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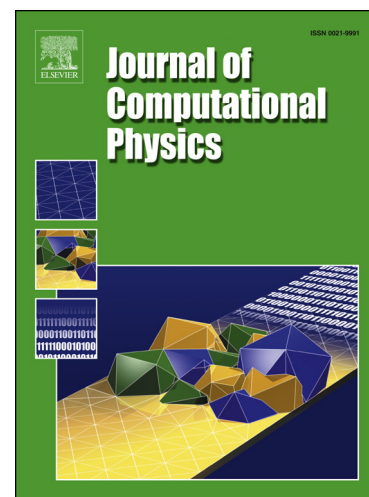
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Highlights

- A new conservative scheme with large-eddy simulation for free-surface turbulent flows.
- Good conservation properties of mass and momentum for free-surface wave and vortical flows.
- Resolving long-term nonlinear wave interactions.
- Capturing complex wave-current-turbulence interactions directly.

A conservative scheme for simulation of free-surface turbulent and wave flows

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Abstract

A numerical scheme with good conservation properties is developed for the simulation of free-surface turbulent and viscous wave flows using a surface-fitted curvilinear grid. The Navier–Stokes equations are written in a strong conservative formulation with respect to the curvilinear coordinates, and are discretized by a pseudo-spectral method in the horizontal directions and a finite-difference method in the vertical direction. Large-eddy simulation (LES) is implemented with the conservative scheme to extend the simulation capability to turbulent flows with higher Reynolds numbers. Fully nonlinear kinematic and dynamic boundary conditions are implemented at the free surface. The numerical scheme is validated using a variety of wave and vortical flow test cases. The results show good agreement with previous theoretical and numerical predictions, whereas the present scheme achieves significant improvement in the conservation of mass and momentum over the non-conservative scheme developed by Yang & Shen [1]. Meanwhile, the present conservative scheme is found to be more stable than the non-conservative scheme for the simulation of sideband waves and broadband waves. The effect of viscous dissipation on the long-term nonlinear wave evolution is also captured by the present scheme. The ability of the present scheme for simulating long-term wave-current-turbulence interaction is demonstrated by the computation of Langmuir circulation, for which the non-conservative

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scheme produces significant errors in mass and momentum conservation and the simulation fails. Flow features of the Langmuir circulation, such as the counter-rotating vortices and converging-diverging zones, have been successfully captured with our numerical scheme. The turbulence statistics also agree with the characteristics of Langmuir circulation.

Keywords: Conservation, Free-surface flow, Wave, Turbulence

1. Introduction

Free-surface fluid flows, especially turbulent flows underneath surface waves, are of great interest to the study of many environmental problems and a wide range of engineering applications. For example, surface waves can significantly modify the characteristics of turbulence in upper oceans [2, 3] and influence a variety of processes, such as the air-sea fluxes of heat, momentum, and mass [2, 4, 5], mixing and transport of pollutants [6, 7, 8], and marine life activities [9, 10]. Waves can affect the subsurface flows through different ways. Wave breaking produces intense turbulent kinetic energy near the surface. On the other hand, non-breaking waves also play an important role in the upper-ocean turbulence, modifying the turbulence through the wave straining [2, 5]. Wave evolution is also an important and yet complex process, which involves nonlinear wave-wave interactions and damping by viscous effect and wave-turbulence interaction [11, 12]. The wave dynamics are often simulated using potential flow models. When the viscous effect, the boundary layer effect, and turbulent flows are involved, it is necessary to resort to models based on the Navier–Stokes equations to resolve the aforementioned effects explicitly [13].

With the increase of computer power, simulations based on the full Navier–Stokes equations that can directly resolve the free surface have been applied to, and proven valuable for the study of free-surface flows [14, 15, 16, 17, 18, 19, 20, 21]. Two classes of numerical methods are usually used, boundary-fitted-grid or arbitrary Lagrangian-Eulerian methods (see e.g. [22, 23, 24, 25, 26, 27, 28, 1, 29]) and fixed-grid methods such as the volume-of-fluid (VOF) method and level-set

method (see e.g. [30, 31]). The fixed-grid methods are able to handle large deformations of the free surface, such as the wave breaking and generation of droplets, with relative ease. The interface is captured on the fixed grid with the VOF or level-set functions. However, the fixed grid makes it difficult to achieve local fine grid resolution around the moving interface, unless adaptive mesh refinement is used, and the interface may become diffused. Therefore, this type of methods is often not as accurate as the boundary-fitted-grid methods for resolving free-surface boundary-layer structures for non-breaking waves [22, 13, 32]. The boundary-fitted-grid methods, which the present paper uses, usually can better resolve the viscous boundary layers and turbulence eddies near the free surface, which is beneficial to the simulation of viscous wave dynamics and turbulent flows. Furthermore, the nonlinear free-surface boundary conditions, including the viscous stresses and surface tension, can be more accurately implemented on the interface as the grid points are distributed on the interface.

The spectral discretization is known to be able to improve the efficiency and accuracy in solving wave problems [33, 34] and turbulent flows [35, 36, 37, 38], and has been combined with the boundary-fitted-grid method for the simulation of free-surface flows. The large-wave simulation (LWS) method [25, 39] uses Fourier series in the horizontal directions and Chebyshev polynomials in the vertical direction. The same discretization method is also used in [14]. The numerical scheme in [1] also uses Fourier series for the discretization in the horizontal direction, but uses a finite-difference scheme for the vertical direction, which allows more flexibility in the vertical grid distribution. The above implementations use the spectral collocation method that is based on the strong formulation of the governing equations. Meanwhile, there exists another class of the implementation of the spectral methods, the spectral element methods, for free-surface flows [23, 26, 28, 21]. The spectral element method incorporates the generality of the finite element method, and provides flexibility in the spatial discretization for problems with complex geometry. Each element uses high degree polynomials as basis functions to achieve a high order of accuracy. Different from the class of spectral collocation method, the spectral element method

is based on weak (or variational) formulations of the governing equations and free-surface boundary conditions.

This paper presents a new numerical scheme that has strong conservation properties for simulation of free-surface turbulent and wave flows on a moving curvilinear coordinate system [1]. The new scheme is a substantial improvement over the non-conservative scheme previously developed in our group by Yang & Shen [1]. In [1], the unsteady three-dimensional Navier–Stokes solver employs an algebraic mapping in the vertical direction for the transformation from the irregular wave-surface-bounded physical domain to a rectangular computational domain. A hybrid pseudo-spectral and finite-difference method for spatial discretization, a fractional-step method for time integration, and the implementation of fully nonlinear free-surface boundary conditions enable accurate simulations for a wide range of applications involving surface waves. The method of [1] has been applied to studies of the turbulent wind over water waves [40, 41] and water turbulence under waves [18, 19]. However, when dealing with more challenging physical problems, we have found that the method of [1] yielded poor mass and momentum conservation that led to wrong numerical predictions or unstable simulations. One of such cases is Langmuir circulation [2, 42], which involves the interactions among rapid progressive surface waves, slowly varying mean current, and turbulence. Over the long-term evolution of the mean current, the numerical method developed in [1] yields accumulated errors in mass and momentum conservation, which eventually contaminate the simulation results.

The conservation of mass, momentum, and kinetic energy has long been the focus of the development of numerical schemes [43, 44, 45]. It has been shown that a conservative scheme produces more accurate results than a non-conservative one, especially for simulations of turbulent flows when a wide range of temporal and spatial scales are present [43, 46]. Good conservation properties also improve the stability of numerical schemes [44, 45]. When the flow is simulated in a time-dependent domain, the moving coordinates can introduce extra numerical errors when a scheme does not obey the discrete conservation

law [47]. Such errors can accumulate in time in the simulations of surface-wave flows because the motion of free surface is driven by the flow itself. While for the simulation of free-surface flows, many numerical methods are based on the non-conservative formulation, e.g., [17, 25, 27, 39, 48, 49, 50, 51, 52], including [1]. The use of a conservative form that conforms to the discrete conservation law is limited to the low-order methods [24, 53, 54, 55].

In the present work, we derive a conservative formulation of the governing equations in curvilinear coordinates for better conservation properties of mass and momentum. The strong formulation of the governing equations and fully nonlinear kinematic and dynamic boundary conditions are solved, and are discretized with a hybrid spectral collocation and finite-difference method. Special treatment is taken for nonlinear terms involving metric coefficients. The improvement of the conservation properties of the new scheme over the one in [1] is illustrated in several canonical test cases, and is shown to be necessary for some applications.

