} = \mathbf{w}\cdot\mathbf{x}_{\alpha_l}, \quad l = 1,2.$$

In summary, the evolution equations for the 3-D water wave problem are as follows:

$$\mathbf{x}_t = \mathbf{w}(\alpha) = (\phi_{\alpha_1})\mathbf{x}^*_{\alpha_1} + (\phi_{\alpha_2})\mathbf{x}^*_{\alpha_2} + (\mathbf{w}_0\cdot\mathbf{n})\mathbf{n}, \tag{19}$$

$$\phi_t = \frac{1}{2}|\mathbf{w}(\alpha)|^2 - \mathbf{g}\cdot\mathbf{x}, \tag{20}$$

$$\phi_{\alpha_l} = \frac{\gamma_l}{2} + P_{l1}(\mathbf{x}_{\alpha_1}\cdot\mathbf{w}_0) + P_{l2}(\mathbf{x}_{\alpha_2}\cdot\mathbf{w}_0), \qquad l = 1,2, \tag{21}$$

where $\mathbf{w}_0$ is defined in (6).

From now on, with $\mathbf{x}(\alpha,t) = (\alpha,0) + s(\alpha,t)$, we assume that $s(\alpha,t)$ and $\phi(\alpha,t)$ are double periodic in α with period 2π. To reduce the computational domain to a single period, we need to replace the original Green's function by a periodic one, which is obtained by summing up all its periodic images

$$\widetilde{G}(\mathbf{x}) = \sum_{\mathbf{m}\in Z^2} G(\mathbf{x} + 2\pi(\mathbf{m},0)), \tag{22}$$

where $\mathbf{m} = (m_1, m_2)$ is a two-dimensional integer index. When the sum is written as in (22), it is strictly divergent. Since only the derivatives of the periodic Green's function will be used, one way to alleviate this difficulty is to express this sum by using the Ewald summation techniques as outlined by Baker, Meiron, and Orszag [2], which converts the derivatives of the periodic Green's function into sums of error functions. Alternatively, one can write this sum with a reflection and with a constant subtracted from each term [4]

$$\widetilde{G}(\mathbf{x}) = \frac{1}{2}\sum_{\mathbf{m}\in Z^2, \mathbf{n}\neq\mathbf{0}} \left(G(\mathbf{x} + 2\pi(\mathbf{m},0)) + G(\mathbf{x} - 2\pi(\mathbf{m},0)) + \frac{1}{2\pi|\mathbf{m}|} \right). \tag{23}$$

The gradient is

$$\nabla\widetilde{G}(\mathbf{x}) = \frac{1}{2}\sum_{\mathbf{m}\in Z^2} \left(\nabla G(\mathbf{x} + 2\pi(\mathbf{m},0)) + \nabla G(\mathbf{x} - 2\pi(\mathbf{m},0))\right). \tag{24}$$

It can be shown that both of these sums converge uniformly in L^1 on bounded sets and $\widetilde{G}(\mathbf{x})$ gives the double periodic Green's function [4].

3. **An Unstable Boundary Integral Method for 3-D Water Waves.** In this section, we will demonstrate that the point vortex method approximation of the 3D water wave equations (2)-(5) and (8)-(9) is numerically unstable. We denote by $\mathbf{x}_j(t)$ the numerical approximation of $\mathbf{x}(\alpha_j,t)$, where $\alpha_j = \mathbf{j}h$, $\mathbf{j}=(j_1,j_2)$ is a 2-D integer index, h is the mesh size. Similarly we define ϕ_j, μ_j, etc. We also need to introduce a discrete derivative operator, D_l^h, which approximates ∂_{α_l}. This could be a center difference derivative operator or a pseudo-spectral derivative operator with smoothing. For the convenience of our later analysis, we express the discrete derivative operator in terms of the discrete Fourier transform. We recall that for a 2π-periodic function,u, the discrete Fourier transform is given by

$$\hat{u}_{\mathbf{k}} = \frac{h^2}{(2\pi)^2} \sum_{(j_1,j_2)=(-N/2+1,-N/2+1)}^{(N/2,N/2)} u(\alpha_j) e^{-i\mathbf{k}\cdot\mathbf{x}_j}, \tag{25}$$

where $h = 2\pi/N$.

The inversion formula is

$$u_{\mathbf{j}} = \sum_{(k_1,k_2)=(-N/2+1,-N/2+1)}^{(N/2,N/2)} \hat{u}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}_j}. \tag{26}$$

In terms of the discrete Fourier transform, we can express the discrete derivative operator as follows:

$$\widehat{(D_l^h f)}_{\mathbf{k}} = ik_l\rho_l(\mathbf{k}h)\hat{f}_{\mathbf{k}}, \qquad k_1,k_2 = -\frac{N}{2}+1,\cdots,\frac{N}{2}, \tag{27}$$

where $\hat{f}_{\mathbf{k}}$ is the discrete 2-D Fourier transform, and $\rho_l(\mathbf{k}h)$ is some non-negative cut-off function depending on the approximation being used. For example, $\rho_l(\mathbf{k}h) = \frac{\sin(k_l h)}{k_l h}$ for a second order center difference derivative operator. In the case of spectral derivative, we require that $\rho_l(\mathbf{x}) = \rho(|\mathbf{x}|)$ satisfies $\rho(r) \geq 0$, $\rho(\pi)=0$, and $\rho(r)=1$ for $0 \leq r \leq \lambda\pi$ with $0<\lambda<1$. The Fourier smoothing is needed here to prevent the aliasing error in the stability analysis, as in the 2-D case [5]. We also denote by S_l^h the spectral derivative operator without smoothing, i.e.

$$\widehat{(S_l^h f)}_{\mathbf{k}} = ik_l\hat{f}_{\mathbf{k}}, \qquad k_1,k_2 = -\frac{N}{2}+1,\cdots,\frac{N}{2}. \tag{28}$$

The point vortex method for 3D water waves is given as follows:

$$\frac{d\mathbf{x}_{\mathbf{i}}}{dt} = \sum_{\mathbf{j}\neq\mathbf{i}} \eta_{\mathbf{j}} \times \nabla_{x'} G(\mathbf{x}_{\mathbf{i}} - \mathbf{x}_{\mathbf{j}})h^2 + \frac{1}{2}\frac{\eta_{\mathbf{i}} \times \mathbf{n}_{\mathbf{i}}}{|D_1^h\mathbf{x}_{\mathbf{i}} \times D_2^h\mathbf{x}_{\mathbf{i}}|} \equiv \mathbf{w}_{\mathbf{i}}, \tag{29}$$

$$\frac{d\phi_{\mathbf{i}}}{dt} = \frac{1}{2}|\mathbf{w}_{\mathbf{i}}|^2 - \mathbf{g}\cdot\mathbf{x}_{\mathbf{i}}, \tag{30}$$

$$\mu_{\mathbf{i}} = 2\phi_{\mathbf{i}} - 2\sum_{\mathbf{j}\neq\mathbf{i}} \mu_{\mathbf{j}}\mathbf{N}_{\mathbf{j}} \cdot \nabla_{x'} G(\mathbf{x}_{\mathbf{i}} - \mathbf{x}_{\mathbf{j}})h^2, \tag{31}$$

where $\eta_{\mathbf{j}} = \gamma_{1\mathbf{j}} D_2^h\mathbf{x}_{\mathbf{j}} - \gamma_{2\mathbf{j}} D_1^h\mathbf{x}_{\mathbf{j}}$, $\mathbf{N}_{\mathbf{j}} = D_1^h\mathbf{x}_{\mathbf{j}} \times D_2^h\mathbf{x}_{\mathbf{j}}$ and $\mathbf{n}_{\mathbf{j}} = \frac{\mathbf{N}_{\mathbf{j}}}{|\mathbf{N}_{\mathbf{j}}|}$, and $\gamma_{l\mathbf{j}} = D_l^h\mu_{\mathbf{j}}$ $(l=1,2)$.

To study the linear stability of the point vortex method, we first introduce the following discrete convolution operators:

$$H_{lh}(f_{\mathbf{i}}) = \frac{1}{2\pi}\sum_{\mathbf{j}\neq\mathbf{i}} \frac{(\alpha_{l\mathbf{i}}-\alpha_{l\mathbf{j}})f_{\mathbf{j}}}{((\alpha_{1\mathbf{i}}-\alpha_{1\mathbf{j}})^2+(\alpha_{2\mathbf{i}}-\alpha_{2\mathbf{j}})^2)^{3/2}}h^2, \qquad l=1,2, \tag{32}$$

and

$$\Lambda_h(f_{\mathbf{i}}) = \frac{1}{2\pi}\sum_{\mathbf{j}\neq\mathbf{i}} \frac{(f_{\mathbf{i}}-f_{\mathbf{j}})}{((\alpha_{1\mathbf{i}}-\alpha_{1\mathbf{j}})^2+(\alpha_{2\mathbf{i}}-\alpha_{2\mathbf{j}})^2)^{3/2}}h^2. \tag{33}$$

These operators will appear in the linear stability analysis around equilibrium. Moreover, we will also use the following discrete operator:

$$R_h = H_{1h}D_1^h + H_{2h}D_2^h. \tag{34}$$

We now examine the linear stability around equilibrium. Let $\mathbf{x} = (\alpha_1, \alpha_2, 0) + \mathbf{x}'$ and $\phi = \frac{1}{2} + \phi'$, where $\mathbf{x}'$ and ϕ' are assumed to be small. Substitute these into the point vortex method, (29)-(31), and neglect nonlinear terms. After some manipulations, we obtain the equations that govern the evolution of the perturbed variables as follows:

$$\frac{d\mathbf{x}'_{\mathbf{i}}}{dt} = \left(D_1^h\mu',\ D_2^h\mu',\ R_h\mu'\right), \tag{35}$$

$$\frac{d\phi'_{\mathbf{i}}}{dt} = -gz'_{\mathbf{i}}, \tag{36}$$

where $\mu' = \phi'_{\mathbf{i}} + \frac{1}{2}(\Lambda_h - R_h)(z'_{\mathbf{i}})$. We will consider the following equations

$$\frac{dz'_{\mathbf{i}}}{dt} = \left(0,\ 0,\ R_h(\phi'_{\mathbf{i}}) + \frac{1}{2}R_h(\Lambda_h - R_h)(z'_{\mathbf{i}})\right), \tag{37}$$

$$\frac{d\phi'_{\mathbf{i}}}{dt} = -gz'_{\mathbf{i}}, \tag{38}$$

where z' is the z-component of $\mathbf{x}' = (x', y', z')$. To study the growth rate of the above linearized equations, we need to study the Fourier symbols of the discrete operators, H_{lh}, Λ_h and R_h. Since these discrete operators are convolution operators, we can compute their Fourier symbols as follows:

$$(\widehat{H_{lh}})_{\mathbf{k}} = -\frac{ik_l}{|\mathbf{k}|}b_l(\mathbf{k}h)\hat{f}_{\mathbf{k}}, \tag{39}$$

$$(\widehat{\Lambda_h})_{\mathbf{k}} = |\mathbf{k}|c(\mathbf{k}h)\hat{f}_{\mathbf{k}}, \tag{40}$$

$$(\widehat{R_h})_{\mathbf{k}} = |\mathbf{k}|d(\mathbf{k}h)\hat{f}_{\mathbf{k}}, \tag{41}$$

(42)

where

$$b_1(\mathbf{k}h) = \frac{1}{2\pi}\sum_{\mathbf{j}\neq\mathbf{0}}\frac{j_1\sin(j_1k_1h)\cos(j_2k_2h)}{(j_1^2+j_2^2)^{3/2}}, \tag{43}$$

$$b_2(\mathbf{k}h) = \frac{1}{2\pi}\sum_{\mathbf{j}\neq\mathbf{0}}\frac{j_2\sin(j_2k_2h)\cos(j_1k_1h)}{(j_1^2+j_2^2)^{3/2}}, \tag{44}$$

$$c(\mathbf{k}h) = \frac{1}{2\pi h|\mathbf{k}|}\sum_{\mathbf{j}\neq\mathbf{0}}\frac{1-\cos(k_1j_1h)\cos(k_2j_2h)}{(j_1^2+j_2^2)^{3/2}}, \tag{45}$$

$$d(\mathbf{k}h) = \frac{k_1b_1\rho_1+k_2b_2\rho_2}{|\mathbf{k}|}. \tag{46}$$

It can be shown that the above infinite series converge. Using the Fourier symbols of the discrete operators, we can easily compute the eigenvalues of the linearized system (37)-(38) as follows:

$$\lambda_1,\lambda_2 = 0, \lambda_3,\lambda_4 = \frac{C|\mathbf{k}|^2}{4}d(c-d)\pm\frac{1}{4}\sqrt{|\mathbf{k}|^4d^2(c-d)^2-16g|\mathbf{k}|d}. \tag{47}$$

If $d(\mathbf{k}h)\neq 0$ and $c(\mathbf{k}h)\neq d(\mathbf{k}h)$, then the unstable eigenvalues can grow as fast as $O(|\mathbf{k}|^2)$ as $|\mathbf{k}|\to\infty$. Our numerical study has demonstrated convincingly that $|d(\mathbf{k}h)|$ and $|c(\mathbf{k}h)-d(\mathbf{k}h)|$ are bounded away from a positive constant for the majority of the Fourier modes. Thus the unstable eigenmodes can indeed grow exponentially fast in frequency space for $t>0$ in a rate proportional to $O(\exp(c_0|\mathbf{k}|^2t)$ for some positive constant c_0. Numerical experiments for 3-D water waves near equilibrium by David Haroldsen [13] also confirmed that numerical solutions of the point vortex method for small analytic perturbation from the equilibrium developed order one oscillation in a short time even though the physical solution was still perfectly smooth at this time. The instability occurred earlier if a finer mesh was used.

It is clear that this instability is caused by violating the compatibility condition, $\Lambda = H_1D_1+H_2D_2$, at the discrete level. While this compatibility can be imposed using a Fourier filtering as in the 2-D case [5], there are four additional compatibility conditions for 3-D water waves that need to be satisfied in order to obtain stability far from equilibrium. We simply do not have enough degree of freedom in filtering the interface variables to satisfy all these compatibility conditions. This is why we need to introduce a different stabilizing technique to obtain a stable 3-D boundary integral method.

4. **A New Stabilizing Technique for 3-D Water Waves.** As we mentioned in the introduction, it is important to separate the treatment of linear stability from that of nonlinear stability when we consider stability of a numerical method for a well-posed initial value problem. It is linear stability that plays the most important role in obtaining convergence of a boundary integral method, as long as the solution is sufficiently smooth. Our stability analysis has two important ingredients. First we derive a leading order approximation of the singular velocity integral. This leading order approximation captures all the leading order contributions of the original velocity integral to linear stability analysis. Moreover, the leading order approximation can be expressed in terms of the Riesz transform, and can be approximated with spectral accuracy. Thus the spectral properties of the original velocity integral are preserved exactly at the discrete level by this leading

order approximation. Secondly, the term consisting of the difference of the original velocity integral and the leading order approximation is less singular and does not contribute to the linear stability. Thus it can be approximated by any consistent quadrature rule such as the point vortex method approximation. Since the leading order approximation in effect has desingularized the velocity integral, we obtain an improved 3rd order accuracy of the (modified) point vortex method approximation for 3-D water waves. The stabilizing technique described above can also be interpreted as a near field correction to the point vortex approximation. Although the near field correction is small in ampltitude, $O(h)$, it contains critical high frequency contribution which stabilizes the point vortex approximation.