The present work also implements large-eddy simulation (LES) for free-surface turbulent flows. The direct numerical simulation (DNS) developed in [1] is restricted to flow problems with relatively low Reynolds numbers. LES, in which only large-scale motions are resolved and small-scale motions are modeled, is an efficient and practical way for simulation of turbulent flows, and has been used in the studies of a variety of environmental flows (see e.g. [8, 56, 57]). However, the application of LES to the free-surface turbulence with appreciable surface deformations like waves is still limited. Hodges & Street [24] developed a method for LES of free-surface turbulent flows based on finite volume discretization, which is less efficient for resolving waves compared with the spectral method. Furthermore, the orthogonal grid transformation used in their work is unnecessarily complicated for many wave problems. The large-wave simulation (LWS) approach developed in [25, 39], which employs an algebraic grid mapping to capture surface deformations, is based on a non-conservative formulation. The LES presented here using the new conservative scheme, which is the first of its kind for flows involving long-term wave-current-turbulence in-

teractions, is shown to be a promising numerical tool for complex free-surface turbulent flows.

The paper is organized as follows: we present the mathematical formulation of the conservative scheme and the LES implementation in section 2; the numerical algorithms are discussed in section 3; then in section 4, we present validation cases and demonstrate applications to the complex wave-current-turbulence interaction problem of Langmuir circulation; finally, conclusions are given in section 5.

2. Formulation

2.1. Governing equations and coordinate transformation

For the non-breaking surface wave problems considered in the present work, the fluid is bounded by an undulating free surface and a flat bottom. The elevation of the free surface, denoted by $\eta(x, y, t)$, is a single-valued function (i.e., the waves are not over-turning nor breaking) of horizontal coordinates (x, y) and time t . The mean surface is set at $z = 0$, and the bottom is located at $z = -\bar{H}$, with $\bar{H}$ being the domain depth. A vertical slice of the domain is shown in Fig. 1a. For a fluid with density ρ and kinematic viscosity ν , its motions are governed by the incompressible continuity equation and Navier-Stokes equations,

$$\frac{\partial u_i}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial(u_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}. \quad (2)$$

Here, u_i ($i = 1, 2, 3$), or (u, v, w) , are the Cartesian velocity components in x -, y - and z -directions, respectively; p is the hydrodynamic pressure, which differs from the total pressure p_{tot} by the hydrostatic pressure $-\rho g z$, i.e., $p = p_{tot} + \rho g z$, with g being the gravitational acceleration. Hereafter, unless specified otherwise, pressure refers to the hydrodynamic pressure p .

To solve the above equations in the wave-surface-bounded domain, a grid mapping is used to transform the physical space to a regular rectangular com-

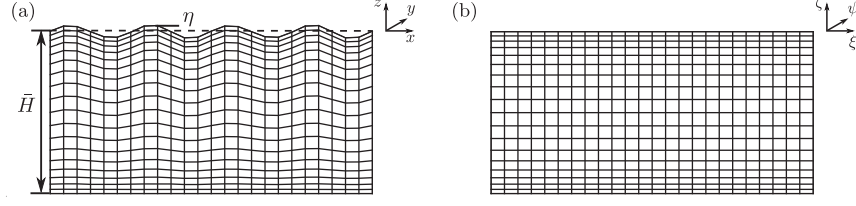


Figure 1: Sketch of the grid transformation: (a) physical space; (b) computational domain. Only one vertical x - z or ξ - ζ plane is shown because the transformation in the y -direction is trivial.

putational domain. We first consider a general time-dependent mapping from the Cartesian physical space (x, y, z, t) (Fig. 1a) to the curvilinear computational domain (ξ, ψ, ζ, τ) (Fig. 1b). The transformation of derivatives is obtained using the chain rule,

$$\frac{\partial}{\partial x_i} = \frac{\partial \xi^k}{\partial x_i} \frac{\partial}{\partial \xi^k}, \quad (3)$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial \xi^k}{\partial t} \frac{\partial}{\partial \xi^k}, \quad (4)$$

where ξ^k ($k = 1, 2, 3$) correspond to the curvilinear coordinates ξ , ψ and ζ , respectively. The transformation satisfies the following metric identity [58]

$$\frac{\partial}{\partial \xi^k} \left(J^{-1} \frac{\partial \xi^k}{\partial x_i} \right) = 0, \quad (5)$$

and the geometric conservation law (GCL) [59, 60],

$$\frac{\partial(J^{-1})}{\partial \tau} - \frac{\partial}{\partial \xi^k} (J^{-1} U_g^k) = 0. \quad (6)$$

Here, $J = \partial(\xi, \psi, \zeta)/\partial(x, y, z)$ is the Jacobian of the transformation; $U_g^j = \dot{x}_k (\partial \xi^j / \partial x_k)$ is the contravariant grid velocity, where $\dot{x}_k$ is the velocity of the curvilinear grid ξ^j in the physical space. By applying the transformation of the derivatives Eq. (3-4) together with the above two identities Eq. (5-6), we obtain the governing equations Eq. (1-2) in the time-dependent curvilinear coordinates

with a strong conservative form [47, 61] as

$$\frac{\partial}{\partial \xi^j} (J^{-1} U^j) = 0, \quad (7)$$

$$\begin{aligned} \frac{\partial(J^{-1} u_i)}{\partial \tau} - \frac{\partial(J^{-1} U_g^j u_i)}{\partial \xi^j} + \frac{\partial(J^{-1} U_j u_i)}{\partial \xi^j} = & -\frac{\partial}{\partial \xi^j} \left(J^{-1} \frac{\partial \xi^j}{\partial x_i} p \right) \\ & + \nu \frac{\partial}{\partial \xi^j} \left(J^{-1} g^{jk} \frac{\partial u_i}{\partial \xi^k} \right). \end{aligned} \quad (8)$$

In the above equations, $g^{ij} = (\partial \xi^i / \partial x_k)(\partial \xi^j / \partial x_k)$ is the metric tensor, and $U^j = u_k(\partial \xi^j / \partial x_k)$ is the contravariant velocity components. Compared with the transformation used in [1], where the chain rule is directly applied to Eq. (1-2), the strong conservative formulation here is expressed using the divergence with respect to the computational coordinates ξ^k , and thus can yield better discrete conservation properties.

In the current work, the same algebraic grid mapping as in [1] is used,

$$\xi = x, \psi = y, \zeta = \frac{z + \bar{H}}{\eta + \bar{H}}, \tau = t. \quad (9)$$

This grid mapping is illustrated in Fig. 1. Fig. 1b shows a vertical plane of the computational grid, and Fig. 1a shows the grid lines in physical space. The mapping defined by Eq. (9) yields the following Jacobian matrix,

$$\begin{bmatrix} \xi_x & \xi_y & \xi_z \\ \psi_x & \psi_y & \psi_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{\zeta \eta_x}{\eta + \bar{H}} & -\frac{\zeta \eta_y}{\eta + \bar{H}} & \frac{1}{\eta + \bar{H}} \end{bmatrix}, \quad (10)$$

and the Jacobian of the transformation $J = 1/(\eta + \bar{H})$. The grid moves only in the z -direction with velocity $\dot{\mathbf{x}} = (0, 0, \zeta \eta_t)$, therefore the contravariant grid velocity $\mathbf{U}_g = (0, 0, \zeta \eta_t / (\eta + \bar{H}))$. Here, the use of an algebraic mapping makes it possible to determine the metric coefficients, J and $\mathbf{U}_g$ analytically. With the transformation defined above, the left hand side of the GCL (Eq. 6) reduces to $\eta_t - \partial(\zeta \eta_t) / \partial \zeta$, where $\zeta \eta_t$ varies linearly with ζ . This means that the left hand side of Eq. (6) equals zero after being discretized by the finite-difference method in the ζ -direction (see section 3), therefore, the discrete GCL is satisfied. We shall also point out that, with the vertical lines fixed, the grid is distorted as

the surface deforms. However, for the simulations of non-breaking wave flows, the grid distortion is typically not large enough to cause significant numerical errors. For example, an extreme case is the theoretical limit of the Stokes wave that has a crest angle of 120° , which is the angle between two lines tangent to the surface at the wave crest. The limiting angle corresponds to a grid distortion angle of about 30° . It has been shown that the numerical errors from the grid non-orthogonality are acceptable when the distortion angle is less than 40° [62, 63]. Therefore, the present non-orthogonal algebraic transformation suffices our applications, and this transformation has also been proven effective in previous non-breaking wave simulations [1, 64, 18].

2.2. Boundary conditions

Periodic boundary conditions are applied in the horizontal directions. At the bottom of the domain, we apply a free-slip boundary condition as

$$\frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = w = 0, \text{ at } z = -\bar{H}. \quad (11)$$

The free-slip boundary condition is used to eliminate the viscous effects of the bottom boundary layer [65] because we mainly focus on deep water wave flows in the present work. We note here that a no-slip bottom with the Dirichlet condition for $\mathbf{u}$ can also be implemented in a straightforward way.

The fluid motions on the free-surface boundary are subject to the kinematic boundary condition (KBC) and dynamic boundary conditions (DBC). The KBC essentially states that the upper boundary is material so that the particles on the surface remain on the surface from a Lagrangian point of view. This constraint is expressed in Eulerian Cartesian coordinates as

$$\eta_t = w - u\eta_x - v\eta_y, \text{ at } z = \eta. \quad (12)$$

The DBCs describe the stress balance across the air-water interface. We express the DBCs in the local surface-following coordinates with unit vectors $(\mathbf{n}, \mathbf{t}_1, \mathbf{t}_2)$. The unit vectors are defined as

$$\mathbf{n} = \frac{(-\eta_x, -\eta_y, 1)}{\sqrt{1 + \eta_x^2 + \eta_y^2}}, \quad \mathbf{t}_1 = \frac{(1, 0, \eta_x)}{\sqrt{1 + \eta_x^2}}, \quad \mathbf{t}_2 = \frac{(0, 1, \eta_y)}{\sqrt{1 + \eta_y^2}}, \quad (13)$$

where $\mathbf{n}$ is the normal vector of the surface pointing from water to air, and $\mathbf{t}_1$ and $\mathbf{t}_2$ are the vectors tangential to the surface in the x - z and y - z planes, respectively. Then the DBCs are given as

$$\sigma_n + \gamma \nabla \cdot \mathbf{n} = \mathbf{n} \cdot \bar{\bar{\boldsymbol{\sigma}}} \cdot \mathbf{n}^T, \quad \sigma_1 = \mathbf{t}_1 \cdot \bar{\bar{\boldsymbol{\sigma}}} \cdot \mathbf{n}^T, \quad \sigma_2 = \mathbf{t}_2 \cdot \bar{\bar{\boldsymbol{\sigma}}} \cdot \mathbf{n}^T, \quad (14)$$

where $(\sigma_n, \sigma_1, \sigma_2)$ is the stress imposed by the air above the interface; and $\bar{\bar{\boldsymbol{\sigma}}} = -(p - \rho g z) \bar{\bar{\mathbf{I}}} + \rho \nu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ is the stress tensor in the water with $\bar{\bar{\mathbf{I}}}$ denoting the identity tensor; it should be pointed out here that the hydrostatic pressure $-\rho g z$ is added to p in $\bar{\bar{\boldsymbol{\sigma}}}$ when considering the boundary conditions. The first equation in Eq. (14) describes the normal stress balance in the $\mathbf{n}$ direction, with $\gamma \nabla \cdot \mathbf{n}$ accounting for the pressure difference caused by surface tension γ ; the second and third equations in Eq. (14) describe the balance of stresses in the $\mathbf{t}_1$ and $\mathbf{t}_2$ directions, respectively.

With Eq. (13), the normal stress balance in Eq. (14) can be rearranged as a Dirichlet boundary condition for the pressure

$$p = \rho g \eta - \sigma_n + \frac{2\rho\nu}{1 + \eta_x^2 + \eta_y^2} \left[-(1 + \eta_y^2) \frac{\partial u}{\partial \xi} - (1 + \eta_x^2) \frac{\partial v}{\partial \psi} + \eta_x \eta_y \left(\frac{\partial u}{\partial \psi} + \frac{\partial v}{\partial \xi} \right) - \eta_x \frac{\partial w}{\partial \xi} - \eta_y \frac{\partial w}{\partial \psi} \right] - \gamma \frac{(1 + \eta_x^2) \eta_{yy} + (1 + \eta_y^2) \eta_{xx} - 2\eta_x \eta_y \eta_{xy}}{(1 + \eta_x^2 + \eta_y^2)^{3/2}}. \quad (15)$$

Here, the derivatives have been transformed to the computational domain using Eq. (3); and a surface-elevation-induced pressure $\rho g \eta$ appears in the above boundary condition for the dynamic pressure p . Without the viscosity, the Eq. (15) is reduced to the dynamic boundary condition in the potential flow theory [66]. The second and third equations in Eq. (14) are expressed as Neumann boundary conditions for velocity components u and v ,

$$\begin{aligned} \frac{\partial u}{\partial \zeta} = & \frac{\eta + \bar{H}}{1 + \eta_x^2 + \eta_y^2} \left[2\eta_x \frac{\partial u}{\partial \xi} + \eta_y \frac{\partial u}{\partial \psi} + \eta_y \frac{\partial v}{\partial \xi} + (\eta_x^2 - 1) \frac{\partial w}{\partial \xi} \right. \\ & \left. + \eta_x \eta_y \frac{\partial w}{\partial \psi} + \sqrt{(1 + \eta_x^2 + \eta_y^2)(1 + \eta_x^2)} \frac{\sigma_1}{\nu} \right] - \eta_x \frac{\partial w}{\partial \zeta}, \end{aligned} \quad (16)$$

$$\begin{aligned} \frac{\partial v}{\partial \zeta} = & \frac{\eta + \bar{H}}{1 + \eta_x^2 + \eta_y^2} \left[\eta_x \frac{\partial v}{\partial \xi} + 2\eta_y \frac{\partial v}{\partial \psi} + \eta_x \frac{\partial u}{\partial \psi} + \eta_x \eta_y \frac{\partial w}{\partial \xi} \right. \\ & \left. + (\eta_y^2 - 1) \frac{\partial w}{\partial \psi} + \sqrt{(1 + \eta_x^2 + \eta_y^2)(1 + \eta_y^2)} \frac{\sigma_2}{\nu} \right] - \eta_y \frac{\partial w}{\partial \zeta}. \end{aligned} \quad (17)$$

The boundary condition for vertical velocity w is intrinsically determined from the continuity equation Eq. (7).

2.3. LES implementation

The LES extends the proposed numerical method to applications of turbulent flows with higher Reynolds numbers. In LES, only turbulent eddies larger than a certain filter scale Δ are resolved, and the effects of eddies at scales smaller than Δ are modeled such that the computational cost is reduced. To simulate free-surface turbulent flows, we implement LES on the wave-surface-fitted grid. The governing equations for the resolved motions are obtained with a filter applied to Eq. (1-2),

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0, \quad (18)$$

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial(\tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^d}{\partial x_j}. \quad (19)$$

Here, $(\tilde{\cdot})$ denotes filtered quantities; $\tau_{ij}^d = \tau_{ij} - \tau_{kk}/3$ is the deviatoric part of the subgrid-scale (SGS) stress $\tau_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$. Using the same transformation technique in section 2.1, we obtain the filtered governing equations in the computational domain as

$$\frac{\partial}{\partial \xi^j} (J^{-1} \tilde{U}^j) = 0, \quad (20)$$

$$\begin{aligned} \frac{\partial(J^{-1} \tilde{u}_i)}{\partial \tau} - \frac{\partial(J^{-1} \tilde{U}_g^j \tilde{u}_i)}{\partial \xi^j} + \frac{\partial(J^{-1} \tilde{U}_j^j \tilde{u}_i)}{\partial \xi^j} &= -\frac{\partial}{\partial \xi^j} \left(\frac{\tilde{p}}{J} \frac{\partial \xi^j}{\partial x_i} \right) \\ &+ \nu \frac{\partial}{\partial \xi^j} \left(\frac{g^{jk}}{J} \frac{\partial \tilde{u}_i}{\partial \xi^k} \right) - \frac{\partial}{\partial \xi^j} \left(\frac{\tau_{ik}^d}{J} \frac{\partial \xi^j}{\partial x_k} \right), \end{aligned} \quad (21)$$

where $\tilde{U}^j = \tilde{u}_k (\partial \xi^j / \partial x_k)$ is the contravariant velocity defined using the filtered velocity.