The leading order approximation of the velocity integral needs to satisfy two properties: (i) It captures all the leading order contributions of the original velocity integral, (ii) It can be evaluated with spectral accuracy. The nonlocal leading order approximations for $\mathbf{x}_{\alpha_l} \cdot \mathbf{w}_0, l = 1,2$ and $\mathbf{w}_0 \cdot \mathbf{n}$ which satisfy these two criteria are given by

$$B_l = \frac{\mathbf{N}(\alpha)}{2} \cdot (\gamma_1(\alpha) H_1 + \gamma_2(\alpha) H_2) \mathbf{x}_{\alpha_l}(\alpha), \qquad l = 1,2 \tag{48}$$

and

$$\begin{aligned} B_{\mathbf{n}} \quad = \quad & \frac{|\mathbf{N}(\alpha)|}{2} \{[H_1(\gamma_1) + H_2(\gamma_2)] \\ & -\gamma_1(\alpha)\mathbf{x}^*_{\alpha_1} \cdot (H_1 D_1 + H_2 D_2)\mathbf{x}(\alpha) \\ & -\gamma_2(\alpha)\mathbf{x}^*_{\alpha_2} \cdot (H_1 D_1 + H_2 D_2)\mathbf{x}(\alpha)\} \, , \end{aligned} \tag{49}$$

where H_1 and H_2 are the Riesz transforms defined in (67) in section 6. The Fourier symbols of the Riesz transforms can be computed explicitly (see section 6). Thus these singular integrals can be evaluated via discrete Fourier transform with spectral accuracy. Moreover, using a special coordinate frame with the property [16]

$$\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2} = \lambda_1(t) |\mathbf{x}_{\alpha_2}|^2, \qquad |\mathbf{x}_{\alpha_1}|^2 = \lambda_2(t) |\mathbf{x}_{\alpha_2}|^2, \tag{50}$$

the Riesz transforms become convolution operators and can be evaluated by Fast Fourier Transform with $O(N^2 \log(N))$ operation counts.

In addition to using a near field correction described above, we also use desingularization to stabilize the aliasing error introduced by the point vortex approximation. In our desingularization, we use the following two identities [2]

$$\int \mathbf{N}(\alpha') \cdot \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) d\alpha' = 0, \tag{51}$$

$$\int \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) \times \mathbf{N}(\alpha') d\alpha' = 0. \tag{52}$$

The use of these identities to reduce the singularity was suggested in [2] and [4]. We define

$$C_l \quad = \quad \gamma_l(\alpha) \int \mathbf{N}(\alpha') \cdot \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) d\alpha', \qquad l = 1,2 \tag{53}$$

$$C_{\mathbf{n}} \quad = \quad \frac{\eta(\alpha)}{|\mathbf{N}(\alpha)|} \cdot \int \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) \times \mathbf{N}(\alpha') d\alpha'. \tag{54}$$

It follows from (51) and (52) that $C_l = 0, l = 1,2$ and $C_{\mathbf{n}} = 0$.

Now we are ready to describe our discretization for the 3-D water wave equations. First we describe the approximation of the normal velocity integral $\mathbf{w}_0 \cdot \mathbf{n}$:

$$\mathbf{w}_0^h \cdot \mathbf{n}^h - C_n^h + (B_{\mathbf{n}}^s - B_{\mathbf{n}}^h) \ , \tag{55}$$

where $\mathbf{w}_0^h, C_{\mathbf{n}}^h, B_{\mathbf{n}}^h$ are the point vortex approximations of $\mathbf{w}_0, C_{\mathbf{n}}, B_{\mathbf{n}}$ respectively, $B_{\mathbf{n}}^s$ is the spectral approximation of $B_{\mathbf{n}}$, and

$$\begin{aligned} \mathbf{w}_0^h &= \sum_{\mathbf{j}\neq\mathbf{i}} \eta_{\mathbf{j}} \times \nabla_{x'} G(\mathbf{x_i} - \mathbf{x_j}) h^2, \\ C_{\mathbf{n}}^h &= \frac{\eta_{\mathbf{i}}}{|\mathbf{N_i}|} \cdot \sum_{\mathbf{j}\neq\mathbf{i}} \mathbf{N_j} \times \nabla_{x'} G(\mathbf{x_i} - \mathbf{x_j}) h^2, \end{aligned}$$

where $\eta_{\mathbf{j}} = \gamma_{1\mathbf{j}} D_2^h \mathbf{x_j} - \gamma_{2\mathbf{j}} D_1^h \mathbf{x_j}$, $\mathbf{N_j} = D_1^h \mathbf{x_j} \times D_2^h \mathbf{x_j}$.

In the discretization of (55), the second term, $-C_n^h$, is a desingularizing term and is introduced to remove the aliasing error associated with the point vortex approximation of $\mathbf{w}_0 \cdot \mathbf{n}$. As noted by Beale in [4], the desingularizing term helps prevent spurious terms from appearing in the stability analysis. The last term in (55) is a near field correction term. This term is small (of order $O(h)$), but it contributes to the stability of the discretization in an essential way.

Next we describe the approximation of the tangential velocity integral $\mathbf{x}_{\alpha_l} \cdot \mathbf{w}_0, l = 1, 2$:

$$D_l^h \mathbf{x_i} \cdot \mathbf{w}_0^h - C_l^h + (B_l^s - B_l^h), \qquad l = 1, 2 \tag{56}$$

where $\mathbf{w}_0^h, C_l^h, B_l^h$ are the point vortex approximations of $\mathbf{w}_0, C_l, B_l$ respectively, B_l^s is the spectral approximation of B_l, and

$$C_l^h = \gamma_{li} \sum_{j\neq i} \mathbf{N}_j \cdot \nabla_{x'} G(\mathbf{x}_i - \mathbf{x}_j) h^2, \qquad l = 1, 2.$$

As in the discretization of the normal velocity, the second term in (56), $-C_l^h$, is a desingularizing term and is introduced to remove the aliasing error associated with the point vortex approximation of $D_l^h \mathbf{x}_i \cdot \mathbf{w}_0$. The last term in (56) is a near field correction term, which contributes to the stability of the discretization.

Now we can state our modified point vortex method for the 3-D water wave problem.

$$\begin{aligned} \frac{d\mathbf{x_i}}{dt} &= D_1^h \phi_{\mathbf{i}} D_1^h \mathbf{x_i}^* + D_2^h \phi_{\mathbf{i}} D_2^h \mathbf{x_i}^* + (\mathbf{w}_0^h \cdot \mathbf{n_i}^h - C_n^h + B_{\mathbf{n}}^s - B_{\mathbf{n}}^h)\mathbf{n_i} \equiv \mathbf{w_i}, && (57) \\ \frac{d\phi_{\mathbf{i}}}{dt} &= \frac{1}{2}|\mathbf{w_i}|^2 - \mathbf{g} \cdot \mathbf{x_i}, && (58) \\ D_l^h \phi_{\mathbf{i}} &= \frac{\gamma_{l\mathbf{i}}}{2} + P_{l1}^h (D_1^h \mathbf{x_i} \cdot \mathbf{w}_0^h - C_1^h + (B_1^s - B_1^h)) + P_{l2}^h (D_2^h \mathbf{x_i} \cdot \mathbf{w}_0^h - C_2^h \\ &\quad + (B_2^s - B_2^h)), \qquad l = 1, 2 && (59) \end{aligned}$$

where $\mathbf{N_i} = D_1^h \mathbf{x_i} \times D_2^h \mathbf{x_i}$ and $\mathbf{n_i} = \frac{\mathbf{N_i}}{|\mathbf{N_i}|}$, D_l^h is a spectral derivative operator, and $P_{lk}^h, l, k = 1, 2$ is a spectral approximation of $P_{lk}, l, k = 1, 2$, which is defined through the discrete Fourier transform of P_{lk}^h as follows: $(\widehat{P_{ij}^h})_{\mathbf{k}} = \frac{k_i k_j}{|\mathbf{k}|^2}$ for $\mathbf{k} \neq \mathbf{0}$, where $\mathbf{k} = (k_1, k_2)$, and $(\widehat{P_{ij}^h})_{\mathbf{k}} = \mathbf{0}$ for $\mathbf{k} = \mathbf{0}$.

Note that because we project the tangential velocity field into $\mathbf{x}_{\alpha_1}^*$ and $\mathbf{x}_{\alpha_2}^*$, we obtain a simplified expression for the discretization of the interface equation (57). On the other hand, since we use the reformulation for the γ_1 and γ_2 equations which involve the tangential velocity $\mathbf{x}_{\alpha_i} \cdot \mathbf{w}_0$, we need to use the near field correction and the desingularization to the tangential velocity field to obtain stability.

The main result of this paper is the following convergence result.

Theorem 1. *Assume that the water wave problem is well-posed and has a smooth solution in C^M $(M \geq 6)$ up to time T. Then the modified point vortex method (57)-(59) is stable and convergent. More precisely, there exists a positive $h_0(T)$ such that for $0 < h \leq h_0(T)$ we have*

$$\|\mathbf{x}(t) - \mathbf{x}(\cdot, t)\|_{l^2} \leq C(T)h^3 , \tag{60}$$

$$\|\gamma_l(t) - \gamma_l(\cdot, t)\|_{l^2} \leq C(T)h^3, \quad l = 1, 2. \tag{61}$$

Here $\|\mathbf{x}\|_{l^2}^2 = \sum_{i,j=1}^{N} |\mathbf{x}_{i,j}|^2 h^2$.

The proof of Theorem 1 will be deferred to Section 5.

5. **Consistency of the modified point vortex method.** In this section, we will prove the consistency of the modified point vortex method for 3-D water waves. Since we approximate the derivative operator and the leading order approximation of the velocity integral with spectral accuracy, it is sufficient to prove the consistency of the point vortex method approximation of the desingularized tangential and normal velocity integrals $\mathbf{x}_{\alpha_l} \cdot \mathbf{w}_0, l = 1, 2$ and $\mathbf{w}_0 \cdot \mathbf{n}$. We will show that the modified point vortex method approximation is third order accurate and has an error expansion in the odd powers of h. First, we introduce a function $\mathbf{v}_l(\alpha, \alpha'), l = 1, 2$ and $\mathbf{v}_\mathbf{n}(\alpha, \alpha')$ as follows:

$$\begin{aligned} \mathbf{v}_l(\alpha, \alpha') &= \mathbf{x}_{\alpha_l}(\alpha) \cdot \eta(\alpha') \times \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) \\ &\quad - \gamma_l(\alpha) \mathbf{N}(\alpha') \cdot \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) \\ &\quad - \frac{\mathbf{N}(\alpha)}{2} \cdot (\gamma_1(\alpha) \frac{\alpha_1 - \alpha_1'}{r^3} + \gamma_2(\alpha) \frac{\alpha_2 - \alpha_2'}{r^3}) \mathbf{x}_{\alpha_l}(\alpha), \qquad l = 1, 2 \end{aligned} \tag{62}$$

and

$$\begin{aligned} \mathbf{v}_\mathbf{n}(\alpha, \alpha') &= \mathbf{n}(\alpha) \cdot \eta(\alpha') \times \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) \\ &\quad - \frac{\eta(\alpha)}{|\mathbf{N}(\alpha)|} \cdot \nabla_{x'} G(\mathbf{x}(\alpha) - \mathbf{x}(\alpha')) \times \mathbf{N}(\alpha') \\ &\quad - \frac{|\mathbf{N}(\alpha)|}{2} ((\frac{\alpha_1 - \alpha_1'}{r^3} \gamma_1 + \frac{\alpha_2 - \alpha_2'}{r^3} \gamma_2)(\alpha) \\ &\quad - \frac{\gamma_1(\alpha)}{2} \mathbf{x}^*_{\alpha_1}(\alpha) \cdot (\frac{\alpha_1 - \alpha_1'}{r^3} D_1 + \frac{\alpha_2 - \alpha_2'}{r^3} D_2) \mathbf{x}(\alpha) \\ &\quad - \frac{\gamma_2(\alpha)}{2} \mathbf{x}^*_{\alpha_2}(\alpha) \cdot (\frac{\alpha_1 - \alpha_1'}{r^3} D_1 + \frac{\alpha_2 - \alpha_2'}{r^3} D_2) \mathbf{x}(\alpha)) , \end{aligned} \tag{63}$$

where $r = |\mathbf{r}|, \mathbf{r} = \mathbf{x}_{\alpha_1}(\alpha)(\alpha_1 - \alpha_1') + \mathbf{x}_{\alpha_2}(\alpha)(\alpha_2 - \alpha_2')$. It is easy to see that $\mathbf{v}_l(\alpha, \alpha')$ and $\mathbf{v}_\mathbf{n}(\alpha, \alpha')$ are the corresponding continuous integrands in the desingularized point vortex approximations of the tangential and normal components of the interface velocity. Then the consistency of the point vortex method approximation of the desingularized tangential and normal velocity integrals is reduced to proving that

$$\int\int \mathbf{v}_l(\alpha_\mathbf{i}, \alpha') d\alpha' - \sum_{\mathbf{j} \neq \mathbf{i}} \mathbf{v}_l(\alpha_\mathbf{i}, \alpha_\mathbf{j}) h^2 = C_3 h^3 + C_5 h^5 + \cdots + C_{2n+1} h^{2n+1} + \tag{64}$$

for $l = 1, 2$, and similarly for the normal component. The error expansion (64) can be proved by using an argument similar to that in [12]. We first break this error estimate into far field and near field estimates using a smooth cut-off function, $f_\delta(|\alpha|)$, which satisfies (i) $f_\delta(|\alpha|) = 1$ for $|\alpha| \le \delta/2$, (ii) $f_\delta(|\alpha|) = 0$ for $|\alpha| \ge \delta$. We will take δ to be small, but independent of h. For the far field estimate, which amounts to replacing $\mathbf{v}_l$ by $\mathbf{v}_l(\alpha, \alpha')g_\delta(|\alpha - \alpha'|)$ with $g_\delta = 1 - f_\delta$, classical error analysis shows that the far field error is of spectral accuracy, $O(h^M)$ (M is the degree of regularity of $\mathbf{x}$ and γ), see, e.g. [9]. For the near field error, we can Taylor expand $\mathbf{v}_l(\alpha, \alpha')$ around $\alpha' = \alpha$. Without loss of generality, we may assume that $\alpha_{\mathbf{i}} = 0$. It is not difficult to show that for $|\alpha'| \le \delta$ small

$$\mathbf{v}_l(0, \alpha') = \mathbf{m}_{-2}(\alpha') + \mathbf{m}_{-1}(\alpha') + \mathbf{m}_0(\alpha') + \mathbf{m}_1(\alpha') + \cdots \tag{65}$$

where $\mathbf{m}_l(\alpha)$ ($l = -2, -1, 0, 1, \cdots$) are homogeneous functions of degree l, and $\mathbf{m}_l(\alpha)$ is odd function of α for l even. Since the cut-off function $f_\delta(|\alpha|)$ is an even function of α, $\mathbf{m}_l(\alpha)f_\delta(|\alpha|)$ is also an odd function of α for l even.

To justify the expansion (65), we Taylor expand $\gamma_l(\alpha')$, $\mathbf{x}_{\alpha_l}(\alpha')$, and $\nabla_{x'}G(\mathbf{x}(0) - \mathbf{x}(\alpha'))$ around $\alpha' = 0$. We have

$$\begin{aligned}
\gamma_l(\alpha') &= \gamma_l(0) + (\gamma_l)_\alpha(0)(\alpha') + \mathbf{m}_2(\alpha') + \cdots, \\
\mathbf{x}_{\alpha_l}(\alpha') &= \mathbf{x}_{\alpha_l}(0) + (\mathbf{x}_{\alpha_l})_\alpha(0)(\alpha') + \mathbf{m}_2(\alpha') + \cdots, \\
\nabla_{x'}G(\mathbf{x}(0) - \mathbf{x}(\alpha')) &= \nabla_{x'}G(\mathbf{r}(0)) - \nabla_{x'}\nabla_{x'}G(\mathbf{r}(0))(\frac{1}{2}(\alpha')^T\nabla\nabla\mathbf{x}(0)(\alpha')) \\
&\quad + \mathbf{m}_0(\alpha') + \cdots,
\end{aligned}$$

where $\mathbf{r}(\alpha) = D_1\mathbf{x}(\alpha)(\alpha_1 - \alpha_1') + D_2\mathbf{x}(\alpha)(\alpha_2 - \alpha_2')$ and $\mathbf{m}_l(\alpha)$ is a generic notation for a homogeneous function of degree l. Substituting the above expansions into the (62), and collecting the terms of the same order give rise to the expansion (65). Moreover, direct calculations show that the homogeneous terms of degree -1 exactly cancel each other. This implies that $\mathbf{m}_{-1}(\alpha) \equiv 0$ in the expansion (65). Since both $\mathbf{m}_{-2}$ and $\mathbf{m}_0$ are odd, they do not contribute to the continuous integral nor the discrete sum. Therefore the first term in the expansion of $\mathbf{v}_l$ that contributes to the error is the $\mathbf{m}_1(\alpha)$ term.

We now show that

$$\int \mathbf{m}_l(\alpha')f_\delta(|\alpha'|)d\alpha' - \sum_{\mathbf{j}\neq 0} \mathbf{m}_l(\alpha_{\mathbf{j}})f_\delta(|\alpha_{\mathbf{j}}|)h^2 = C_{l+2}h^{l+2} + O(h^M), \quad \text{for} \quad l \ge 1. \tag{66}$$

The proof follows closely that of [12]. Using the homogeneity of $\mathbf{m}_l$, we can write

$$\sum_{\mathbf{j}\neq 0} \mathbf{m}_l(\alpha_{\mathbf{j}})f_\delta(|\alpha_{\mathbf{j}}|)h^2 = h^{l+2}S_l(h), \quad \text{with} \quad S_l(h) = \sum_{\mathbf{j}\neq \mathbf{0}} \mathbf{m}_l(\mathbf{j})f_\delta(|\mathbf{j}|h).$$

Since S_l is a finite sum due to the cut-off f_δ, we may differentiate $S_l(h)$ with respect to h. We have

$$\frac{d}{dh}S_l(h) = \sum_{\mathbf{j}\neq \mathbf{0}} \mathbf{m}_l(\mathbf{j})\frac{d}{dr}f_\delta(|\mathbf{j}|h)|\mathbf{j}| = h^{-(l+3)}\sum_{\mathbf{j}\neq \mathbf{0}} \mathbf{m}_l(\mathbf{j}h)\frac{d}{dr}f_\delta(|\mathbf{j}|h)|\mathbf{j}h|h^2.$$

The sum is a trapezoidal rule approximation to

$$\int \mathbf{m}_l(y)\frac{d}{dr}f_\delta(|y|)|y|dy.$$

Note that the integrand is a smooth function with compact support since $\frac{d}{dr}f_\delta(|y|)$ vanishes near the origin and has a compact support. It is well-known that the trapezoidal rule gives spectral accuracy for such smooth integrand with compact support [9]. That is

$$\sum_{\mathbf{j}\neq\mathbf{0}} \mathbf{m}_l(\mathbf{j}h)\frac{d}{dr}f_\delta(|\mathbf{j}|h)|\mathbf{j}h|h^2 = \int \mathbf{m}_l(y)\frac{d}{dr}f_\delta(|y|)|y|dy + O(h^M).$$

On the other hand, using the polar coordinate, we obtain

$$\begin{aligned}\int \mathbf{m}_l(y)\frac{d}{dr}f_\delta(|y|)|y|dy &= \int_0^{2\pi}\int_0^\infty r^l\mathbf{m}_l(\theta)\frac{d}{dr}f_\delta(r)r^2 drd\theta \\ &= \int_0^{2\pi}\mathbf{m}_l(\theta)d\theta\int_0^\infty r^{l+2}\frac{d}{dr}f_\delta(r)dr \\ &= -(l+2)\int_0^{2\pi}\mathbf{m}_l(\theta)d\theta\int_0^\infty r^l f_\delta(r)rdr \\ &= -(l+2)\int \mathbf{m}_l(y)f_\delta(|y|)dy,\end{aligned}$$

where we have used the homogeneity of $\mathbf{m}_l$. Thus we have

$$\frac{d}{dh}S_l(h) = -(l+2)h^{-(l+3)}\int \mathbf{m}_l(y)f_\delta(|y|)dy + O(h^M).$$

Integrating the above equation from h to 1 gives

$$S_l(h) = -C_{l+2} + h^{-(l+2)}\int \mathbf{m}_l(y)f_\delta(|y|)dy + O(h^M),$$

where C_{l+2} is an integration constant. This implies that

$$\begin{aligned}\int \mathbf{m}_l(y)f_\delta(|y|)dy - \sum_{\mathbf{j}\neq\mathbf{0}}\mathbf{m}_l(\alpha_\mathbf{j})f_\delta(|\alpha_\mathbf{j}|)h^2 &= \int \mathbf{m}_l(y)f_\delta(|y|)dy - h^{(l+2)}S_l(h) \\ &= C_{l+2}h^{(l+2)} + O(h^M),\end{aligned}$$

for all $l \geq 1$. Observe that $C_l = 0$ for l even due to the oddness of $\mathbf{m}_l$. Thus we obtain an error expansion in the odd powers of h. This proves the consistency of the modified point vortex method.

6. **Properties of some singular integral operators.** Before we proceed to analyze the stability of our 3-D boundary integral method, we need to study the spectral properties of certain singular integral operators. We first define the Riesz transform (which is the 2-D analogue of the Hilbert transform) and the Λ operator

$$H_l(f) = \frac{1}{2\pi}\int\int \frac{(\alpha_l - \alpha_l')f(\alpha')}{r^3}d\alpha', \qquad l = 1,2, \tag{67}$$

$$\Lambda(f) = \frac{1}{2\pi}\int\int \frac{f(\alpha) - f(\alpha')}{r^3}d\alpha', \tag{68}$$

where $r = |\mathbf{r}|$, and

$$\mathbf{r} = \mathbf{x}_{\alpha_1}(\alpha)(\alpha_1 - \alpha_1') + \mathbf{x}_{\alpha_2}(\alpha)(\alpha_2 - \alpha_2').$$

The Fourier transform of a 2-D function f is defined by

$$\hat{f}(\xi) = (2\pi)^{-2}\int\int f(x)e^{-i\mathbf{x}\cdot\xi}d\mathbf{x}. \tag{69}$$

The inverse transform is given by

$$f(\mathbf{x}) = \int\int \hat{f}(\xi) e^{i\mathbf{x}\cdot\xi} d\xi. \tag{70}$$

Note that the Riesz transforms defined in (67) are not a convolution operator. They are pseudo-differential operators. Their 'Fourier symbols' depend on the free surface $\mathbf{x}(\alpha)$. Nonetheless, we can still characterize their spectral properties via the Fourier transform. The result is summarized in the following lemma.

Lemma 6.1. *The Riesz transforms have the following spectral representation:*

$$(H_1 f)(\alpha) = \frac{-i}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|^2} \int\int \frac{(|\mathbf{x}_{\alpha_2}|^2 \xi_1 - (\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2})\xi_2)\hat{f}(\xi) e^{i\xi\cdot\alpha}}{(|\mathbf{x}_{\alpha_2}|^2 \xi_1^2 - 2(\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2})\xi_1\xi_2 + |\mathbf{x}_{\alpha_1}|^2 \xi_2^2)^{1/2}} d\xi, \tag{71}$$

$$(H_2 f)(\alpha) = \frac{-i}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|^2} \int\int \frac{(|\mathbf{x}_{\alpha_1}|^2 \xi_2 - (\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2})\xi_1)\hat{f}(\xi) e^{i\xi\cdot\alpha}}{(|\mathbf{x}_{\alpha_2}|^2 \xi_1^2 - 2(\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2})\xi_1\xi_2 + |\mathbf{x}_{\alpha_1}|^2 \xi_2^2)^{1/2}} d\xi. \tag{72}$$

Proof: In the special case of an orthogonal parametrization of the free surface, i.e. $\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2} = 0$, this result has been obtained in Lemma 3.1 of [18]. The result for a non-orthogonal parametrization can be obtained in a similar way. We express f in terms of his Fourier transform and substitute it into the Riesz transforms. We obtain

$$\begin{aligned}(H_1 f)(\alpha) &= \frac{1}{2\pi} \int\int \hat{f}(\xi) d\xi \int\int \frac{(\alpha_1 - \alpha_1')e^{i\xi\cdot\alpha'}}{r^3} d\alpha' \\ &= \frac{1}{2\pi} \int\int \hat{f}(\xi) e^{i\xi\cdot\alpha} d\xi \int\int \frac{\alpha_1' e^{-i\xi\cdot\alpha'}}{(|\mathbf{x}_{\alpha_1}|^2 \alpha_1'^2 + 2\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2} \alpha_1'\alpha_2' + |\mathbf{x}_{\alpha_2}|^2 \alpha_2'^2)^{3/2}} d\alpha'.\end{aligned} \tag{73}$$

We define

$$\Phi(\xi_1, \xi_2) = \int\int \frac{\alpha_1' e^{-i\xi\cdot\alpha'}}{(|\mathbf{x}_{\alpha_1}|^2 \alpha_1'^2 + 2\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2} \alpha_1'\alpha_2' + |\mathbf{x}_{\alpha_2}|^2 \alpha_2'^2)^{3/2}} d\alpha'.$$

By making a change of variables from α' to β',

$$\beta_1' = \frac{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|}{|\mathbf{x}_{\alpha_2}|} \alpha_1', \quad \beta_2' = \frac{\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2}}{|\mathbf{x}_{\alpha_2}|} \alpha_1' + |\mathbf{x}_{\alpha_2}| \alpha_2',$$

and using the identity

$$|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|^2 + (\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_1})^2 = |\mathbf{x}_{\alpha_1}|^2 |\mathbf{x}_{\alpha_2}|^2, \tag{74}$$

we can show that

$$\Phi\left(\frac{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|}{|\mathbf{x}_{\alpha_2}|}\xi_1 + \frac{\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2}}{|\mathbf{x}_{\alpha_2}|}\xi_2, |\mathbf{x}_{\alpha_2}|\xi_2\right) = \frac{|\mathbf{x}_{\alpha_2}|}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|^2} \int\int \frac{\beta_1' e^{-i\xi\cdot\beta'}}{(\beta_1'^2 + \beta_2'^2)^{3/2}} d\beta'.$$

It has been shown in [23] (pp. 57-58) that the Fourier transform of the Riesz kernel $\frac{\beta_1}{(\beta_1^2+\beta_2^2)^{3/2}}$ is given by

$$\int\int \frac{\beta_1' e^{-i\xi\cdot\beta'}}{(\beta_1'^2 + \beta_2'^2)^{3/2}} d\beta' = -2\pi \frac{i\xi_1}{(\xi_1^2 + \xi_2^2)^{1/2}}.$$

Therefore, we obtain

$$\Phi(\xi_1,\xi_2) = \frac{-2\pi i}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^2}\frac{(|\mathbf{x}_{\alpha_2}|^2\xi_1 - (\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})\xi_2)}{(|\mathbf{x}_{\alpha_2}|^2\xi_1^2 - 2(\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})\xi_1\xi_2 + |\mathbf{x}_{\alpha_1}|^2\xi_2^2)^{1/2}}.$$

By (73), we have

$$(H_1 f)(\alpha) = \frac{-i}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^2}\int\int\frac{(|\mathbf{x}_{\alpha_2}|^2\xi_1 - (\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})\xi_2)\hat{f}(\xi)e^{i\xi\cdot\alpha}}{(|\mathbf{x}_{\alpha_2}|^2\xi_1^2 - 2(\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})\xi_1\xi_2 + |\mathbf{x}_{\alpha_1}|^2\xi_2^2)^{1/2}}d\xi.$$

Using the same argument, we can get the expression of $(H_2 f)(\alpha)$. This proves Lemma 6.1.

Lemma 6.2. *The* Λ *operator satisfies the following compatibility condition:*

$$\Lambda = H_1 D_1 + H_2 D_2. \tag{75}$$

where $D_l = \partial_{\alpha_l}$. *Moreover,* ΛH_l *is a local derivative operator to the leading order:*

$$\Lambda H_1(f) = -\frac{1}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^4}\left(|\mathbf{x}_{\alpha_2}|^2 D_1 - (\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_1})D_2\right)f + A_0(f), \tag{76}$$

$$\Lambda H_2(f) = -\frac{1}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^4}\left(|\mathbf{x}_{\alpha_1}|^2 D_2 - (\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})D_1\right)f + A_0(f), \tag{77}$$

where $A_0(f)$ *is a bounded operator from* H^s *to* H^s.

Proof: The identity (75) can be verified directly by using integration by parts. Using (75) and Lemma 6.1, we obtain

$$(\Lambda f)(\alpha) = \frac{1}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^2}\int(|\mathbf{x}_{\alpha_2}|^2\xi_1^2 - 2(\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})\xi_1\xi_2 + |\mathbf{x}_{\alpha_1}|^2\xi_2^2)^{1/2}\hat{f}(\xi)e^{i\xi\cdot\alpha}d\xi. \tag{78}$$

Define the commutator operator as follows:

$$[\Lambda, g](f) = \Lambda(gf) - g\Lambda(f).$$

It is easy to show that the commutator operator $[\Lambda, g] = A_0$ is a bounded operator for g smooth. Now using (78), Lemma 6.1, and $[\Lambda, g] = A_0$, we have

$$\begin{aligned}
\Lambda H_1(f) &= -\frac{i}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^4}\int(|\mathbf{x}_{\alpha_2}|^2\xi_1 - (\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2})\xi_2)\hat{f}(\xi)e^{i\xi\cdot\alpha}d\xi + A_0(f)\\
&= -\frac{|\mathbf{x}_{\alpha_2}|^2}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^4}\int\int i\xi_1\hat{f}(\xi)e^{i\xi\cdot\alpha}d\xi + \frac{\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2}}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^4}\int\int i\xi_2\hat{f}(\xi)e^{i\xi\cdot\alpha}d\xi\\
&\quad + A_0(f)\\
&= -\frac{1}{|\mathbf{x}_{\alpha_1}\times\mathbf{x}_{\alpha_2}|^4}\left(|\mathbf{x}_{\alpha_2}|^2 D_1 - (\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_1})D_2\right)f + A_0(f).
\end{aligned}$$

This proves (76). The proof of (77) follows similarly. This completes the proof of Lemma 6.2.

Now we can describe the spectral discretization of $H_l, l = 1, 2$ defined in section 4. Using the explicit Fourier representation of H_l in Lemma 6.1, we can define our spectral discretization of the H_l operator, denoted as H_l^s. To this end, it is sufficient to give a spectral discretization of the Riesz transform. We denote by H_l^s the spectral discretization of the Riesz transform H_l,

$$(H_{1,h}^s f)(\alpha_{\mathbf{j}}) = -\frac{i}{|D_1^h\mathbf{x}\times D_2^h\mathbf{x}|^2}\sum_{\mathbf{k}\in K_N}\frac{(|D_2^h\mathbf{x}|^2 k_1 - (D_1^h\mathbf{x}\cdot D_2^h\mathbf{x})k_2)\hat{f}_{\mathbf{k}}e^{i\mathbf{k}\cdot\alpha_{\mathbf{j}}}}{(|D_2^h\mathbf{x}|^2 k_1^2 - 2(D_1^h\mathbf{x}\cdot D_2^h\mathbf{x})k_1k_2 + |D_1^h\mathbf{x}|^2 k_2^2)^{1/2}},$$

$$(H^s_{2,h}f)(\alpha_{\mathbf{j}}) = -\frac{i}{|D^h_1\mathbf{x}\times D^h_2\mathbf{x}|^2}\sum_{\mathbf{k}\in K_N}\frac{(|D^h_1\mathbf{x}|^2k_2-(D^h_1\mathbf{x}\cdot D^h_2\mathbf{x})k_1)\hat{f}_{\mathbf{k}}e^{i\mathbf{k}\cdot\alpha_{\mathbf{j}}}}{(|D^h_2\mathbf{x}|^2k_1^2-2(D^h_1\mathbf{x}\cdot D^h_2\mathbf{x})k_1k_2+|D^h_1\mathbf{x}|^2k_2^2)^{1/2}},$$

where $D^h_l\mathbf{x} = D^h_l\mathbf{x}(\alpha_j)$ and $K_N = \{\mathbf{k} : \mathbf{k} \neq \mathbf{0}, -N/2+1 \leq k_l \leq N/2, l = 1,2\}$.