2.3.1. SGS model

A Smagorinsky model is used to determine the SGS stress as

$$\tau_{ij}^d = -2\nu_t \tilde{S}_{ij} = -2C_0 |\tilde{S}| \tilde{S}_{ij}. \quad (22)$$

Here, $\tilde{S}_{ij}$ is the strain rate tensor based on the filtered velocity, $\tilde{S}_{ij} = (\tilde{u}_{i,j} + \tilde{u}_{j,i})/2$, and $|\tilde{S}|$ is the magnitude of the strain rate defined as $|\tilde{S}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$. The Smagorinsky coefficient C_0 is dynamically determined using a Lagrangian scale-dependent model [67, 68]. A traditional dynamic Smagorinsky model uses plane-averaging in the process of determining C_0 to improve the numerical stability, assuming there exist homogeneous planes in the turbulent flows [69, 70]. This assumption, however, often does not hold in flows with complex geometry, such as surface waves, which can be highly inhomogeneous. In the dynamic Lagrangian SGS model, the averaging is performed in the Lagrangian frame, i.e., following the pathlines of the fluid particles with diminishing weight on older history [67]. In addition, the assumption of the scale-invariance of C_0 in traditional models does not always hold, e.g. in the near-wall regions of many geophysical flows. The SGS model we adopt dynamically determines the scale-dependence of C_0 . This dynamic Lagrangian scale-dependent model is shown to perform well for heterogeneous geophysical flows [68, 71, 72].

2.3.2. Free-surface boundary conditions

The implementation of the bottom boundary free-slip conditions is trivial, and therefore we only discuss the LES treatment for the free-surface boundary conditions. The evolution of the filtered surface elevation $\tilde{\eta}$ is governed by the filtered KBC,

$$\tilde{\eta}_t = \tilde{w} - \tilde{u}\tilde{\eta}_x - \tilde{v}\tilde{\eta}_y - K_x - K_y. \quad (23)$$

Compared with the non-filtered KBC in Eq. (12), the extra terms $K_x = \widetilde{u\eta_x} - \tilde{u}\tilde{\eta}_x$ and $K_y = \widetilde{v\eta_y} - \tilde{v}\tilde{\eta}_y$ account for the effects of SGS surface elevations. As pointed out by Hodges and Street [24], the small-scale fluctuations of the free surface are related to the dynamics of near-surface small-scale motions, which involve the effects of pressure fluctuations, viscous layer, and surface tension. The present computational framework can be used to perform DNS experiments to help understand the flow physics and the modeling of free-surface SGS kinematics. However, the development of such models is not the main focus of the current work. In the large wave simulation [25], the SGS kinematics terms

were found to be negligible. Hodges and Street [24] also neglected the terms in their implementation of LES of free-surface turbulent flows. Here, we also choose to omit the SGS kinematics terms K_x and K_y .

For consistency, in the treatment of the free-surface DBCs, we also omit the SGS contributions generated from nonlinear terms, e.g. η_x^2 in Eq. (15). The complete filtered dynamic boundary conditions with the SGS terms omitted are

$$\begin{aligned} \tilde{p} = \rho g \tilde{\eta} + \frac{2\rho(\nu + \nu_t)}{1 + \tilde{\eta}_x^2 + \tilde{\eta}_y^2} \left[-(1 + \tilde{\eta}_y^2) \frac{\partial \tilde{u}}{\partial \xi} - (1 + \tilde{\eta}_x^2) \frac{\partial \tilde{v}}{\partial \psi} + \tilde{\eta}_x \tilde{\eta}_y \left(\frac{\partial \tilde{u}}{\partial \psi} + \frac{\partial \tilde{v}}{\partial \xi} \right) \right. \\ \left. - \tilde{\eta}_x \frac{\partial \tilde{w}}{\partial \xi} - \tilde{\eta}_y \frac{\partial \tilde{w}}{\partial \psi} \right] - \gamma \frac{(1 + \tilde{\eta}_x^2) \tilde{\eta}_{yy} + (1 + \tilde{\eta}_y^2) \tilde{\eta}_{xx} - 2 \tilde{\eta}_x \tilde{\eta}_y \tilde{\eta}_{xy}}{(1 + \tilde{\eta}_x^2 + \tilde{\eta}_y^2)^{3/2}}, \quad (24) \end{aligned}$$

$$\begin{aligned} \frac{\partial \tilde{u}}{\partial \zeta} = \frac{\tilde{\eta} + \bar{H}}{1 + \tilde{\eta}_x^2 + \tilde{\eta}_y^2} \left[2 \tilde{\eta}_x \frac{\partial \tilde{u}}{\partial \xi} + \tilde{\eta}_y \frac{\partial \tilde{u}}{\partial \psi} + \tilde{\eta}_y \frac{\partial \tilde{v}}{\partial \xi} + (\tilde{\eta}_x^2 - 1) \frac{\partial \tilde{w}}{\partial \xi} \right. \\ \left. + \tilde{\eta}_x \tilde{\eta}_y \frac{\partial \tilde{w}}{\partial \psi} + \sqrt{(1 + \tilde{\eta}_x^2 + \tilde{\eta}_y^2)(1 + \tilde{\eta}_x^2)} \frac{\sigma_1}{\nu + \nu_t} \right] - \tilde{\eta}_x \frac{\partial \tilde{w}}{\partial \zeta}, \quad (25) \end{aligned}$$

$$\begin{aligned} \frac{\partial \tilde{v}}{\partial \zeta} = \frac{\tilde{\eta} + \bar{H}}{1 + \tilde{\eta}_x^2 + \tilde{\eta}_y^2} \left[\tilde{\eta}_x \frac{\partial \tilde{v}}{\partial \xi} + 2 \tilde{\eta}_y \frac{\partial \tilde{v}}{\partial \psi} + \tilde{\eta}_x \frac{\partial \tilde{u}}{\partial \psi} + \tilde{\eta}_x \tilde{\eta}_y \frac{\partial \tilde{w}}{\partial \xi} \right. \\ \left. + (\tilde{\eta}_y^2 - 1) \frac{\partial \tilde{w}}{\partial \psi} + \sqrt{(1 + \tilde{\eta}_x^2 + \tilde{\eta}_y^2)(1 + \tilde{\eta}_y^2)} \frac{\sigma_2}{\nu + \nu_t} \right] - \tilde{\eta}_y \frac{\partial \tilde{w}}{\partial \zeta}. \quad (26) \end{aligned}$$

3. Numerical Methods

Following [1], a hybrid pseudo-spectral and finite-difference method is employed for spatial discretization. Since periodic conditions are imposed in the horizontal directions and this work is aimed at simulating flows with waves, the spectral method based on Fourier series is a natural choice for the discretization in the horizontal directions (ξ, ψ) . A collocated arrangement for all flow variables is used in the horizontal planes (ξ, ψ) . In the vertical direction ζ , we use a finite-difference scheme with second-order accuracy for discretization such that the grid distribution can be more flexible (e.g., clustered near the boundary with a derived grid stretching ratio). A staggered grid is adopted in the ζ -direction to avoid the odd-even decoupling, as shown in Fig. 2. The velocity w and contravariant velocity W are located at the cell face; the horizontal velocity u and

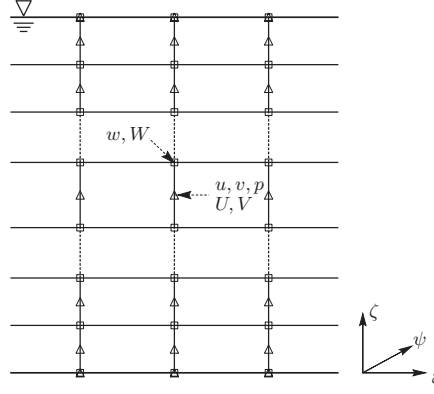


Figure 2: Sketch of the staggered grid layout. The velocity (u, v) , the contravariant velocity (U, V) , and the pressure p are defined at nodes marked with Δ ; the velocity w and contravariant velocity W are defined at nodes marked with $\square$. Only one vertical $\xi - \zeta$ plane is shown.

v are located at the cell center, so is the pressure p ; the contravariant velocity U and V are located at the same nodes as u and v . Horizontal velocities (u, v) and (U, V) , and pressure p are also defined at the boundary. The boundary nodes are needed for the KBC and DBCs of the free-surface flows.