Remark 6.1 If we evaluate directly the above spectral discretization of the Riesz transform, it will cost $O(N^4 \log N)$ operations which are comparable to the operation count of the point vortex method approximation using direct summations. On the other hand, it is possible to reduce the Riesz transform, H_l, to a convolution operator by introducing a generalized arclength parametrization for the free surface. Such a generalized arclength parametrization can be obtained by imposing

$$\mathbf{x}_{\alpha_1}\cdot\mathbf{x}_{\alpha_2} = \lambda_1(t)|\mathbf{x}_{\alpha_2}|^2, \qquad |\mathbf{x}_{\alpha_1}|^2 = \lambda_2(t)|\mathbf{x}_{\alpha_2}|^2.$$

It can be shown that such a parametrization exists, at least for near equilibrium initial data [16]. Our numerical experiments have indicated that this parametrization exists quite generically even for large perturbations from the equilibrium [16]. Once we have found such parametrization of the free surface initially, this property is preserved in time by adding two tangential velocities dynamically. We refer the reader to [16] for more details. Using this generalized arclength frame, the Riesz transform now becomes a convolution operator. In fact, we now have

$$\begin{aligned}
(H^s_{1,h}f)(\alpha_{\mathbf{j}}) &= -\frac{|D^h_2\mathbf{x}|\, i}{|D^h_1\mathbf{x}\times D^h_2\mathbf{x}|^2}\sum_{\mathbf{k}\in K_N}\frac{(k_1-\lambda_1(t)k_2)\hat{f}_{\mathbf{k}}e^{i\mathbf{k}\cdot\alpha_{\mathbf{j}}}}{(k_1^2-2\lambda_1(t)k_1k_2+\lambda_2(t)k_2^2)^{1/2}},\\
(H^s_{2,h}f)(\alpha_{\mathbf{j}}) &= -\frac{|D^h_2\mathbf{x}|\, i}{|D^h_1\mathbf{x}\times D^h_2\mathbf{x}|^2}\sum_{\mathbf{k}\in K_N}\frac{(k_2-\lambda_1(t)k_1)\hat{f}_{\mathbf{k}}e^{i\mathbf{k}\cdot\alpha_{\mathbf{j}}}}{(k_1^2-2\lambda_1(t)k_1k_2+\lambda_2(t)k_2^2)^{1/2}},
\end{aligned}$$

which can be evaluated by Fast Fourier Transform with $O(N^2 \log N)$ operation count.

7. **Stability of the modified point vortex method for 3-D water waves.** In this section, we will analyze stability the modified point vortex method. We first consider the linear variation of the modified point vortex method approximation to the tangential and normal velocity integral, i.e. the terms $\mathbf{x}_{\alpha_l}\cdot\mathbf{w}_0, l = 1,2$ and $\mathbf{w}_0\cdot\mathbf{n}$. Denote the errors in $\mathbf{x}_{\mathbf{j}}, \gamma_{l\mathbf{j}}$ and $\phi_{\mathbf{j}}$ by $\dot{\mathbf{x}}_{\mathbf{j}} = \mathbf{x}_{\mathbf{j}} - \mathbf{x}(\alpha_{\mathbf{j}})$, $\dot{\gamma}_{l\mathbf{j}} = \gamma_{l\mathbf{j}} - \gamma_l(\alpha_{\mathbf{j}}), l = 1,2$, and $\dot{\phi}_{\mathbf{j}} = \phi_{\mathbf{j}} - \phi(\alpha_{\mathbf{j}})$ respectively. $\dot{E}_{pvm}(\mathbf{j})$, $\dot{E}_{near}(\mathbf{j})$, and $\dot{E}_{local}(\mathbf{j})$ are defined similarly. We sometimes also use the notation, $Er(f)(\mathbf{j}) = f(\alpha_{\mathbf{j}}) - f_{\mathbf{j}}$ when the quantity f consists of several terms. Further, we define

$$\begin{aligned}
E^l(\alpha_{\mathbf{i}}) &\equiv \Bigg(-\mathbf{x}_{\alpha_l}(\alpha)\cdot\int\!\!\int \eta(\alpha')\times\nabla_{\mathbf{x}'}G(\mathbf{x}(\alpha)-\mathbf{x}(\alpha'))d\alpha'\\
&\quad + D^h_l\mathbf{x}_{\mathbf{i}}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\eta_j\times\nabla_{x'}G(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}})h^2\\
&\quad - \gamma_{l\mathbf{i}}\sum_{\mathbf{j}\neq\mathbf{i}}\mathbf{N}_j\cdot\nabla_{x'}G(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}})h^2\Bigg) + (B^s_l - B^p_l)\\
&\equiv E^l_{pvm} + E^l_{near}, \qquad l = 1,2, \qquad (79)
\end{aligned}$$

and

$$
\begin{aligned}
E^{\mathbf{n}}(\alpha_{\mathbf{i}}) &\equiv \Big(-\mathbf{n}(\alpha)\cdot\int\int\eta(\alpha')\times\nabla_{\mathbf{x}'}G(\mathbf{x}(\alpha)-\mathbf{x}(\alpha'))d\alpha' \\
&\quad +\mathbf{n}_{\mathbf{i}}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\eta_j\times\nabla_{x'}G(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}})h^2 \\
&\quad -\frac{\eta_i}{|\mathbf{N}_{\mathbf{i}}|}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\nabla_{x'}G(\mathbf{x}_{\mathbf{i}}-\mathbf{x}_{\mathbf{j}})\times\mathbf{N}_{\mathbf{j}}h^2\Big)+(B^s_{\mathbf{n}}-B^p_{\mathbf{n}}) \\
&\equiv E^{\mathbf{n}}_{pvm}+E^{\mathbf{n}}_{near},
\end{aligned} \tag{80}
$$

where $B^p_l, l=1,2,\mathbf{n}$ denotes the point vortex method approximation of B_l, and B^s_l denotes the spectral approximation of B_l using the exact Fourier symbols of B_l. Stability analysis of our approximations to the tangential and normal velocity integrals is to estimate E_l and $E_{\mathbf{n}}$ in terms of $\dot{\mathbf{x}}_{\mathbf{j}}$ and $\dot\gamma_{l\mathbf{j}}$, etc.

The first term on the right hand side of (79) and (80) measures the stability error due to the point vortex method approximation of the velocity integral. So we call it E^l_{pvm} $(l=1,2)$ and $E^{\mathbf{n}}$. The second term on the right hand side is due to the contribution of a near field correction. So we term it E^l_{near} $(l=1,2)$ and $E^{\mathbf{n}}$.

We first study the linear variation of $E^l_{pvm}, l=1,2$. Direct calculations show that the linear variation of $E^l_{pvm}, l=1,2$, denoted as $\dot E^l_{pvm}$, is given by

$$
\begin{aligned}
\dot E^1_{pvm}(\mathbf{i}) &= D^h_1\dot{\mathbf{x}}_{\mathbf{i}}\cdot\mathbf{w}^h_0+K^h_1\dot\gamma_1-K^h_2\dot\gamma_2 \\
&\quad +\frac{\mathbf{N}_{\mathbf{i}}}{2}\cdot(\gamma_{1\mathbf{i}}H^p_{1,h}+\gamma_{2\mathbf{i}}H^p_{2,h})D^h_1\dot{\mathbf{x}}_{\mathbf{i}} \\
&\quad +O(h)(\dot\gamma_{\mathbf{i}})+A_0(\dot{\mathbf{x}}_{\mathbf{i}}),
\end{aligned} \tag{81}
$$

$$
\begin{aligned}
\dot E^2_{pvm}(\mathbf{i}) &= D^h_2\dot{\mathbf{x}}_{\mathbf{i}}\cdot\mathbf{w}^h_0+K^h_3\dot\gamma_1-K^h_4\dot\gamma_2 \\
&\quad +\frac{\mathbf{N}_i}{2}\cdot(\gamma_{1\mathbf{i}}H^p_{1,h}+\gamma_{2\mathbf{i}}H^p_{2,h})D^h_2\dot{\mathbf{x}}_{\mathbf{i}} \\
&\quad +O(h)(\dot\gamma_{\mathbf{i}})+A_0(\dot{\mathbf{x}}_{\mathbf{i}}),
\end{aligned} \tag{82}
$$

$$
\begin{aligned}
\dot E^{\mathbf{n}}_{pvm}(\mathbf{i}) &= \dot{\mathbf{n}}\cdot\mathbf{w}^h_0+\frac{|\mathbf{N}_{\mathbf{i}}|}{2}\Big(H^p_{1,h}(\dot\gamma_{1\mathbf{i}})+H^p_{2,h}(\dot\gamma_{2\mathbf{i}}) \\
&\quad -\gamma_{1\mathbf{i}}D^h_1\mathbf{x}^*_{\mathbf{i}}\cdot(H^p_{1,h}D^h_1+H^p_{2,h}D^h_2)\dot{\mathbf{x}}_{\mathbf{i}} \\
&\quad -\gamma_{2i}D^h_2\mathbf{x}^*_{\mathbf{i}}\cdot(H^p_{1,h}D^h_1+H^p_{2,h}D^h_2)\dot{\mathbf{x}}_{\mathbf{i}}\Big) \\
&\quad +A_{-1}(\dot\gamma_{\mathbf{i}})+A_0(\dot{\mathbf{x}}_{\mathbf{i}}),
\end{aligned} \tag{83}
$$

where $\gamma l\mathbf{i}=\gamma_l(\alpha_{\mathbf{i}})$ (l=1,2), K^h_l is a point vortex method approximation of K_l $(l=1,2,3,4)$, $\mathbf{w}^h_0$ is a point vortex method approximation of $\mathbf{w}_0$, A_0 is a bounded operator from l^p to l^p, and A_{-1} is a smoothing operator of order one, i.e. $D^h_l A_{-1}=A_{-1}(D^h_l)=A_0$. We defer to Appendix C to give a more detailed derivation of the above error estimates.

Next we estimate the linear variation of the near field term E_{near}. Direct calculations show that the linear variation of E_{near}, denoted as $\dot E^l_{near}$(l=1,2) and $\dot E^{\mathbf{n}}_{near}$, is given by

$$\begin{aligned}
\dot{E}^1_{near}(\mathbf{i}) &= \frac{\mathbf{N_i}}{2}\cdot(\gamma_{1\mathbf{i}}H^s_{1,h}+\gamma_{2i}H^s_{2,h})D^h_1\dot{\mathbf{x}}_\mathbf{i} \\
&\quad -\frac{\mathbf{N_i}}{2}\cdot(\gamma_{1\mathbf{i}}H^p_{1,h}+\gamma_{2\mathbf{i}}H^p_{2,h})D^h_1\dot{\mathbf{x}}_\mathbf{i} \\
&\quad +O(h)(\dot{\gamma}_\mathbf{i})+A_0(\dot{\mathbf{x}}_\mathbf{i}). \qquad (84)\\
\dot{E}^2_{near}(\mathbf{i}) &= \frac{\mathbf{N_i}}{2}\cdot(\gamma_{1\mathbf{i}}H^s_{1,h}+\gamma_{2\mathbf{i}}H^s_{2,h})D^h_2\dot{\mathbf{x}}_\mathbf{i} \\
&\quad -\frac{\mathbf{N_i}}{2}\cdot(\gamma_{1\mathbf{i}}H^p_{1,h}+\gamma_{2\mathbf{i}}H^p_{2,h})D^h_2\dot{\mathbf{x}}_\mathbf{i} \\
&\quad +O(h)(\dot{\gamma}_\mathbf{i})+A_0(\dot{\mathbf{x}}_\mathbf{i}). \qquad (85)\\
\dot{E}^\mathbf{n}_{near}(\mathbf{i}) &= \frac{|\mathbf{N_i}|}{2}\big(H^s_{1,h}(\dot{\gamma}_{1\mathbf{i}})+H^s_{2,h}(\dot{\gamma}_{2\mathbf{i}}) \\
&\quad -\gamma_{1\mathbf{i}}D^h_1\mathbf{x}^*_\mathbf{i}\cdot(H^s_{1,h}D^h_1+H^s_{2,h}D^h_2)\dot{\mathbf{x}}_\mathbf{i} \\
&\quad -\gamma_{2i}D^h_2\mathbf{x}^*_\mathbf{i}\cdot(H^s_{1,h}D^h_1+H^s_{2,h}D^h_2)\dot{\mathbf{x}}_\mathbf{i}\big) \\
&\quad -\frac{|\mathbf{N_i}|}{2}\Big(H^p_{1,h}(\dot{\gamma}_{1\mathbf{i}})+H^p_{2,h}(\dot{\gamma}_{2\mathbf{i}}) \\
&\quad -\gamma_{1i}D^h_1\mathbf{x}^*_\mathbf{i}\cdot(H^p_{1,h}D^h_1+H^p_{2,h}D^h_2)\dot{\mathbf{x}}_\mathbf{i} \\
&\quad -\gamma_{2i}D^h_2\mathbf{x}^*_\mathbf{i}\cdot(H^p_{1,h}D^h_1+H^p_{2,h}D^h_2)\dot{\mathbf{x}}_\mathbf{i}\Big) \\
&\quad +A_{-1}(\dot{\gamma}_\mathbf{i})+A_0(\dot{\mathbf{x}}_\mathbf{i})\ . \qquad (86)
\end{aligned}$$

Again, we defer to Appendix C to give a more detailed derivation of the above error estimates.

By adding $\dot{E}^l_{pvm}$ and $\dot{E}^l_{near}$ $(l=1,2)$ and adding $\dot{E}^\mathbf{n}_{pvm}$ and $\dot{E}^\mathbf{n}_{near}$, we obtain after some cancellations that

$$\begin{aligned}
\dot{E}^1_{pvm}(\mathbf{i})+\dot{E}^1_{near}(\mathbf{i}) &= D^h_1\dot{\mathbf{x}}_\mathbf{i}\cdot\mathbf{w}^h_0+K^h_1\dot{\gamma}_1-K^h_2\dot{\gamma}_2 \\
&\quad +\frac{\mathbf{N_i}}{2}\cdot(\gamma_{1\mathbf{i}}H^s_{1,h}+\gamma_{2\mathbf{i}}H^s_{2,h})D^h_1\dot{\mathbf{x}}_\mathbf{i} \\
&\quad +O(h)(\dot{\gamma}_\mathbf{i})+A_0(\dot{\mathbf{x}}_\mathbf{i}), \qquad (87)\\
\dot{E}^2_{pvm}(\mathbf{i})+\dot{E}^2_{near}(\mathbf{i}) &= D^h_2\dot{\mathbf{x}}_\mathbf{i}\cdot\mathbf{w}^h_0+K^h_3\dot{\gamma}_1-K^h_4\dot{\gamma}_2 \\
&\quad +\frac{\mathbf{N_i}}{2}\cdot(\gamma_{1\mathbf{i}}H^s_{1,h}+\gamma_{2\mathbf{i}}H^s_{2,h})D^h_2\dot{\mathbf{x}}_\mathbf{i} \\
&\quad +O(h)(\dot{\gamma}_\mathbf{i})+A_0(\dot{\mathbf{x}}_\mathbf{i}), \qquad (88)\\
\dot{E}^\mathbf{n}_{pvm}(\mathbf{i})+\dot{E}^\mathbf{n}_{near}(\mathbf{i}) &= \dot{\mathbf{n}}\cdot\mathbf{w}^h_0+\frac{|\mathbf{N_i}|}{2}\big(H^s_{1,h}(\dot{\gamma}_{1\mathbf{i}})+H^s_{2,h}(\dot{\gamma}_{2\mathbf{i}}) \\
&\quad -\gamma_{1\mathbf{i}}D^h_1\mathbf{x}^*_\mathbf{i}\cdot(H^s_{1,h}D^h_1+H^s_{2,h}D^h_2)\dot{\mathbf{x}}_\mathbf{i} \\
&\quad -\gamma_{2\mathbf{i}}D^h_2\mathbf{x}^*_\mathbf{i}\cdot(H^s_{1,h}D^h_1+H^s_{2,h}D^h_2)\dot{\mathbf{x}}_\mathbf{i}\big) \\
&\quad +A_{-1}(\dot{\gamma}_\mathbf{i})+A_0(\dot{\mathbf{x}}_\mathbf{i}). \qquad (89)
\end{aligned}$$

Projection of errors into local normal and tangent vectors.

As we can see from (87)–(89), the leading order error terms of the tangential and normal velocity components can be naturally expressed in terms of the local normal and tangent vectors. This suggests that we project the interface errors into the local normal and tangent vectors instead of using the original (x,y,z) coordinate. In the local normal and tangent coordinates, the equations that govern the growth of the leading order errors greatly simplify and we can identify cancellation of interface errors in certain tangent direction. This makes it easier to obtain stability by performing energy estimates.

On the other hand, we have from (59) that

$$\begin{aligned} D_l^h \dot{\phi}_{\mathbf{i}} &= \frac{\dot{\gamma}_{l\mathbf{i}}}{2} + P_{l1}^h Er((D_1^h \mathbf{x}_{\mathbf{i}} \cdot \mathbf{w}_0^h - C_1^h) + (B_1^s - B_1^h)) \\ &+ P_{l2}^h Er((D_2^h \mathbf{x}_{\mathbf{i}} \cdot \mathbf{w}_0^h - C_2^h) + (B_2^s - B_2^h)), \end{aligned} \tag{90}$$

where $Er(f) = f(\alpha_{\mathbf{j}}) - f_{\mathbf{j}}$ denotes the error of f. Using (87) and (88) , and the definition of $E_{pvm}(\mathbf{i})$ and $E_{near}(\mathbf{i})$, we get

$$\left(\frac{I}{2} + A_h + O(h)\right) \dot{\gamma}_{\mathbf{i}} = \bigtriangledown^h \dot{\phi}_{\mathbf{i}} - \bigtriangledown^h \dot{\mathbf{x}}_{\mathbf{i}} \cdot \mathbf{w}_0^h + \frac{\mathbf{N}_{\mathbf{i}}}{2} \cdot (\gamma_{1\mathbf{i}} H_{1,h}^s + \gamma_{1\mathbf{i}} H_{1,h}^s) \bigtriangledown^h \dot{\mathbf{x}}_{\mathbf{i}} \tag{91}$$

where A_h is two by two matrix, $A_h = (a_{ij}^h)$ with a_{ij} given by

$$\begin{aligned} a_{11}^h &= P_{11}^h K_1^h + P_{12}^h K_3^h, \qquad a_{12}^h = P_{11}^h K_2^h + P_{12}^h K_4^h \ , \\ a_{21}^h &= P_{21}^h K_1^h + P_{22}^h K_3^h, \qquad a_{22}^h = P_{21}^h K_2^h + P_{22}^h K_4^h \ . \end{aligned}$$

We can show that $\frac{1}{2}I + A_h + O(h)$ is invertible by using the invertibility of the corresponding continuous operator and the fact that the kernel of A_h approximates that of A to the leading order. The following lemma, which is proved in Appendix A, concerns the solvability of (91).

Lemma 7.1. *Given $\mathbf{x}(\alpha, t)$ smooth for $0 \le t \le T$, the operator $I + 2A_h$ is invertible for h sufficiently small, and the norm of $(I+2A_h)^{-1}$ as an operator on L_h^2 is bounded uniformly in h and t.*

Since K_l is an integral operator with weakly singular kernel, one can verify that $K_l^h(\dot{\phi})$ is a smoothing operator of order one, i.e. $K_l^h(\dot{\phi}) = A_{-1}(\dot{\phi})$ $(l = 1, 2, 3, 4)$. We defer to Appendix B to prove this property (see also [4] for proof of a similar result). We can show that the invertibility of $(\frac{1}{2}I + A_h)$ and the fact $K_l^h(\dot{\phi}) = A_{-1}(\dot{\phi})$ $(l = 1, 2, 3, 4)$ imply

$$\begin{aligned} \frac{\dot{\gamma}_{l\mathbf{i}}}{2} &= D_l^h \dot{\phi}_{\mathbf{i}} - \left(D_l^h \dot{\mathbf{x}}_{\mathbf{i}} \cdot \mathbf{w}_0(\alpha_{\mathbf{i}}) + \frac{\mathbf{N}_{\mathbf{i}}}{2} \cdot (\gamma_{1\mathbf{i}} H_{1,h}^s + \gamma_{2\mathbf{i}} H_{2,h}^s) D_l^h \dot{\mathbf{x}}_{\mathbf{i}} \right) \\ &+ A_0(\dot{\phi}_{\mathbf{i}}) + A_0(\dot{\mathbf{x}}_{\mathbf{i}}), \end{aligned} \tag{92}$$

which can be rewritten as

$$\begin{aligned} \frac{\dot{\gamma}_{l\mathbf{i}}}{2} &= D_l^h (\dot{F}_{\mathbf{i}} + E_{local}(\alpha_{\mathbf{i}}) \cdot \dot{\mathbf{x}}_{\mathbf{i}}) + \frac{\mathbf{N}_{\mathbf{i}}}{2} \cdot (\gamma_{1\mathbf{i}} H_{1,h}^s + \gamma_{2\mathbf{i}} H_{2,h}^s) D_l^h \dot{\mathbf{x}}_{\mathbf{i}} \\ &\quad + A_0(\dot{\mathbf{x}}_{\mathbf{i}}) + A_0(\dot{F}_{\mathbf{i}}), \end{aligned} \tag{93}$$

where

$$\dot{F}_{\mathbf{i}} = \dot{\phi}_{\mathbf{i}} - \mathbf{w}(\alpha_{\mathbf{i}}) \cdot \dot{\mathbf{x}}_{\mathbf{i}}, \tag{94}$$

and

$$\begin{aligned}E_{local}(\alpha) &= \mathbf{w}(\alpha) - \mathbf{w}_0(\alpha)\\ &= \phi_{\alpha_1}\mathbf{x}^*_{\alpha_1} + \phi_{\alpha_1}\mathbf{x}^*_{\alpha_2} + (\mathbf{w}_0\cdot\mathbf{n})\mathbf{n}\\ &\quad -((\mathbf{w}_0\cdot\mathbf{x}_{\alpha_1})\mathbf{x}^*_{\alpha_1} + (\mathbf{w}_0\cdot\mathbf{x}_{\alpha_2})\mathbf{x}^*_{\alpha_2} + (\mathbf{w}_0\cdot\mathbf{n})\mathbf{n})\\ &= ((\phi_{\alpha_1} - \mathbf{w}_0\cdot\mathbf{x}_{\alpha_1})\mathbf{x}^*_{\alpha_1} + (\phi_{\alpha_2} - \mathbf{w}_0\cdot\mathbf{x}_{\alpha_2})\mathbf{x}^*_{\alpha_2}\\ &= \frac{\gamma_1}{2}\mathbf{x}^*_{\alpha_1} + \frac{\gamma_2}{2}\mathbf{x}^*_{\alpha_2}\,. \end{aligned}\tag{95}$$

It follows from (93) that $A_{-1}(\dot\gamma_{\mathbf{i}}) = A_0(\dot F_{\mathbf{i}}) + A_0(\dot{\mathbf{x}}_{\mathbf{i}})$. From the definition of E_{local}, we have

$$E_{local}\cdot\dot{\mathbf{x}}_{\mathbf{i}} \;=\; \frac{1}{2}\left(\gamma_{1\mathbf{i}}D^h_1\mathbf{x}^*_i + \gamma_{2\mathbf{i}}D^h_2\mathbf{x}^*_i\right)\cdot\dot{\mathbf{x}}_{\mathbf{i}}. \tag{96}$$

Substituting (93) into (89) and using (96), we obtain after some cancellations that

$$\begin{aligned}\dot E^{\mathbf{n}}_{pvm}(\mathbf{i}) + \dot E^{\mathbf{n}}_{near}(\mathbf{i}) &= \dot{\mathbf{n}}\cdot\mathbf{w}^h_0 + |D^h_1\mathbf{x}_{\mathbf{i}}\times D^h_2\mathbf{x}_{\mathbf{i}}|(H^s_{1,h}D^h_1 + H^s_{2,h}D^h_2)\dot F_{\mathbf{i}}\\ &+ \frac{|\mathbf{N}_i|^2}{2}\mathbf{n}_{\mathbf{i}}\cdot(\gamma_{1\mathbf{i}}H^s_{1,h} + \gamma_{2\mathbf{i}}H^s_{2,h})(H^s_{1,h}D^h_1 + H^s_{2,h}D^h_2)\dot{\mathbf{x}}_{\mathbf{i}}\\ &+ A_0(\dot{\mathbf{x}}_{\mathbf{i}}) + A_0(\dot F_{\mathbf{i}}).\end{aligned}\tag{97}$$

Furthermore, direct calculations show that

$$\begin{aligned}\dot E_{local}(\mathbf{i})\cdot\mathbf{n}_{\mathbf{i}} &= \frac{\gamma_{1\mathbf{i}}}{2|\mathbf{N}_{\mathbf{i}}|^2}\left((D^h_2\mathbf{x}\times\mathbf{n})_{\mathbf{i}}\times D^h_2\mathbf{x}_{\mathbf{i}}\cdot D^h_1\dot{\mathbf{x}}_{\mathbf{i}} - (D^h_2\mathbf{x}\times\mathbf{n})_{\mathbf{i}}\times D^h_1\mathbf{x}_{\mathbf{i}}\cdot D^h_2\dot{\mathbf{x}}_{\mathbf{i}}\right)\\ &\quad+\frac{\gamma_{2\mathbf{i}}}{2|\mathbf{N}_{\mathbf{i}}|^2}\left((\mathbf{n}\times D^h_1\mathbf{x})_{\mathbf{i}}\times D^h_1\mathbf{x}_{\mathbf{i}}\cdot D^h_2\dot{\mathbf{x}}_{\mathbf{i}} - (\mathbf{n}\times D^h_1\mathbf{x})_{\mathbf{i}}\times D^h_2\mathbf{x}_{\mathbf{i}}\cdot D^h_1\dot{\mathbf{x}}_{\mathbf{i}}\right)\\ &= \frac{\gamma_{1\mathbf{i}}}{2|\mathbf{N}_{\mathbf{i}}|^2}\mathbf{n}_{\mathbf{i}}\cdot\left(|D^h_2\mathbf{x}_{\mathbf{i}}|^2D^h_1\dot{\mathbf{x}}_{\mathbf{i}} - (D^h_2\mathbf{x}_{\mathbf{i}}\cdot D^h_1\mathbf{x}_{\mathbf{i}})\cdot D^h_2\dot{\mathbf{x}}_{\mathbf{i}}\right)\\ &\quad+\frac{\gamma_{2\mathbf{i}}}{2\mathbf{N}_{\mathbf{i}}|^2}\mathbf{n}_{\mathbf{i}}\cdot\left(|D^h_1\mathbf{x}_{\mathbf{i}}|^2D^h_2\dot{\mathbf{x}}_{\mathbf{i}} - (D^h_1\mathbf{x}_{\mathbf{i}}\cdot D^h_2\mathbf{x}_{\mathbf{i}})D^h_1\dot{\mathbf{x}}_{\mathbf{i}}\right).\end{aligned}\tag{98}$$

Using (97), (98) and Lemma 4.2, we obtain after canceling the local terms that

$$\begin{aligned}\dot{\mathbf{w}}_{\mathbf{i}}\cdot\mathbf{n}_{\mathbf{i}} &= Er\left(D^h_1\phi_{\mathbf{i}}D^h_1\mathbf{x}^*_{\mathbf{i}} + D^h_2\phi_{\mathbf{i}}D^h_2\mathbf{x}^*_{\mathbf{i}} + (\mathbf{w}^h_0\cdot\mathbf{n}^h_{\mathbf{i}} - C^h_n + B^s_{\mathbf{n}} - B^h_{\mathbf{n}})\mathbf{n}_{\mathbf{i}}\right)\cdot\mathbf{n}_{\mathbf{i}}\\ &= Er(D^h_1\phi_{\mathbf{i}}D^h_1\mathbf{x}^*_{\mathbf{i}} + D^h_2\phi_{\mathbf{i}}D^h_2\mathbf{x}^*_{\mathbf{i}})\cdot\mathbf{n}_{\mathbf{i}} + \dot E^{\mathbf{n}}_{pvm}(\mathbf{i}) + \dot E^{\mathbf{n}}_{near}(\mathbf{i})\\ &= -(D^h_1\phi_{\mathbf{i}}D^h_1\mathbf{x}^*_{\mathbf{i}} + D^h_2\phi_{\mathbf{i}}D^h_2\mathbf{x}^*_{\mathbf{i}})\cdot\dot{\mathbf{n}}_{\mathbf{i}} + \dot E^{\mathbf{n}}_{pvm}(\mathbf{i}) + \dot E^{\mathbf{n}}_{near}(\mathbf{i})\\ &= -E_{local}\cdot\dot{\mathbf{n}}_{\mathbf{i}} - \left(\mathbf{w}^h_0\cdot D^h_1\mathbf{x}_{\mathbf{i}})D^h_1\mathbf{x}^*_{\mathbf{i}} + (\mathbf{w}^h_0\cdot D^h_2\mathbf{x}_{\mathbf{i}})D^h_2\mathbf{x}^*_{\mathbf{i}}\right)\cdot\dot{\mathbf{n}}_{\mathbf{i}} + \dot E^{\mathbf{n}}_{pvm}(\mathbf{i})\\ &\quad+\dot E^{\mathbf{n}}_{near}(\mathbf{i})\\ &= \dot E_{local}\cdot\mathbf{n}_{\mathbf{i}} - \mathbf{w}^h_0\cdot\dot{\mathbf{n}}_{\mathbf{i}} + \dot E^{\mathbf{n}}_{pvm}(\mathbf{i}) + \dot E^{\mathbf{n}}_{near}(\mathbf{i})\\ &= |D^h_1\mathbf{x}_{\mathbf{i}}\times D^h_2\mathbf{x}_{\mathbf{i}}|(H^s_{1,h}D^h_1 + H^s_{2,h}D^h_2)\dot F_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) + A_0(\dot F).\end{aligned}\tag{99}$$

Here $Er(f) = f(\alpha_{\mathbf{j}}) - f_{\mathbf{j}}$ as it was defined earlier. This completes our error estimate for the normal velocity component.

The error estimate for the tangential velocity component is much easier. Note that equation (57) implies

$$D^h_l\phi_{\mathbf{i}} = D^h_l\mathbf{x}_{\mathbf{i}}\cdot\mathbf{w}_{\mathbf{i}}.$$

Thus we have

$$D^h_l\dot\phi_{\mathbf{i}} = D^h_l\dot{\mathbf{x}}_{\mathbf{i}}\cdot\mathbf{w}_{\mathbf{i}} + D^h_l\mathbf{x}_{\mathbf{i}}\cdot\dot{\mathbf{w}}_{\mathbf{i}}, \tag{100}$$

which implies

$$\dot{\mathbf{w}}_{\mathbf{i}} \cdot D_l^h \mathbf{x}(\alpha_{\mathbf{i}}) = D_l^h(\dot{F}) + A_0(\dot{\mathbf{x}}_{\mathbf{i}}). \tag{101}$$

This completes the error estimate for the tangential velocity component.

Derivation of the error equations in the normal and tangent coordinates.

We are ready to perform energy estimates to obtain stability. As in the 2-D case [5], we need to first derive the error equations in the local normal and tangent coordinates. Let $\mathbf{t}^1$, $\mathbf{t}^2$, and $\mathbf{n}$ be the local unit tangent and normal vectors respectively. Denote by $\dot{x}^{\mathbf{t}^l} = \dot{\mathbf{x}} \cdot \mathbf{t}^l$ $(l = 1, 2)$, and $\dot{x}^{\mathbf{n}} = \dot{\mathbf{x}} \cdot \mathbf{n}$. After projecting the error equations into the local tangent and normal vectors, we obtain

$$\frac{\partial \dot{x}_{\mathbf{i}}^{\mathbf{t}^1}}{\partial t} = \frac{1}{|D_1^h \mathbf{x}_{\mathbf{i}}|} D_1^h \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) \tag{102}$$

$$\frac{\partial \dot{x}_{\mathbf{i}}^{\mathbf{t}^2}}{\partial t} = \frac{1}{|D_2^h \mathbf{x}_{\mathbf{i}}|} D_2^h \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) \tag{103}$$

$$\frac{\partial \dot{x}_{\mathbf{i}}^{\mathbf{n}}}{\partial t} = |D_1^h \mathbf{x}_{\mathbf{i}} \times D_2^h \mathbf{x}_{\mathbf{i}}| \left(H_{1,h}^s D_1^h + H_{2,h}^s D_2^h \right) \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) + A_0(\dot{F}), \tag{104}$$

where we have used (99)-(101).

we will need to express the evolution equation for $\dot{F}_i$ in the new variables. From the definition of $\dot{F}_i$ (see (94)), we have

$$(\dot{F}_{\mathbf{i}})_t = (\dot{\phi}_{\mathbf{i}})_t - \mathbf{w}(\alpha_{\mathbf{i}}) \cdot (\dot{\mathbf{x}}_{\mathbf{i}})_t - \mathbf{w}_t(\alpha_{\mathbf{i}}) \cdot \dot{\mathbf{x}}_{\mathbf{i}}. \tag{105}$$

To evaluate $(\dot{\phi}_{\mathbf{i}})_t$, we compare the continuous Bernoulli equation with its discrete approximation, i.e.

$$(\phi_{\mathbf{i}})_t = \frac{1}{2}|\mathbf{w}_{\mathbf{i}}|^2 - \mathbf{g} \cdot \mathbf{x}_{\mathbf{i}}, \tag{106}$$

$$(\phi(\alpha_{\mathbf{i}}))_t = \frac{1}{2}|\mathbf{w}(\alpha_{\mathbf{i}})|^2 - \mathbf{g} \cdot \mathbf{x}(\alpha_{\mathbf{i}}). \tag{107}$$