3.1. Free surface advancing

The Navier–Stokes equations are solved in an undulating domain with the surface elevation η . To obtain η , the KBC is integrated over time using a second-order Runge–Kutta method in a prediction-correction style. This scheme consists of two stages updating the free surface from the current time step (n) to the next time step $(n + 1)$:

- prediction:

$$\eta^{(n+1)*} = \eta^{(n)} + \Delta t \eta_t^{(n)}, \quad (27)$$

- correction:

$$\eta^{(n+1)} = \eta^{(n+1)*} + \frac{\Delta t}{2} \left(\eta_t^{(n+1)*} - \eta_t^{(n)} \right). \quad (28)$$

The first stage Eq. (27) is essentially a forward Euler method, and $\eta_t^{(n)}$ is evaluated using Eq. (12) with η and (u, v, w) from the current time step (n) . The $\eta^{(n+1)*}$ obtained from Eq. (27) is a first-order prediction of surface elevation at time step $(n+1)$. The Navier–Stokes equations are advanced to time step $(n+1)$ on the grid with elevation $\eta^{(n+1)*}$ to obtain velocity $u_i^{(n+1)*}$. The velocity $u_i^{(n+1)*}$ is then used at the correction stage Eq. (28) for the calculation of $\eta^{(n+1)}$ with second-order accuracy.

3.2. Navier–Stokes equations solution

The solution of the incompressible Navier–Stokes equations Eq. (7-8) is based on the fractional-step method [73] with modifications for free-surface flows. The fractional-step method consists of two steps, of which the first step is to obtain an intermediate velocity $\hat{u}_i$ by integrating the momentum equation Eq. (8) without the pressure. The intermediate velocity $\hat{u}_i$ is not solenoidal. In the second step, $\hat{u}_i$ is projected onto a divergence-free space, using pseudo-pressure ϕ , to satisfy the continuity equation.

The integration of the momentum equation in the first step is calculated by

$$\frac{(J^{-1})^{(n+1)}\hat{u}_i - (J^{-1}u_i)^{(n)}}{\Delta t} = \frac{3R_i^{(n)} - R_i^{(n-1)}}{2}. \quad (29)$$

Here, the superscript (n) denotes that the corresponding terms are evaluated at time step (n) . An Adam-Bashforth scheme with second-order accuracy is used for temporal integration. On the right hand side of Eq. (29), $R_i^{(n)}$ represents all terms in the momentum equation other than the temporal derivatives and pressure terms,

$$R_i^{(n)} = \frac{\partial(J^{-1}U_g^j u_i)^{(n)}}{\partial \xi^j} - \frac{\partial(J^{-1}U_j u_i)^{(n)}}{\partial \xi^j} + \nu \frac{\partial}{\partial \xi^j} \left(J^{-1} g^{jk} \frac{\partial u_i}{\partial \xi^k} \right)^{(n)}. \quad (30)$$

Additionally, SGS stress terms are also included in R_i when LES equations are solved. The viscous terms are treated explicitly. Although the explicit treatment may pose a restriction on the time step, this restriction is alleviated when the viscous effect is relatively small, such as in high Reynolds number flows.

In the second step of the fractional-step method, we correct the intermediate velocity $\hat{u}_i$ using

$$u_i^{(n+1)} = \hat{u}_i - \Delta t \left[J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial x_i} \frac{\phi}{J} \right) \right]^{(n+1)}, \quad (31)$$

to make the final velocity field $u_i^{(n+1)}$ satisfy the solenoidal condition

$$\frac{\partial (J^{-1} U^j)^{(n+1)}}{\partial \xi^j} = 0. \quad (32)$$

By substituting Eq. (31) into Eq. (29), we obtain the pseudo-pressure ϕ related to the hydrodynamic pressure p as

$$\phi^{(n+1)} = p^{(n+1/2)}. \quad (33)$$

Applying the divergence operator $D[\cdot]$ defined as

$$D[\cdot] = J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial x_i} \frac{\cdot}{J} \right)$$

to Eq. (31) yields a Poisson equation for the pseudo-pressure ϕ

$$J \frac{\partial}{\partial \xi^j} \left[\frac{\partial \xi^j}{\partial x_i} \frac{\partial}{\partial \xi^k} \left(\frac{\partial \xi^k}{\partial x_i} \frac{\phi}{J} \right) \right]^{(n+1)} = D^{(n+1)}[\hat{u}_i]. \quad (34)$$

If we substitute the grid transformation coefficients in Eq. (10) into the above equation, we obtain

$$\begin{aligned} & \frac{\partial^2 \Phi^{(n+1)}}{\partial \xi^2} + \frac{\partial^2 \Phi^{(n+1)}}{\partial \psi^2} + \frac{\partial}{\partial \xi} \left(\frac{\partial \zeta_x \Phi}{\partial \zeta} \right)^{(n+1)} + \frac{\partial}{\partial \psi} \left(\frac{\partial \zeta_y \Phi}{\partial \zeta} \right)^{(n+1)} \\ & + \frac{\partial}{\partial \zeta} \left[\zeta_x \left(\frac{\partial \Phi}{\partial \xi} + \frac{\partial \zeta_x \Phi}{\partial \zeta} \right) + \zeta_y \left(\frac{\partial \Phi}{\partial \psi} + \frac{\partial \zeta_y \Phi}{\partial \zeta} \right) + \zeta_z \frac{\partial \zeta_z \Phi}{\partial \zeta} \right]^{(n+1)} = \\ & \frac{\partial J^{-1} \hat{u}}{\partial \xi} + \frac{\partial J^{-1} \hat{v}}{\partial \psi} + \frac{\partial}{\partial \zeta} \left(\zeta_x^{(n+1)} \frac{\hat{u}}{J} + \zeta_y^{(n+1)} \frac{\hat{v}}{J} + \zeta_z^{(n+1)} \frac{\hat{w}}{J} \right), \end{aligned} \quad (35)$$

where $\Phi^{(n+1)} = (J^{-1} \phi)^{(n+1)}$. To make use of the spectral discretization in the horizontal directions, we use an iterative method to solve the Poisson equation.

During the iteration, the equation to solve is

$$\begin{aligned} & \frac{\partial^2 \Phi^{(m+1)}}{\partial \xi^2} + \frac{\partial^2 \Phi^{(m+1)}}{\partial \psi^2} + \frac{1}{H^2} \frac{\partial^2 \Phi^{(m+1)}}{\partial \zeta^2} = \frac{1}{H^2} \frac{\partial^2 \Phi^{(m)}}{\partial \zeta^2} - \frac{\partial}{\partial \xi} \left(\frac{\partial \zeta_x \Phi}{\partial \zeta} \right)^{(m)} \\ & - \frac{\partial}{\partial \psi} \left(\frac{\partial \zeta_y \Phi}{\partial \zeta} \right)^{(m)} - \frac{\partial}{\partial \zeta} \left[\zeta_x \left(\frac{\partial \Phi}{\partial \xi} + \frac{\partial \zeta_x \Phi}{\partial \zeta} \right) + \zeta_y \left(\frac{\partial \Phi}{\partial \psi} + \frac{\partial \zeta_y \Phi}{\partial \zeta} \right) + \zeta_z \frac{\partial \zeta_z \Phi}{\partial \zeta} \right]^{(m)} \\ & + \frac{\partial J^{-1} \hat{u}}{\partial \xi} + \frac{\partial J^{-1} \hat{v}}{\partial \psi} + \frac{\partial}{\partial \zeta} \left(\zeta_x^{(n+1)} \frac{\hat{u}}{J} + \zeta_y^{(n+1)} \frac{\hat{v}}{J} + \zeta_z^{(n+1)} \frac{\hat{w}}{J} \right). \end{aligned} \quad (36)$$

Here, the superscripts $(m + 1)$ and (m) denote the solution from the $(m + 1)$ -th and m -th iterations, respectively. Compared to the original Eq. (35), all nonlinear terms are moved to the right hand side of the equation as source terms, which are evaluated using values from the previous iteration. An extra term $(\bar{H}^{-2})\partial^2\Phi^{(n+1)}/\partial\zeta^2$ is added on both sides of the equation so that the terms on the left are entirely linear for the Fourier transformation of Φ . With this treatment, the pseudo-spectral method can be used to discretize the horizontal directions ξ and ψ , and yields a group of ordinary differential equations in terms of ζ , which can then be solved using a tridiagonal matrix solver. When the iteration converges, the modified equation Eq. (36) is equivalent to the original Eq. (35).

3.2.1. Boundary conditions for intermediate velocity

In Eq. (29), the right hand side R_i can be directly calculated from Eq. (30) for each internal nodes, therefore the intermediate velocity $\hat{u}_i$ at the internal nodes can be obtained using Eq. (29). However, $\hat{u}_i$ on the boundary needs to be determined using boundary conditions.