Subtracting (107) from (106), we obtain

$$(\dot{\phi}_{\mathbf{i}})_t = \dot{\mathbf{w}}_{\mathbf{i}} \cdot \mathbf{w}(\alpha_{\mathbf{i}}) - \mathbf{g} \cdot \dot{\mathbf{x}}_{\mathbf{i}} + \frac{1}{2}|\dot{\mathbf{w}}_{\mathbf{i}}|^2. \tag{108}$$

Substituting (108) into (105), we have after some cancellations

$$(\dot{F}_{\mathbf{i}})_t = -(\mathbf{w}_t(\alpha_{\mathbf{i}}) + \mathbf{g}) \cdot \dot{\mathbf{x}}_{\mathbf{i}} + \frac{1}{2}|\dot{\mathbf{w}}_{\mathbf{i}}|^2. \tag{109}$$

Noting that the Lagrangian velocity $\mathbf{w}$ satisfies the Euler equations in the fluid domain in the form

$$\mathbf{w}_t = -\nabla p - \mathbf{g}.$$

Thus we have

$$(\dot{F}_{\mathbf{i}})_t = \nabla p \cdot \dot{\mathbf{x}}_{\mathbf{i}} + \frac{1}{2}|\dot{\mathbf{w}}_{\mathbf{i}}|^2. \tag{110}$$

Moreover, $p = 0$ on the interface so that ∇p is in the normal direction. We have

$$\nabla p \cdot \dot{\mathbf{x}}_{\mathbf{i}} = -c(\alpha_{\mathbf{i}}) \dot{\mathbf{x}}_{\mathbf{i}}^{\mathbf{n}}, \tag{111}$$

where $c(\alpha) = -\nabla p \cdot \mathbf{n} = (\mathbf{w}_t + \mathbf{g}) \cdot \mathbf{n}$. Hence the evolution equation for $\dot{F}$ becomes

$$(\dot{F}_{\mathbf{i}})_t = -c(\alpha_{\mathbf{i}}) \dot{\mathbf{x}}_{\mathbf{i}}^{\mathbf{n}} + \frac{1}{2}|\dot{\mathbf{w}}_{\mathbf{i}}|^2. \tag{112}$$

Now the whole set of evolution equations for $\dot{x}^{\mathbf{t}^l}$ $(l = 1, 2)$, $\dot{x}^{\mathbf{n}}$, and $\dot{F}$ is given by

$$\frac{\partial \dot{x}_{\mathbf{i}}^{\mathbf{t}^1}}{\partial t} = \frac{1}{|D_1^h \mathbf{x_i}|} D_1^h \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) \tag{113}$$

$$\frac{\partial \dot{x}_{\mathbf{i}}^{\mathbf{t}^2}}{\partial t} = \frac{1}{|D_2^h \mathbf{x_i}|} D_2^h \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) \tag{114}$$

$$\frac{\partial \dot{x}_{\mathbf{i}}^{\mathbf{n}}}{\partial t} = |D_1^h \mathbf{x_i} \times D_2^h \mathbf{x_i}| \left(H_{1,h}^s D_1^h + H_{2,h}^s D_2^h \right) \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) + A_0(\dot{F}) \tag{115}$$

$$(\dot{F}_{\mathbf{i}})_t = -c(\alpha_{\mathbf{i}}) \dot{x}_{\mathbf{i}}^{\mathbf{n}} + \frac{1}{2} |\dot{\mathbf{w}}_{\mathbf{i}}|^2. \tag{116}$$

Thus, we have reduced the error estimates for the full nonlinear, nonlocal water wave equations into a simple linear and almost local system for the variation quantities. The only nonlocality in the leading order terms comes from the discrete Riesz transform $H_{l,h}^s (l = 1, 2)$. The lower order terms are nonlocal, but they are smoother than the principal linearized terms. This simplification helps us identify and balance the most important terms in our energy estimates.

The energy estimates (113)-(116) can be obtained directly. As in the two dimensional case, the normal variation plays an essential role. The tangential variations only contribute to the lower order terms. To see this, we make the following change of variables for the tangential variations $\dot{x}_{\mathbf{i}}^{\mathbf{t}^1}$ and $\dot{x}_{\mathbf{i}}^{\mathbf{t}^2}$:

$$\dot{\delta}_{\mathbf{i}}^1 = \dot{x}_{\mathbf{i}}^{\mathbf{t}^1} + \frac{|D_1^h \mathbf{x_i} \times D_2^h \mathbf{x_i}|}{|D_1^h \mathbf{x_i}|} \left[|D_1^h \mathbf{x_i}|^2 H_{1,h}^s + (D_1^h \mathbf{x_i} \cdot D_2^h \mathbf{x_i}) H_{2,h}^s \right] \dot{x}_{\mathbf{i}}^{\mathbf{n}} \tag{117}$$

$$\dot{\delta}_{\mathbf{i}}^2 = \dot{x}_{\mathbf{i}}^{\mathbf{t}^2} + \frac{|D_1^h \mathbf{x_i} \times D_2^h \mathbf{x_i}|}{|D_2^h \mathbf{x_i}|} \left[|D_2^h \mathbf{x_i}|^2 H_{2,h}^s + (D_1^h \mathbf{x_i} \cdot D_2^h \mathbf{x_i}) H_{1,h}^s \right] \dot{x}_{\mathbf{i}}^{\mathbf{n}}. \tag{118}$$

Using Lemma 4.2 and the identity (74), we have

$$\Lambda(|\mathbf{x}_{\alpha_1}|^2 H_1 + (\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2}) H_2)(f) = -\frac{1}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_1}|^2} D_1 f + A_0(f) \tag{119}$$

$$\Lambda(|\mathbf{x}_{\alpha_2}|^2 H_2 + (\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2}) H_1)(f) = -\frac{1}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_1}|^2} D_2 f + A_0(f). \tag{120}$$

It follows from (119) and (120) that the leading order terms in $d\dot{\delta}_{\mathbf{i}}^l/dt$ cancel each other. We get

$$\frac{d\dot{\delta}_{\mathbf{i}}^1}{dt} = A_0(\dot{\mathbf{x}}) + A_0(\dot{F}), \tag{121}$$

$$\frac{d\dot{\delta}_{\mathbf{i}}^2}{dt} = A_0(\dot{\mathbf{x}}) + A_0(\dot{F}). \tag{122}$$

As a result, the error equations simplify further to the leading order,

$$\frac{d\dot{\delta}_{\mathbf{i}}^1}{dt} = A_0(\dot{\mathbf{x}}) + A_0(\dot{F}), \tag{123}$$

$$\frac{d\dot{\delta}_{\mathbf{i}}^2}{dt} = A_0(\dot{\mathbf{x}}) + A_0(\dot{F}), \tag{124}$$

$$\frac{\partial \dot{\mathbf{x}}_{\mathbf{i}}^{\mathbf{n}}}{\partial t} = |D_1^h \mathbf{x_i} \times D_2^h \mathbf{x_i}| \Lambda_h^s \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) + A_0(\dot{F}) \tag{125}$$

$$(\dot{F}_{\mathbf{i}})_t = -c(\alpha_{\mathbf{i}}) \dot{\mathbf{x}}_{\mathbf{i}}^{\mathbf{n}} + \frac{1}{2} |\dot{\mathbf{w}}_{\mathbf{i}}|^2, \tag{126}$$

where $\Lambda_h^s = H_{1,h}^s D_1^h + H_{2,h}^s D_2^h$.

Energy estimates and convergence analysis

In the above estimates, we only study the linear stability of the modified point vortex approximation. To obtain convergence, we also need to obtain nonlinear stability. To this end, we use Strang's technique [24], which can be summarized as follows. In proving convergence, there are two steps, consistency and stability. In the consistency step, we usually use the exact solution of the continuum water wave equations to construct "exact particles" $\mathbf{x}(\alpha_{\mathbf{i}}, t)$ and vortex sheet strengths $\gamma_l(\alpha_{\mathbf{i}}, t)$. Denote by $R(t)$ (the consistency error) the amount by which these exact particles fail to satisfy the modified point vortex equations. In our case, we have $R(t) = O(h^3)$. Strang's idea is not to use the exact particles, but to construct "smooth particles" ($\tilde{\mathbf{x}}(\alpha_{\mathbf{i}}, t) = \mathbf{x}(\alpha_{\mathbf{i}}, t) + h^3 \mathbf{x}_3(\alpha_{\mathbf{i}}, t)$, $\tilde{\gamma}_l(\alpha_{\mathbf{i}}, t) = \gamma_l(\alpha_{\mathbf{i}}, t) + h^3 \gamma_{l3}(\alpha_{\mathbf{i}}, t)$ for some smooth $\mathbf{x}_3$ and γ_{l3}) that are $O(h^3)$ perturbations of the exact particles, which satisfy the discrete equations more accurately: $R(t) = O(h^r)$ for $r \geq 5$ as long as the continuous solution is sufficiently smooth. Existence of such smooth particles is guaranteed by the existence of the error expansion we obtained for the consistency error in section 5. The perturbed solution, $\mathbf{x}_3$ and γ_{l3}, basically satisfies the linearized water wave equations with coefficients depending the exact solution of the water wave equations. Then, in the stability step, we bound $e(t)$, the difference between the smooth particles and the particles computed by the modified point vortex method. As observed by Strang in [24], if the numerical method is linearly stable, nonlinear stability can be obtained by using the smallness of the error $e(t)$. This greatly simplifies the nonlinear stability analysis.

To illustrate, we define

$$T^* = \sup\{t \mid t \leq T,\ \|\dot{\mathbf{x}}\|_{l^2} \leq h^3,\ \|\dot{\gamma}\|_{l^2} \leq h^2\}.$$

Here the errors $\dot{\mathbf{x}}$ and $\dot{\gamma}$ are with respect to the "smooth" particles $\tilde{\mathbf{x}}(\alpha, t)$ and the smooth vortex vortex strengths $\tilde{\gamma}(\alpha, t)$ [24, 4, 8]. Since $h^2 |\dot{\mathbf{x}}_{\mathbf{i}}|^2 \leq \|\dot{\mathbf{x}}\|_{l^2}^2$, we conclude that

$$\|\dot{\mathbf{x}}\|_\infty \leq \frac{1}{h} \|\dot{\mathbf{x}}\|_{l^2} \leq h^2, \quad \text{for } t \leq T^* . \tag{127}$$

Similarly we have

$$\|\dot{\gamma}\|_\infty \leq h, \quad \text{for } t \leq T^*,$$

and

$$\|D_l^h \dot{\mathbf{x}}\|_\infty \leq \frac{1}{h} \|D_l^h \dot{\mathbf{x}}\|_{l^2} \leq \frac{2\pi}{h^2} \|\dot{\mathbf{x}}\|_{l^2} \leq 2\pi h, \quad l = 1, 2, \quad \text{for } t \leq T^*.$$

A typical nonlinear term has the following form:

$$E_{\mathbf{i}}^{NL} = \sum_{\mathbf{j} \neq \mathbf{i}} \frac{\dot{\gamma}_{l\mathbf{j}} |\dot{\mathbf{x}}_{\mathbf{i}} - \dot{\mathbf{x}}_{\mathbf{j}}|^2}{|(\mathbf{x}(\alpha_{\mathbf{i}}) - \mathbf{x}(\alpha_{\mathbf{j}})) + (\dot{\mathbf{x}}_{\mathbf{i}} - \dot{\mathbf{x}}_{\mathbf{j}})|^3} h^2.$$

We assume that the exact water wave solution is smooth and non-self-intersecting. Thus we have

$$|\mathbf{x}(\alpha_{\mathbf{i}}) - \mathbf{x}(\alpha_{\mathbf{j}})| \geq c|\alpha_{\mathbf{i}} - \alpha_{\mathbf{j}}| \geq ch, \quad \text{for } \mathbf{j} \neq \mathbf{i}.$$

Therefore, for h small and $t \leq T^*$, we have from (127) that

$$|\mathbf{x}(\alpha_{\mathbf{i}}) - \mathbf{x}(\alpha_{\mathbf{j}})) + (\dot{\mathbf{x}}_{\mathbf{i}} - \dot{\mathbf{x}}_{\mathbf{j}})| \geq c|\alpha_{\mathbf{i}} - \alpha_{\mathbf{j}}| - 2h^2 \geq \frac{c}{2} |\alpha_{\mathbf{i}} - \alpha_{\mathbf{j}}|.$$

Thus, for $t \le T^*$, we get

$$\|E^{NL}\|_{l^2} \le \|\dot{\gamma}\|_\infty \|\dot{\mathbf{x}}\|_{l^2} \max_{\mathbf{i}} \sum_{\mathbf{j}\ne\mathbf{i}} \frac{Ch^2}{|\alpha_{\mathbf{i}} - \alpha_{\mathbf{j}}|^3} \le \frac{C}{h} \|\dot{\gamma}\|_\infty \|\dot{\mathbf{x}}\|_{l^2} \le C\|\dot{\mathbf{x}}\|_{l^2}, \tag{128}$$

where we have used Young's inequality. This shows that $E^{NL} = A_0(\dot{\mathbf{x}})$. Other nonlinear terms can be treated similarly.

Combining the consistency and stability steps, we obtain the following new error equations,

$$\frac{d\dot{\delta}^1_{\mathbf{i}}}{dt} = A_0(\dot{\mathbf{x}}) + A_0(\dot{F}) + O(h^r), \tag{129}$$

$$\frac{d\dot{\delta}^2_{\mathbf{i}}}{dt} = A_0(\dot{\mathbf{x}}) + A_0(\dot{F}) + O(h^r), \tag{130}$$

$$\frac{\partial \dot{\mathbf{x}}^{\mathbf{n}}_{\mathbf{i}}}{\partial t} = |D^h_1 \mathbf{x}_{\mathbf{i}} \times D^h_2 \mathbf{x}_{\mathbf{i}}| \Lambda^s_h \dot{F}_{\mathbf{i}} + A_0(\dot{\mathbf{x}}) + A_0(\dot{F}) + O(h^r), \tag{131}$$

$$\frac{d\dot{F}_{\mathbf{i}}}{dt} = -c(\alpha_{\mathbf{i}})\dot{\mathbf{x}}^{\mathbf{n}}_{\mathbf{i}} + \frac{1}{2}|\dot{\mathbf{w}}_{\mathbf{i}}|^2, \tag{132}$$

where we still use the same notation, $\dot{\mathbf{x}}$, to denote the error between the particles computed by the modified point vortex method and the smooth particles $\tilde{\mathbf{x}}$, and $r \ge 5$ by construction.

To perform energy estimate, we first define a discrete $H^{1/2}$ norm. From (78), we have

$$(\Lambda f)(\alpha) = \int g^2(\xi, \alpha) \hat{f}(\xi) e^{i\xi\cdot\alpha} d\xi, \tag{133}$$

where $g(\xi, \alpha)$ is defined as

$$g(\xi, \alpha) = \frac{1}{|\mathbf{x}_{\alpha_1} \times \mathbf{x}_{\alpha_2}|} (|\mathbf{x}_{\alpha_2}|^2 \xi_1^2 - 2(\mathbf{x}_{\alpha_1} \cdot \mathbf{x}_{\alpha_2})\xi_1\xi_2 + |\mathbf{x}_{\alpha_1}|^2 \xi_2^2)^{1/4} \tag{134}$$

Introduce a function $\psi(\alpha)$ defined as follows

$$\psi(\alpha) = \int g(\xi, \alpha) \widehat{f(\xi)} e^{i\xi\cdot\alpha} d\xi.$$

We can show that if f is a real function, so is ψ. To see this, we compute the complex conjugate of ψ. We have

$$\overline{\psi(\alpha)} = \int g(\xi, \alpha) \overline{\widehat{f(\xi)}} e^{-i\xi\cdot\alpha} d\xi = \int g(\xi, \alpha) \widehat{f(-\xi)} e^{-i\xi\cdot\alpha} d\xi \tag{135}$$

$$= \int g(-\xi, \alpha) \widehat{f(\xi)} e^{i\xi\cdot\alpha} d\xi = \psi(\alpha), \tag{136}$$

where we have used the fact that g is an even function of ξ and $\overline{\widehat{f(\xi)}} = \widehat{f(-\xi)}$ since f is real.

By using the same argument as in the proof of Lemma 3.2 in [18], we can show that the Λ operator satisfies the following estimate:

$$(\Lambda f, f) - (\psi, \psi) = (A_0(f), f), \tag{137}$$

where (f, g) is the usual inner product in L^2, and A_0 is a bounded operator in L^2. Furthermore, we assume that $|(A_0(f), f)| \le c_0 \|f\|_{L^2}$. Define a generalized $H^{1/2}$ norm as follows:

$$\|f\|^2_{H^{1/2}} = ((\Lambda + dI)f, f),$$

where $d = c_0 + 1$. It follows from (137) that

$$\begin{aligned}((\Lambda + dI)f, f) &= (\Lambda f, f) + d(f, f)\\ &= (\psi, \psi) + (A_0(f), f) + d(f, f)\\ &\geq (\psi, \psi) + (f, f)\\ &\geq 0.\end{aligned}$$

Recall that $\psi(\alpha) = \int g(\xi, \alpha)\hat{f}(\xi)e^{i\xi\cdot\alpha}d\xi$, and $|g(\xi, \alpha)| \leq c|\xi|^{1/2}$. Thus we also have

$$((\Lambda + dI)f, f) \leq C\|f\|^2_{H^{1/2}}.$$

Since Λ_h^s is a spectral approximation of Λ, we can introduce a discrete $H^{1/2}$ norm as follows:

$$\|f\|_{H_h^{1/2}} = ((\Lambda_h^s + dI)f, f)_h^{1/2}, \tag{138}$$

where $(\cdot, \cdot)_h$ is the inner product associated with the discrete l^2 norm. Then the above derivation for the continuous case can be carried out in the same way for the discrete norm.

By assumption of the theorem, the problem is well-posed. It has been shown by Wu [26] that the coefficient $c(\alpha)$ in (126) is positive

$$c(\alpha) \geq c_0 > 0.$$

To obtain our energy estimate, we multiply (129) by $\dot{\delta}^1_{\mathbf{i}}$, (130) by $\dot{\delta}^2_{\mathbf{i}}$, (131) by $\frac{c(\alpha_{\mathbf{i}})}{|D_1^h\mathbf{x_i} \times D_2^h\mathbf{x_i}|}\dot{\mathbf{x}}^{\mathbf{n}}$, (132) by $(\Lambda_h^s + dI)\dot{F}_{\mathbf{i}}$, we then add and sum in $\mathbf{i}$. Let

$$y_0^2(t) = \|\left(\frac{c(\alpha_{\mathbf{i}})}{|D_1^h\mathbf{x_i} \times D_2^h\mathbf{x_i}|}\right)^{1/2}\dot{\mathbf{x}}^{\mathbf{n}}(t)\|^2_{l^2} + \|\dot{\delta}^1(t)\|^2_{l^2} + \|\dot{\delta}^2(t)\|^2_{l^2} + \|\dot{F}(t)\|^2_{H_h^{1/2}},$$

where

$$\|\dot{F}(t)\|^2_{H_h^{1/2}} = ((\Lambda_h^s + dI)\dot{F}(t), \dot{F}(t))_h.$$

We obtain

$$\begin{aligned}\frac{1}{2}\frac{dy_0^2}{dt} &= (\Lambda_h^s\dot{F}, c\dot{\mathbf{x}}^{\mathbf{n}})_h - (c\dot{\mathbf{x}}^{\mathbf{n}}, (\Lambda_h^s + dI)\dot{F})_h\\ &+ (f_1, \dot{\delta}^1)_h + (f_2, \dot{\delta}^2)_h + (f_3, \dot{\mathbf{x}}^{\mathbf{n}})_h + (f_4, (\Lambda_h^s + dI)\dot{F})_h,\end{aligned} \tag{139}$$

where

$$\|f_j\|_{l^2} \leq C(\|\dot{\mathbf{x}}^{\mathbf{n}}\|_{l^2} + \|\dot{\delta}^1\|_{l^2} + \|\dot{\delta}^2\|_{l^2} + \|\dot{F}\|_{l^2} + h^r), \quad j = 1, 2, 3,$$

and $f_4 = \frac{1}{2}|\dot{\mathbf{w}}_{\mathbf{i}}|^2$.

Note that $\dot{\mathbf{w}}_{\mathbf{i}} = \frac{d\dot{\mathbf{x}}_{\mathbf{i}}}{dt}$. Using the estimate on $\frac{d\dot{\mathbf{x}}_{\mathbf{i}}}{dt}$ and the fact that $\|\dot{\mathbf{x}}\|_\infty \leq h^2$ and $\|\dot{\gamma}\|_\infty \leq h$ for $t \leq T^*$, we can show that $\|\dot{\mathbf{w}}\|_\infty \leq c\, h|\log(h)|$. Therefore, we obtain

$$\begin{aligned}|(\quad &(\Lambda_h^s + dI)\dot{F}, |\dot{\mathbf{w}}_{\mathbf{i}}|^2)_h| \leq \|(\Lambda_h^s + dI)\dot{F}\|_{l^2}\|\, |\dot{\mathbf{w}}|^2\|_{l^2}\\ \leq \quad &c\, h\,|\log(h)|\, \|(\Lambda_h^s + dI)\dot{F}\|_{l^2}\left(\|(\Lambda_h^s + dI)\dot{F}\|_{l^2} + \|\dot{F}\|_{l^2} + \|\dot{\mathbf{x}}\|_{l^2} + h^r\right).\end{aligned}$$

It follows from the spectral property of Λ_h^s that

$$\|(\Lambda_h^s + dI)\dot{F}\|_{l^2} \leq Ch^{-1/2}\|\dot{F}\|_{H_h^{1/2}}.$$

As a consequence, we get

$$|((\Lambda_h^s + dI)\dot{F}, |\dot{\mathbf{w}}_{\mathbf{i}}|^2)_h| \le C\|\dot{F}\|_{H^{1/2}}(y_0(t) + ch^r).$$

Now we are ready to complete the convergence analysis. Note that the two leading order terms in the righthand side of (139) containing the Λ_h^s operator cancels each other and the entire right-hand side is bounded by $y_0(t)(y_0(t) + Ch^r)$. Hence we obtain

$$\frac{dy_0^2}{dt} \le C_0\, y_0(t)(y_0(t) + h^r),$$

for some constant C_0. The Gronwall inequality then implies

$$y_0(t) \le C(T)h^r, \quad t \le T^*. \tag{140}$$

In terms of the original variables, we have

$$\|\dot{\mathbf{x}}\|_{l^2} \le B(T)h^r, \quad \|\dot{\gamma}\|_{l^2} \le B(T)h^{r-1}, \quad t \le T^*, \tag{141}$$

where we have used (93) for $\dot{\gamma}$. Since $r \ge 5$, for h small enough, we get

$$\|\dot{\mathbf{x}}\|_{l^2} \le B(T)h^5 < \frac{1}{2}h^3, \quad \|\dot{\gamma}\|_{l^2} \le B(T)h^4 < \frac{1}{2}h^2.$$

It follows from the definition of T^* that

$$T^* = T.$$

This implies that estimate (141) is valid for the entire time interval $0 \le t \le T$. Since the smooth particles and the smooth vortex sheet strengths are order $O(h^3)$ perturbations from the exact particles and vortex sheet strengths, i.e. $\tilde{\mathbf{x}}(\alpha, t) = \mathbf{x}(\alpha, t) + O(h^3)$ and $\tilde{\gamma}_l(\alpha, t) = \gamma_l(\alpha, t) + O(h^3)$ $(l = 1, 2)$ by construction, we conclude that

$$\|\mathbf{x}(t) - \mathbf{x}(\cdot, t)\|_{l^2} \le Ch^3, \quad 0 \le t \le T, \tag{142}$$

$$\|\gamma_l(t) - \gamma_l(\cdot, t)\|_{l^2} \le Ch^3, \quad 0 \le t \le T. \tag{143}$$

This completes the convergence proof of the modified point vortex method for 3-D water waves.

Appendix A. Proof of Lemma 7.1

Proof of Lemma 7.1: The invertibility of of $I + 2A_h$ will follow from that of the operator $I + 2A$ of which it is an approximation, where A is the two by two matrix operator acting on periodic functions of α. We have discussed the invertibility of $I + 2A$, and now we treat A_h as a perturbation of A.

We would like to extend the discrete operator $P_{rs}^h K_l^h(\gamma_k)_{\mathbf{j}}, r, s, , k = 1, 2, l = 1, 2, 3, 4$ to a continuous operator in such a way that the L^2 norm of the extended continuous operator is the same as the discrete l^2 norm of the discrete operator and that the extended operator P_{rs}^h is a bounded operator. We do this in two steps. In the first step, we extend $f_{\mathbf{j}} = K_l^h(\gamma_k)_{\mathbf{j}}$ as a piecewise constant function in L^2 using the same method as in Lemma 6.1 of [4].

In the second step, we will extend $P_{rs}^h f(\alpha)$ for periodic function f defined in $[-\pi, \pi)^2$. Keep in mind that we need to define our extension in such a way that the L^2 norm of the extended operator should be the same as the discrete l^2 norm of the original discrete operator. Let $B_{\mathbf{j}} = \{\alpha \in [-\pi, \pi)^2 : 0 \le \alpha_l - (\alpha_{\mathbf{j}})_l < h, l = 1, 2\}$

for $\mathbf{j} \in I$, where I is the two-dimensional integer set. Define the average of f over $B_\mathbf{j}$ as follows:

$$\bar{f}_\mathbf{j} = \frac{1}{|B_\mathbf{j}|} \int_{B_\mathbf{j}} f(x)dx.$$

Since $f(\alpha)$ is a piecewise constant function on $B_\mathbf{j}$ from our step 1, we have

$$\bar{f}_\mathbf{j} = f_\mathbf{j}.$$

Let I_N be a two-dimensional integer set defined by

$$I_N = \{(j_1, j_2), \ | - N/2 + 1 \le j_1 \le N/2, \ -N/2 + 1 \le j_2 \le N/2\}.$$

Using the discrete Fourier transform, we have

$$\widehat{\bar{f}}(\mathbf{k}) = h^2 \sum_{\mathbf{j} \in I_N} \bar{f}_\mathbf{j} e^{i\mathbf{k}\cdot\alpha_\mathbf{j}},$$

and

$$\hat{f}(\mathbf{k}) = h^2 \sum_{\mathbf{k} \in I_N} f_\mathbf{j} e^{i\mathbf{k}\cdot\alpha_\mathbf{j}}.$$

Since $\bar{f}_\mathbf{j} = f_\mathbf{j}$, we have $\widehat{\bar{f}}(\mathbf{k}) = \hat{f}(\mathbf{k})$. Now we define the extension of P_{12}^h as follows:

$$P_{12}^h f(\alpha) = \sum_{\mathbf{k} \in I_N} \frac{k_1 k_2}{|\mathbf{k}|^2} \widehat{\bar{f}}(\mathbf{k}) e^{i\mathbf{k}\cdot\alpha}.$$

We claim that

$$\|P_{12}^h f(\alpha)\|_{L^2} = \|P_{12}^h f(\alpha_\mathbf{j})\|_{l^2}, \tag{144}$$

for any piecewise constant function $f(\alpha)$.

Proof of (144): Using Parseval equality and the fact $\widehat{\bar{f}}(\mathbf{k}) = \hat{f}(\mathbf{k})$, we have

$$\begin{aligned}
\|P_{12}^h f(\alpha)\|_{L^2}^2 &= \|\sum_{\mathbf{k} \in I_N} \frac{k_1 k_2}{|\mathbf{k}|^2} \widehat{\bar{f}}(\mathbf{k}) e^{i\mathbf{k}\cdot\alpha}\|_{L^2}^2 \\
&= \sum_{\mathbf{k} \in I_N} |\frac{k_1 k_2}{|\mathbf{k}|^2} \widehat{\bar{f}}(\mathbf{k})|^2 \\
&= \sum_{\mathbf{k} \in I_N} |\frac{k_1 k_2}{|k|^2} \hat{f}(\mathbf{k})|^2.
\end{aligned}$$

On the other hand, using the discrete Parseval equality, we get

$$\begin{aligned}
\|P_{12}^h f(\alpha_\mathbf{j})\|_{l^2}^2 &= \|\sum_{\mathbf{k} \in I_N} \frac{k_1 k_2}{|\mathbf{k}|^2} \hat{f}(\mathbf{k}) e^{i\mathbf{k}\cdot\alpha_\mathbf{j}}\|_{l^2} \\
&= \sum_{\mathbf{k} \in I_N} |\frac{k_1 k_2}{|\mathbf{k}|^2} \hat{f}(\mathbf{k})|^2.
\end{aligned}$$

Thus we have

$$\|P_{12}^h \bar{K}_l^h(\gamma_k)(\alpha)\|_{L^2} = \|P_{12}^h \bar{K}_l^h(\gamma_k)_\mathbf{j}\|_{l^2}, \qquad l = 1, 2, 3, 4.$$

Similar result applies to other P_{rs}^h operators, $r, s = 1, 2$.

Next we will prove

$$\|P_{rs}^h f(\alpha)\|_{L^2} \le \|f\|_{L^2}, \tag{145}$$

for any L^2 function $f(\alpha)$.

Proof of (145): From the definition of the extension operator and using the Parseval equality, we get

$$\begin{aligned}\|P_{12}^h f(\alpha)\|_{L^2}^2 &= \|\sum_{\mathbf{k}\in I_N} \frac{k_1k_2}{|\mathbf{k}|^2}\widehat{\bar{f}}(\mathbf{k})e^{i\mathbf{k}\cdot\alpha}\|_{L^2} = \sum_{\mathbf{k}\in I_N} |\frac{k_1k_2}{|\mathbf{k}|^2}\widehat{\bar{f}}(\mathbf{k})|^2 \\ &\le \sum_{\mathbf{k}\in I_N} |\widehat{\bar{f}}(\mathbf{k})|^2 = h^2\sum_{\mathbf{k}\in I_N} |\bar{f}_{\mathbf{j}}|^2 \le \sum_{\mathbf{j}\in I_N}\int_{B_{\mathbf{j}}} |f(\alpha)|^2 d\alpha = \|f\|_{L^2}^2.\end{aligned}$$

Using (144)-(145), and arguing as in the proof of Lemma 6.1 in [4], we can show that

$$\|A - A_h\|_{L_h^2} = O(h|\log h|).$$

Finally, it follows from Theorem 1.37 in [7] that $(\frac{1}{2}I + A^h + O(h))^{-1}$ exists and is bounded since the unperturbed operator $(\frac{1}{2}I + A)^{-1}$ exists and is bounded.

Appendix B. Proof of $K_l^h(\dot{\phi}) = A_{-1}(\dot{\phi})$ $(l = 1, 2, 3, 4)$

Proof of $K_l^h(\dot{\phi}) = A_{-1}(\dot{\phi})$ $(l = 1, 2, 3, 4)$.

Similar to the regularized Green's function G_h in [4], we define

$$G_h(\mathbf{x}) = -(4\pi r)^{-1}s(r/h), \qquad r = |\mathbf{x}|,$$

with s chosen so that $s(r)$ is smooth and

$$s(r) = \begin{cases} 0, & r < c/2, \\ 1, & r > 3c/4, \end{cases}$$

where the constant c is chosen such that $|\mathbf{x}(\alpha,t) - x(\alpha',t)| \ge c|\alpha - \alpha'|$. Therefore, G_h is smooth, for $h > 0$ and we have $G_h(\mathbf{x}) = h^{-1}G_1(\mathbf{x}/h)$. Letting $\psi = \Delta G_1$, we find

$$\psi(\mathbf{x}) = \Delta G_1(\mathbf{x}) = -(4\pi r)^{-1}s''(r), \qquad r = |\mathbf{x}|,$$

and correspondingly

$$\Delta G_h(\mathbf{x}) = \psi_h(\mathbf{x}) = h^{-3}\psi(|\mathbf{x}|/h),$$

which approximates the Dirac delta function as $h \longrightarrow 0$.