As pointed out in section 2.2, in this study the bottom is a free-slip boundary. The implementation of a free-slip boundary is thoroughly discussed in the literature (e.g. [74]). The bottom boundary conditions of intermediate velocity $\hat{u}$ are

$$\frac{\partial \hat{u}}{\partial \zeta} = \frac{\partial \hat{v}}{\partial \zeta} = \hat{w} = 0. \quad (37)$$

At the free surface, the velocity at time $(n + 1)$ should satisfy the DBCs given by Eq. (16) and (17),

$$\begin{aligned} \frac{\partial u^{(n+1)}}{\partial \zeta} = & \frac{\eta + \bar{H}}{1 + \eta_x^2 + \eta_y^2} \left[2\eta_x \frac{\partial u^{(n+1)}}{\partial \xi} + \eta_y \frac{\partial u^{(n+1)}}{\partial \psi} + \eta_y \frac{\partial v^{(n+1)}}{\partial \xi} + \eta_x \eta_y \frac{\partial w^{(n+1)}}{\partial \psi} \right. \\ & \left. + (\eta_x^2 - 1) \frac{\partial w^{(n+1)}}{\partial \xi} + \sqrt{(1 + \eta_x^2 + \eta_y^2)(1 + \eta_x^2)} \frac{\sigma_1}{\nu} \right] - \eta_x \frac{\partial w^{(n+1)}}{\partial \zeta}, \quad (38) \end{aligned}$$

$$\begin{aligned} \frac{\partial v^{(n+1)}}{\partial \zeta} = & \frac{\eta + \bar{H}}{1 + \eta_x^2 + \eta_y^2} \left[\eta_x \frac{\partial v^{(n+1)}}{\partial \xi} + 2\eta_y \frac{\partial v^{(n+1)}}{\partial \psi} + \eta_x \frac{\partial u^{(n+1)}}{\partial \psi} + \eta_x \eta_y \frac{\partial w^{(n+1)}}{\partial \xi} \right. \\ & \left. + (\eta_y^2 - 1) \frac{\partial w^{(n+1)}}{\partial \psi} + \sqrt{(1 + \eta_x^2 + \eta_y^2)(1 + \eta_y^2)} \frac{\sigma_2}{\nu} \right] - \eta_y \frac{\partial w^{(n+1)}}{\partial \zeta}. \quad (39) \end{aligned}$$

The derivatives $\partial u^{(n+1)}/\partial \zeta$ and $\partial v^{(n+1)}/\partial \zeta$ are evaluated explicitly, with $u_i^{(n+1)}$ on the right hand of Eq. (38) and (39) estimated by

$$u_i^{(n+1)} = 2u_i^{(n)} - u_i^{(n-1)} + O(\Delta t^2).$$

Meanwhile, substituting Eq. (31) into the left hand side of Eq. (38) and (39) about $\hat{u}$ and $\hat{v}$ yields

$$\frac{\partial u^{(n+1)}}{\partial \zeta} = \frac{\partial \hat{u}}{\partial \zeta} - \Delta t \frac{\partial}{\partial \zeta} \left[J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial x} \frac{\phi^{(n+1)}}{J} \right) \right], \quad (40)$$

$$\frac{\partial v^{(n+1)}}{\partial \zeta} = \frac{\partial \hat{v}}{\partial \zeta} - \Delta t \frac{\partial}{\partial \zeta} \left[J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial y} \frac{\phi^{(n+1)}}{J} \right) \right]. \quad (41)$$

With $\phi^{(n+1)}$ estimated by

$$\phi^{(n+1)} = \phi^{(n)} + O(\Delta t),$$

we obtain the vertical gradient of the intermediate velocity $\hat{u}$ and $\hat{v}$ at the boundary as

$$\frac{\partial \hat{u}}{\partial \zeta} = \frac{\partial u^{(n+1)}}{\partial \zeta} + \Delta t \frac{\partial}{\partial \zeta} \left[J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial x} \frac{\phi^{(n)}}{J} \right) \right] + O(\Delta t^2), \quad (42)$$

$$\frac{\partial \hat{v}}{\partial \zeta} = \frac{\partial v^{(n+1)}}{\partial \zeta} + \Delta t \frac{\partial}{\partial \zeta} \left[J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial y} \frac{\phi^{(n)}}{J} \right) \right] + O(\Delta t^2). \quad (43)$$

The derivatives $\partial \hat{u}/\partial \zeta$ and $\partial \hat{v}/\partial \zeta$ are estimated using one-sided stencil as

$$\frac{\partial \hat{u}}{\partial \zeta} = \frac{8\hat{u}_{Nz} - 9\hat{u}_{Nz-1} + \hat{u}_{Nz-2}}{6(\zeta_{Nz} - \zeta_{Nz-1})} + O(\Delta z^2), \quad (44)$$

$$\frac{\partial \hat{v}}{\partial \zeta} = \frac{8\hat{v}_{Nz} - 9\hat{v}_{Nz-1} + \hat{v}_{Nz-2}}{6(\zeta_{Nz} - \zeta_{Nz-1})} + O(\Delta z^2). \quad (45)$$

The velocity at the free-surface boundary nodes is denoted by subscript Nz , and the second and the third off-boundary nodes are denoted by $Nz-1$ and $Nz-2$, respectively (see Fig. 2 for the grid arrangement). The boundary intermediate velocity $\hat{u}_{Nz}$ and $\hat{v}_{Nz}$ are solved from Eq. (42-45). After $\hat{u}_{Nz}$ and $\hat{v}_{Nz}$ are obtained, the intermediate velocity $\hat{w}$ is calculated from Eq. (35), where $\phi^{(n+1)}$ is estimated using $\phi^{(n)}$, which we have shown yields second-order accuracy in time. Using Eq. (35) to determine $\hat{w}$ is consistent with the conservative formulation.

3.2.2. Boundary conditions for pseudo-pressure

The Poisson equation for pseudo-pressure $\phi^{(n+1)}$ is solved subject to the Dirichlet boundary condition at the free surface according to Eq. (33),

$$\phi^{(n+1)} = p^{(n+1/2)} = \frac{1}{2}(p^{(n)} + p^{(n+1)}), \quad \text{at } z = \eta, \quad (46)$$

where $p^{(n)}$ and $p^{(n+1)}$ are calculated from the pressure Dirichlet boundary condition Eq. (15). Here, $p^{(n+1)}$ involves the velocity u_i at time step $(n+1)$, which is estimated by Eq. (31) with the intermediate velocity $\hat{u}_i$ and the pseudo-pressure $\phi^{(n)}$ as

$$u_i^{(n+1)} = \hat{u}_i - \Delta t \left[J \frac{\partial}{\partial \xi^j} \left(\frac{\partial \xi^j}{\partial x_i} \frac{\phi^{(n)}}{J} \right) \right] + O(\Delta t^2). \quad (47)$$

The compatible boundary condition for $\phi^{(n+1)}$ at the bottom boundary is [74]

$$\frac{\partial \phi^{(n+1)}}{\partial \phi} = 0, \quad \text{at } z = -\bar{H}. \quad (48)$$

3.3. Summary of solution procedure

The simulation of free-surface flows generally follows the solution procedure used in [1]. From time step (n) to the next time step $(n+1)$, the procedure is:

1. The free surface elevation $\eta^{(n)}$ is advanced to $\eta^{(n+1)*}$ by Eq. (27) using $u^{(n)}$.
2. Obtain intermediate velocity $\hat{u}_i$ in the updated domain with surface elevation $\eta^{(n+1)*}$ using Eq. (29).
3. Solve $\phi^{(n+1)*}$ from pressure Poisson equation Eq. (35), and correct intermediate velocity $\hat{u}_i$ to $u^{(n+1)*}$ using Eq. (31).
4. The free surface elevation $\eta^{(n+1)*}$ is corrected to $\eta^{(n+1)}$ by Eq. (28) using $u^{(n+1)*}$.
5. Repeat steps 2-4 to solve the Navier–Stokes equations on the corrected domain with surface elevation $\eta^{(n+1)}$, and obtain $u_i^{(n+1)}$ and $\phi^{(n+1)}$.

We note here that compared to [1], the present numerical scheme, including discretization and boundary conditions, is adapted accordingly to the conservative formulation, and is thus able to improve the conservation properties of the scheme, which we show in the next section.

4. Results

In this section, we first validate and test the accuracy of the conservative scheme. Then we test the performance of the conservative scheme against the non-conservative one in [1], with a focus on the difference in conservation properties. Both laminar and turbulent free-surface flows are tested, and the results are shown in the following subsections.