Since $\bigtriangledown_{\mathbf{x}} G_h(\mathbf{0}) = \mathbf{0}$ by the definition of G_h, we can rewrite K_1^h as follows:

$$\begin{aligned} K_1^h(\dot{\phi}) &= \sum_{\mathbf{j}\ne\mathbf{i}} D_1^h\mathbf{x}_{\mathbf{i}} \times D_2^h\mathbf{x}_{\mathbf{j}} \cdot \bigtriangledown_{\mathbf{x}'} G(\mathbf{x}_{\mathbf{i}} - \mathbf{x}_{\mathbf{j}})\dot{\phi}_{\mathbf{j}}h^2 \\ &= \sum_{\mathbf{j}} D_1^h\mathbf{x}_{\mathbf{i}} \times D_2^h\mathbf{x}_{\mathbf{j}} \cdot \bigtriangledown_{\mathbf{x}'} G_h(\mathbf{x}_{\mathbf{i}} - \mathbf{x}_{\mathbf{j}})\dot{\phi}_{\mathbf{j}}h^2 \\ &\equiv \sum_{\mathbf{j}} K_h(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}})\dot{\phi}_{\mathbf{j}}h^2. \end{aligned}$$

The following proof is similar to the proof of Theorem 5.1 in [4]. We first split the regularized Green's function into a far-field part and local part, in order to focus attention on the latter. We wish to restrict the local analysis to a small neighborhood of the singularity in which the coordinate mapping is well approximated by its linearization. Let $J(\alpha)$ be the Jacobian matrix $\frac{\partial \mathbf{x}}{\partial \alpha}$ at α. It can be shown that there is some δ_0 small enough with $\delta_0 < \pi/2$ so that for all α and α' satisfying $|\alpha - \alpha'| \le \delta_0$ we have

$$|J(\alpha)(\alpha - \alpha')|/2 \le |\mathbf{x}(\alpha) - \mathbf{x}(\alpha')| \le 2|J(\alpha)(\alpha - \alpha')|.$$

It follows from the above inequalities and the fact that the Jacobian matrix $J(\alpha)$ is nonsingular that there exists $r_0 > 0$ with $r_0 < \pi/2$ so that $|\mathbf{x}(\alpha) - \mathbf{x}(\alpha')| \le r_0$ implies $|\alpha - \alpha'| \le \delta_0$. We can also assume that $|J(\alpha)(\alpha - \alpha')| \le \delta_0$ implies $|\alpha - \alpha'| \le \delta_0$. We now choose a cut-off function ζ so that $\zeta(\mathbf{x}) = 1$ for $\mathbf{x}$ near 0 and $\zeta(\mathbf{x}) = 0$ for $|\mathbf{x}| > r_0$. We write the regularized Kernel function as $K_h = \zeta K_h + (1-\zeta)K_h$. The far-field part $K_h^\infty = (1-\zeta)K_h$ is smooth. Consequently a discrete integral operator with kernel $D^m K_h^\infty(\mathbf{x_i}, \mathbf{x_j})$ is l^2-bounded, uniformly in h, where D^m is a derivative operator of any order m. The local term K_h when evaluated on the surface is

$$K_h(\mathbf{x}(\alpha), \mathbf{x}(\alpha'))\zeta(\mathbf{x}(\alpha) - \mathbf{x}(\alpha'))$$

for $|\alpha - \alpha'| \le \pi$; the remaining terms in the sum (those corresponding to $|\alpha - \alpha'| > \pi$) are zero because the small support of ζ. Thus the boundedness properties of a discrete operator with $D^m K_h(\mathbf{x_i}, \mathbf{x_j})$ reduce to consideration of $D^m K_h^0(\mathbf{x_i}, \mathbf{x_j})$, where $K_h^0(\mathbf{x_i}, \mathbf{x_j}) = K_h(\mathbf{x_i}, \mathbf{x_j})\zeta(\mathbf{x_i} - \mathbf{x_j})$.

We now consider the boundedness properties of the operator K_1^h. Because of the above remark, we can replace K_h by K_h^0. We will make a Taylor expansion of the kernel. We treat $\mathbf{x_i} - \mathbf{x_j}$ as a perturbation of its linearization $\mathbf{y}_{ij} = J_\mathbf{i}(\alpha_\mathbf{i} - \alpha_\mathbf{j})$, where $J_\mathbf{i} = J(\alpha_\mathbf{i})$. Thus we can write $DG_h(\mathbf{x_i} - \mathbf{x_j})$ as an expansion in terms $D^{m+1}G_h(\mathbf{y}_{ij})(\mathbf{z_{ij}})^\mathbf{m}$, summed over $\mathbf{m}$ with remainder, where $\mathbf{z_{ij}} = \mathbf{x}(\alpha_\mathbf{i}) - x(\alpha_\mathbf{j}) - \mathbf{y_{ij}}$, and $\mathbf{m}$ is a multi-index. We can further expand $\mathbf{z_{ij}}$ in powers of $\alpha_\mathbf{i} - \alpha_\mathbf{j}$, quadratic or higher. We can also expand $D_2\mathbf{x_j}$ as $D_2\mathbf{x_i}$ plus powers of $\alpha_\mathbf{i} - \alpha_\mathbf{j}$. We then have a linear combination of terms for K_h. A typical term for $|\alpha_\mathbf{i} - \alpha_\mathbf{j}| \le \pi$ is given by

$$D_\mathbf{x}^{m+1} G_h(J_\mathbf{i}(\alpha_\mathbf{i} - \alpha_\mathbf{j}))(\alpha_\mathbf{i} - \alpha_\mathbf{j})^{\mathbf{p}+\mathbf{l}}. \tag{146}$$

Here $\mathbf{p}, \mathbf{l}$ are some multi-indices, with $|\mathbf{p}| \ge 2|\mathbf{m}|, |\mathbf{l}| \ge 0$. For a discrete integral operator with (146) as a kernel, we can derive boundedness properties of this operator by estimating the Fourier transform of the kernel $\alpha^{\mathbf{p}+\mathbf{l}} D_\mathbf{x}^m G_h(J_\mathbf{i}\alpha)$ with respect to α. The relevant estimates have been stated in the lemma 5.3 in [4]. These estimates and the previous remarks show that the operator with kernel (146) gains $|\mathbf{p}| + |\mathbf{l}| - |\mathbf{m}|$ derivatives, i.e., it is of order $|\mathbf{m}| - |\mathbf{p}| - |\mathbf{l}|$ in l^2 in the sense defined above. The first term, with $\mathbf{m} = \mathbf{p} = \mathbf{l} = \mathbf{0}$ vanishes because $D_l\mathbf{x}(\alpha_\mathbf{i}) \cdot N(\alpha_\mathbf{i}) = 0$ $(l = 1, 2)$, and the others are of order -1 or less since $|\mathbf{p}| \ge 2|\mathbf{m}|$. This proves that $K_1^h(\dot\phi) = A_{-1}(\dot\phi)$. Similar argument applies to K_l^h for $l = 2, 3, 4$.

Appendix C. Derivation of (81)-(86)

Estimates for $\dot{E}_{pvm}^l$ (l=1,2)

By the definition of $E_{pvm}^1(\mathbf{i})$, we have

$$
\begin{aligned}
\dot{E}^1_{pvm}(\mathbf{i}) \;=\;& D^h_1\dot{\mathbf{x}}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\eta_\mathbf{j}\times\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&+D^h_1\mathbf{x}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}(\dot\gamma_{1\mathbf{j}}D^h_2\mathbf{x}_\mathbf{j}-\dot\gamma_{2\mathbf{j}}D^h_1\mathbf{x}_\mathbf{j})\times\bigtriangledown_{x'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&+D^h_1\mathbf{x}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}(\gamma_{1\mathbf{j}}D^h_2\dot{\mathbf{x}}_\mathbf{j}-\gamma_{2\mathbf{j}}D^h_1\dot{\mathbf{x}}_\mathbf{j})\times\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&+D^h_1\mathbf{x}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\eta_\mathbf{j}\times Er(\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j}))h^2\\
&-\dot\gamma_{1\mathbf{i}}\sum_{\mathbf{j}\neq\mathbf{i}}N_\mathbf{j}\cdot\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&-\gamma_{1\mathbf{i}}\sum_{\mathbf{j}\neq\mathbf{i}}(D^h_1\dot{\mathbf{x}}_\mathbf{j}\times D^h_2\mathbf{x}_\mathbf{j}+D^h_1\mathbf{x}_\mathbf{j}\times D^h_2\dot{\mathbf{x}}_\mathbf{j})\cdot\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&-\gamma_{1\mathbf{i}}\sum_{\mathbf{j}\neq i}N_\mathbf{j}\cdot Er(\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j}))h^2,
\end{aligned}
$$

where $Er(f)=f(\alpha_\mathbf{j})-f_\mathbf{j}$. The first term is $D^h_1\dot{x}_\mathbf{i}\cdot w^h_0$; the second term is $K^h_1\dot\gamma_1-K^h_2\dot\gamma_2$; the fourth and seventh terms cancel each other to the leading order; the fifth term gives $O(h)\dot\gamma_\mathbf{i}$. Combining the third and sixth terms, we can obtain $\frac{\mathbf{N}_\mathbf{i}}{2}\cdot(\gamma_{1\mathbf{i}}H^p_{1,h}+\gamma_{2\mathbf{i}}H^p_{2,h})D^h_1\dot{\mathbf{x}}_\mathbf{i}$ to the leading order.

Similarly, we can derive (83) for $\dot{E}^2_{pvm}(\mathbf{i})$.

Estimates for $\dot{E}^n_{pvm}$

By the definition of $E^\mathbf{n}_{pvm}(\mathbf{i})$, we have

$$
\begin{aligned}
\dot{E}^\mathbf{n}_{pvm}(\mathbf{i}) \;=\;& \dot{\mathbf{n}}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\eta_\mathbf{j}\times\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&+\mathbf{n}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}(\dot\gamma_{1\mathbf{j}}D^h_2\mathbf{x}_\mathbf{j}-\dot\gamma_{2\mathbf{j}}D^h_1\mathbf{x}_\mathbf{j})\times\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&+\mathbf{n}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}(\gamma_{1\mathbf{j}}D^h_2\dot{\mathbf{x}}_\mathbf{j}-\gamma_{2j}D^h_1\dot{\mathbf{x}}_\mathbf{j})\times\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})h^2\\
&+\mathbf{n}_\mathbf{i}\cdot\sum_{\mathbf{j}\neq\mathbf{i}}\eta_\mathbf{j}\times Er(\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j}))h^2\\
&-Er(\frac{\eta_\mathbf{i}}{|\mathbf{N}_\mathbf{i}|})\sum_{\mathbf{j}\neq\mathbf{i}}\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})\times\mathbf{N}_\mathbf{j}h^2\\
&-\frac{\eta_\mathbf{i}}{|\mathbf{N}_\mathbf{i}|}\sum_{\mathbf{j}\neq\mathbf{i}}\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j})\times(D^h_1\dot{\mathbf{x}}_\mathbf{j}\times D^h_2\mathbf{x}_\mathbf{j}+D^h_1\mathbf{x}_\mathbf{j}\times D^h_2\dot{\mathbf{x}}_\mathbf{j})h^2\\
&-\frac{\eta_\mathbf{i}}{|\mathbf{N}_\mathbf{i}|}\sum_{\mathbf{j}\neq\mathbf{i}}Er(\bigtriangledown_{\mathbf{x}'}G(\mathbf{x}_\mathbf{i}-\mathbf{x}_\mathbf{j}))\times\mathbf{N}_\mathbf{j}h^2,
\end{aligned}
$$

where we have used the notation $Er(f)=f(\alpha_\mathbf{j})-f_\mathbf{j}$. The first term is $\dot{\mathbf{n}}_\mathbf{i}\cdot w^h_0$; the second term is $\frac{|\mathbf{N}_\mathbf{i}|}{2}(H^h_{1,p}(\dot\gamma_{1\mathbf{i}})+H^h_{2,p}(\dot\gamma_{2\mathbf{i}}))$; the fourth and seventh terms cancel each other to the leading order; the fifth term gives $O(h)\dot\gamma_\mathbf{i}+O(h)A_1(\dot{\mathbf{x}})=A_{-1}(\dot\gamma_\mathbf{i})+A_0(\dot{\mathbf{x}})$. Combining the third and sixth terms, we obtain to the leading order the following error terms:

$$-\gamma_{1\mathbf{i}} D_1^h \mathbf{x}_\mathbf{i}^* \cdot (H_{1,h}^p D_1^h + H_{2,h}^h D_2^h)\dot{\mathbf{x}}_\mathbf{i} - \gamma_{2\mathbf{i}} D_2^h \mathbf{x}_\mathbf{i}^* \cdot (H_{1,h}^p D_1^h + H_{2,h}^h D_2^h)\dot{\mathbf{x}}_\mathbf{i}.$$

Putting all the leading order estimates together, we get the desired estimates for $\dot{E}_{pvm}^{\mathbf{n}}$.

Estimates for $\dot{E}_{near}$

By the definition of $E_{near}^1(\mathbf{i})$, we have

$$\begin{aligned}\dot{E}_{near}^1(\mathbf{i}) \quad = \quad & Er(\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot (H_{1,h}^s - H_{1,h}^p) D_1^h \mathbf{x}_\mathbf{i} + Er(\frac{\mathbf{N_i}}{2}\gamma_{2\mathbf{i}}) \cdot (H_{2,h}^s - H_{2,h}^p) D_1^h \mathbf{x}_\mathbf{i} \\ & + (\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot Er(H_{1,h}^s - H_{1,h}^p) D_1^h \mathbf{x}_\mathbf{i} + (\frac{\mathbf{N_i}}{2}\gamma_{2\mathbf{i}}) \cdot Er(H_{2,h}^s - H_{2,h}^p) D_1^h \mathbf{x}_\mathbf{i} \\ & (\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot (H_{1,h}^s - H_{1,h}^p) D_1^h \dot{\mathbf{x}}_\mathbf{i} + (\frac{\mathbf{N_i}}{2}\gamma_{2\mathbf{i}}) \cdot (H_{2,h}^s - H_{2,h}^p) D_1^h \dot{\mathbf{x}}_\mathbf{i},\end{aligned}$$

where we have used the notation $Er(f) = f(\alpha_\mathbf{j}) - f_\mathbf{j}$. The first term is $O(h)(\dot{\gamma}_\mathbf{i}) + O(h)A_1(\dot{\mathbf{x}}_\mathbf{i}) = O(h)(\dot{\gamma}_\mathbf{i}) + A_0(\dot{\mathbf{x}}_\mathbf{i})$; the second term is of the same order; the fifth and sixth terms are the terms that we would like to get. We claim that the third and fourth terms are $O(h)A_1(\dot{\mathbf{x}}_\mathbf{i}) = A_0(\dot{\mathbf{x}}_\mathbf{i})$. Let us study the third term in some details. It can be expressed as follows:

$$\begin{aligned}& (\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot (D_1^h \mathbf{x}_\mathbf{i} \cdot D_1^h \dot{\mathbf{x}}_\mathbf{i})(H_{1,11,h}^s - H_{1,11,h}^p) D_1^h \mathbf{x}_\mathbf{i} \\ & + (\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot (D_1^h \mathbf{x}_\mathbf{i} \cdot D_2^h \dot{\mathbf{x}}_\mathbf{i})(H_{1,12,h}^s - H_{1,12,h}^p) D_1^h \mathbf{x}_\mathbf{i} \\ & + (\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot (D_2^h \mathbf{x}_\mathbf{i} \cdot D_1^h \dot{\mathbf{x}}_\mathbf{i})(H_{1,21,h}^s - H_{1,21,h}^p) D_1^h \mathbf{x}_\mathbf{i} \\ & + (\frac{\mathbf{N_i}}{2}\gamma_{1\mathbf{i}}) \cdot (D_2^h \mathbf{x}_\mathbf{i} \cdot D_2^h \dot{\mathbf{x}}_\mathbf{i})(H_{1,22,h}^s - H_{1,22,h}^p) D_1^h \mathbf{x}_\mathbf{i}\end{aligned}$$

where the operator $H_{1,lm}, l, m = 1, 2$ is an integral operator with the following kernel

$$\frac{(\alpha_1 - \alpha_1')(\alpha_l - \alpha_l')(\alpha_m - \alpha_m')}{|r|^5},$$

and

$$r = D_1^h \mathbf{x}_\mathbf{i}(\alpha_1 - \alpha_1') + D_2^h \mathbf{x}_\mathbf{i}(\alpha_2 - \alpha_2').$$

As a consequence, we can show that the third term is $O(h)A_1(\dot{\mathbf{x}}_\mathbf{i}) = A_0(\dot{\mathbf{x}}_\mathbf{i})$. Similarly, we can show that the fourth term is of the same order. This completes the derivation for $\dot{E}_{near}^1$. Using a similar argument, we can derive (83) and (84) for $\dot{E}_{near}^2(\mathbf{i})$ and $\dot{E}_{near}^{\mathbf{n}}(\mathbf{i})$ respectively.

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