4.1. Decaying vortex

We first carry out a simulation of a two-dimensional decaying vortex to test the accuracy of the conservative scheme. The analytic solution of the problem with $\rho = 1$ and $\nu = 1$ is given by [73]

$$\begin{aligned} u(x, z, t) &= -\cos x \sin z e^{-2t}, \\ w(x, z, t) &= \sin x \cos z e^{-2t}, \\ p(x, z, t) &= -0.25(\cos 2x + \cos 2z)e^{-4t}. \end{aligned} \tag{49}$$

The solution is defined in the domain $x \in [0, 2\pi]$, $z \in [-\pi/2, \pi/2]$. The periodic boundary condition in the x -direction is automatically satisfied for this problem. On the lower boundary $z = -\pi/2$, the exact solution gives $w = 0$ and $\partial u / \partial z = 0$ so that we can apply the free-slip condition there. On the upper boundary $z = \pi/2$, we apply the pressure Dirichlet boundary condition using the exact solution and zero tangential stress condition.

Because the theoretical solution is sinusoidal with respect to x and the Fourier-based pseudo-spectral method is used in the horizontal direction, the numerical error due to the spatial discretization mainly comes from the finite-difference discretization in the vertical direction. The spatial discretization error is studied using three sets of uniform grids with different vertical resolutions, 32×40 , 32×80 , and 32×160 . The initial condition of the domain is given by the analytic solution, then the flow field is advanced in time with a fixed Courant number $\Delta t / \Delta z = 0.005$ (velocity scale is 1). The numerical solutions are compared to the analytic solution at time $t = 0.4$. Table 1 shows the errors

	32×40	32×80	32×160	Convergence rate
<i>u</i>				
L_∞ error	$3.97e-4$	$9.88e-5$	$2.47e-5$	2.00
L_2 error	$1.67e-4$	$4.12e-5$	$1.03e-5$	2.01
<i>w</i>				
L_∞ error	$3.41e-4$	$8.51e-5$	$2.13e-5$	2.00
L_2 error	$9.22e-5$	$2.30e-5$	$5.76e-6$	2.00
<i>p</i>				
L_∞ error	$3.53e-3$	$8.93e-4$	$2.17e-4$	2.02
L_2 error	$1.81e-3$	$4.53e-4$	$1.13e-4$	2.00

Table 1: L_∞ and L_2 errors of velocity (u, w) and pressure p for the decaying vortex for different grid resolutions with a fixed Courant number of 0.5.

of velocity (u, w) and pressure p between the numerical and analytic solutions. The errors are evaluated in both L_∞ and L_2 norms. It is clear that the present numerical scheme successfully predicts the theoretical solution. The convergence rates obtained using least-square regression shows that a second-order spatial accuracy is achieved for all variables.

The error contributed by the temporal discretization is small compared to that from the spatial discretization due to the small time steps restricted by numerical stability limitations. To study the temporal accuracy of the present scheme, we set up simulations on the same grid 32×80 with four time steps, $\Delta t_1 = 3 \times 10^{-4}$, $\Delta t_2 = 2.5 \times 10^{-4}$, $\Delta t_3 = 2 \times 10^{-4}$, and $\Delta t_4 = 2 \times 10^{-5}$. The last one with a much smaller time step serves as the reference solution. The errors of the other sets of solutions are defined based on the reference solution so that the spatial discretization error is eliminated [27]. The results of the temporal error analysis are shown in Table 2. The errors are evaluated at $t = 0.051$. It is evident that the scheme also achieves an overall second-order accuracy for temporal discretization.

	Δt_1	Δt_2	Δt_3	Convergence rate
<i>u</i>				
L_∞ error	$1.48e-7$	$1.02e-7$	$6.53e-8$	2.02
L_2 error	$7.46e-8$	$5.15e-8$	$3.27e-8$	2.03
<i>w</i>				
L_∞ error	$1.50e-7$	$1.04e-7$	$6.62e-8$	2.02
L_2 error	$7.33e-8$	$5.07e-8$	$3.22e-8$	2.03
<i>p</i>				
L_∞ error	$3.22e-7$	$2.06e-7$	$1.32e-7$	2.10
L_2 error	$1.45e-7$	$9.57e-8$	$6.02e-8$	2.12

Table 2: L_∞ and L_2 errors of velocity (u, w) and pressure p for the decaying vortex for different time steps on a 32×80 grid.

4.2. Surface waves

4.2.1. Theoretical two-dimensional progressive waves

The numerical performance of the conservative scheme for free-surface wave flows is first tested using three theoretical progressive wave solutions, including the linear viscous wave, Stokes wave, and Crapper capillary wave. The performance is compared with the non-conservative formulation in terms of the conservation of mass and momentum.

The linear viscous wave is used to test the performance of the present method for small-amplitude waves. The velocity of a viscous linear wave is $(u_\phi + u_\nu, w_\phi + w_\nu)$, where the subscript ϕ denotes the potential part of the velocity, and the subscript ν denotes rotational part. The surface elevation and the velocity are

given by [75],

$$\begin{aligned}
 \eta(x, z, t) &= a_0 \exp(-2\nu k^2 t) \sin(kx + \omega t), \\
 u_\phi(x, z, t) &= -\omega a_0 \exp(kz - 2\nu k^2 t) \sin(kx + \omega t), \\
 w_\phi(x, z, t) &= \omega a_0 \exp(kz - 2\nu k^2 t) \cos(kx + \omega t), \\
 u_\nu(x, z, t) &= 2\nu k \beta a_0 \exp(\beta z - 2\nu k^2 t) [\sin(kx + \beta z + \omega t) - \cos(kx + \beta z + \omega t)], \\
 w_\nu(x, z, t) &= -2\nu k^2 a_0 \exp(\beta z - 2\nu k^2 t) \sin(kx + \beta z + \omega t).
 \end{aligned} \tag{50}$$

Here, a_0 is the initial amplitude of the wave; k is the wavenumber; $\beta = \sqrt{\omega/2\nu}$ is a depth dependence coefficient related to viscous effects; and ω is the angular frequency determined from the dispersion relationship $\omega = \sqrt{gk}$. For the linear approximation to be effective, a small wave steepness $a_0 k = 0.01$ is chosen. We choose the characteristic timescale to be the inverse of wave frequency ω^{-1} , and the lengthscale to be k^{-1} . The Froude number, which quantifies the relative importance of the inertia and gravity forcing in the flow, is thus $\text{Fr} = (\omega k^{-1})/\sqrt{gk^{-1}} = 1$. We consider cases with two different Reynolds numbers, $\text{Re} = \omega/\nu k^2 = 100$ and $\text{Re} = 500$, to examine the viscous effect on the wave evolution. A higher Reynolds number corresponds to a fluid with lower viscosity or a wave with longer wavelength.

The Stokes wave is a nonlinear potential wave solution suitable for waves with moderate-to-large steepness. The simulation is initialized with a 5th-order Stokes solution [76]. The velocity is calculated from velocity potential ϕ as $(u, w) = (\partial\phi/\partial x, \partial\phi/\partial z)$. The potential $\phi(x, z)$ is solved from $\nabla^2\phi = 0$ with the Dirichlet boundary condition $\phi(x, \eta) = \Phi^S$ at the surface $z = \eta$. The surface elevation η and surface potential Φ^S are given by Equations (17-18) in [76]. Length and time are normalized by the characteristic length k^{-1} and frequency $\omega = \sqrt{gk}$, respectively. Therefore, the Froude number $\text{Fr} = (\omega k^{-1})/\sqrt{gk^{-1}} = 1$, and the Reynolds number is defined as $\text{Re} = \omega/\nu k^2$. We consider a relatively steep Stokes wave with steepness $a_0 k = 0.35$. Under such wave steepness, the wave nonlinearity is no longer negligible, and the deformation of the wave surface is sufficiently large to cover most non-breaking wave applications. We mainly

focus on the case with $Re = 500$, while another case with a lower Reynolds number $Re = 100$ is simulated for comparison.

The capillary wave is used to test the surface tension in the free-surface boundary condition. The initial condition is given by Crapper's solution [77]. The surface elevation η and the surface velocity potential Φ^S satisfies

$$\begin{aligned}\frac{x}{\lambda} &= \frac{\Phi^S}{c\lambda} - \frac{2}{\pi} \frac{A \sin(2\pi\Phi^S/c\lambda)}{1 + A^2 + 2A \cos(2\pi\Phi^S/c\lambda)}, \\ \frac{\eta}{\lambda} &= \frac{2}{\pi} - \frac{2}{\pi} \frac{1 + A \cos(2\pi\Phi^S/c\lambda)}{1 + A^2 + 2A \cos(2\pi\Phi^S/c\lambda)},\end{aligned}\quad (51)$$

where λ is the wavelength, $c = \sqrt{k\gamma/\rho} \sqrt{(1 - A^2)/(1 + A^2)}$ is the phase speed, and $A = 2 \left(\sqrt{1 + (ak)^2/4} - 1 \right) / ak$ is a dimensionless coefficient. The surface potential Φ^S is calculated from the first equation in Eq. (51) using the Newton's method. Then η is determined from the second equation of the above formula. With the surface potential Φ^S and elevation η determined, the velocity field is initialized in the same way as in the simulation of Stokes wave. For the capillary wave, we normalize the length using k^{-1} , and the time using the linear frequency of a capillary wave $\omega = \sqrt{\gamma k^3/\rho}$, which leads to a unit Weber number $We = \rho(\omega/k)^2 k^{-1}/\gamma = 1$. We consider the wave with steepness $a_0 k = 0.35$ at two Reynolds numbers $Re = \omega/\nu k^2 = 500$ and $Re = 100$.

The size of the computational domain for both types of waves is $L_x \times \bar{H} = 2\pi \times 3.5$, discretized by a uniform grid of size 64×200 . With a minimum (half) grid size $\Delta z_{min} = 8.75 \times 10^{-3}$ at the surface, the grid is able to resolve the viscous Stokes boundary layer with a thickness of the order of magnitude $k\delta \sim O(\sqrt{2/Re}) = 0.07$. The wavelength for both cases is set to 2π so that there is one period of wave in the domain. The depth $\bar{H}$ meets the deep water wave condition.

Fig. 3 shows the decay of the amplitude of the linear wave due to viscous dissipation over time. The results from the conservative scheme and the non-conservative scheme are similar. For $Re = 500$, the decay rate agrees well with the theoretical solution Eq. (50). For $Re = 100$, the wave decays at a faster rate compared to the case with $Re = 500$ because of the increased viscous

effects. However, the decay rate is slightly lower than the theoretical prediction in Eq. (50). The small deviation from the linear viscous wave theory is because the Reynolds number is assumed to be much larger than 1 in the theory [75].

Figs. 4a and 4b show the surface elevation profiles for the Stokes wave and the capillary wave, respectively. The nonlinearity of both types of waves can be clearly seen. For the Stokes wave, the wave profile is sharper at the crest and flatter at the wave trough, as shown in Fig. 4a; by contrast, the capillary wave shown in Fig. 4b has a sharp trough and a flattened trough. Both the conservative scheme and the non-conservative scheme give numerical predictions that agree well with the theoretical solution. The results indicate that the present method can capture the features of nonlinear gravity and capillary waves.

The viscous decay of the Stokes wave and the capillary wave is shown in Figs. 5a and 5b, respectively. It can be seen that the evolution of the amplitudes of both types of waves follows the theoretical exponential decay $\exp(-2\nu k^2 t)$. As the Reynolds number decreases, the increased viscous dissipation results in a faster decay of waves. We shall also point out here that the amplitudes oscillate during the wave evolution, indicating the existence of standing wave components. This is mostly due to the mismatch between the viscous flow solver and the initial wave field that is based on the potential flow theory [78], as the amplitude of oscillation is more significant at $Re = 100$.

Next, we examine the conservation of mass and momentum for the present conservative scheme and the previous non-conservative scheme. Only the $Re = 500$ cases are shown. For the linear viscous wave, Fig. 6a shows the change of mean surface, an indicator of the total volume. After four wave periods at $t/T = 4$, the mean surface obtained using the non-conservative scheme approaches 10^{-6} while the conservative scheme keeps the volume change under 10^{-11} . Fig. 7a and 8a show similar comparisons of the mass conservation for the Stokes wave and the capillary wave, respectively. With an increased grid deformations associated with the larger wave steepness, the deviation of the mean surface in both cases reaches an order of 10^{-3} after four wave periods when the non-conservative scheme is used, whereas the deviation in the conservative

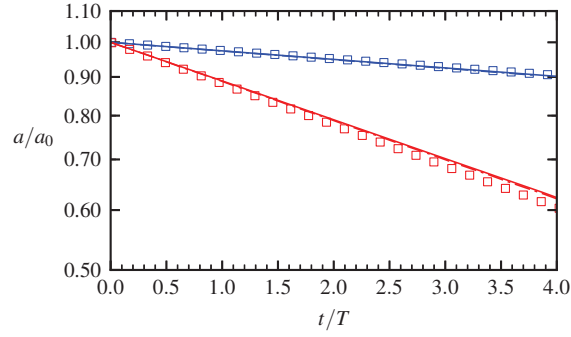


Figure 3: Decay of the amplitude of linear viscous wave for $\text{Re} = 500$ (blue) and $\text{Re} = 100$ (red): —, solution obtained using the conservative scheme; - - -, solution obtained using the non-conservative scheme; $\square$, theoretical solution. The amplitude a is normalized by the initial amplitude a_0 , and time t is normalized by wave period T . The vertical axis is in logarithmic scale.

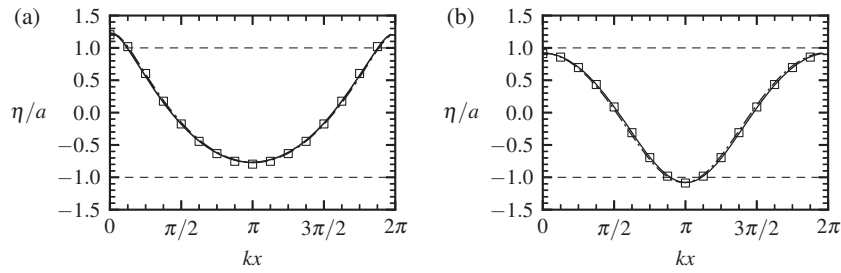


Figure 4: Normalized surface elevation of (a) Stokes wave and (b) capillary wave for $\text{Re} = 500$ after four wave periods $t/T = 4$: —, solution obtained using the conservative scheme; - - -, solution obtained using the non-conservative scheme; $\square$, theoretical solution.

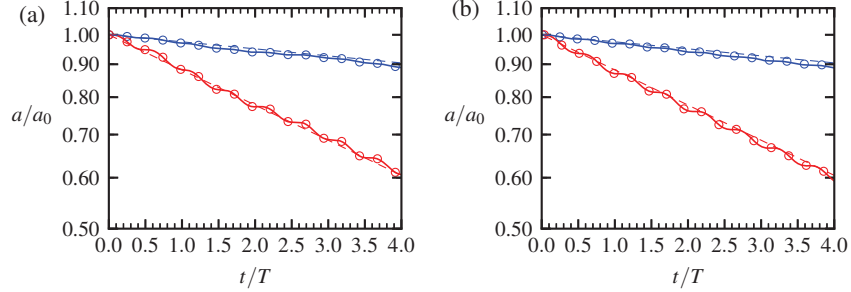


Figure 5: Decay of the amplitude of (a) Stokes wave and (b) capillary wave for $Re = 500$ (blue) and $Re = 100$ (red): —, solution obtained using the conservative scheme; $\circ$, solution obtained using the non-conservative scheme; — — — —, theoretical decay $a/a_0 = \exp(-2\nu k^2 t)$.

scheme is merely of order 10^{-11} . Figs. 6b, 7b and 8b compare the variation of the total u -momentum $M = \int u dx dz$ with time for the above three types of waves, respectively. Because no external stress is applied on the boundaries, the total momentum should remain unchanged. However, M keeps increasing when the non-conservative scheme is used as shown in Figs. 6b, 7b and 8b. On the other hand, the error of momentum M in the conservative scheme is negligible. The above comparisons show that the conservative scheme performs much better than the non-conservative scheme in terms of the conservation of mass and momentum. The advantage becomes more obvious when the surface deformation is increased.

The convergence test for the surface wave cases is also performed for the conservative scheme on three sets of uniform grids: (1) 64×50 ; (2) 64×100 ; and (3) 64×200 . Because of the nonlinear and viscous effects, the theoretical wave solution does not exactly match the numerical solution. We therefore define the error $\epsilon_{i,j}$ as the difference between the numerical solutions obtained on two different grids. Table 3 shows the error and convergence rate for the two types of waves. For the linear wave cases, a convergence rate close to 2 is achieved. While for Stokes wave and the capillary wave, as the wave steepness is increased, the order of accuracy is slightly decreased because of the larger grid deformation.

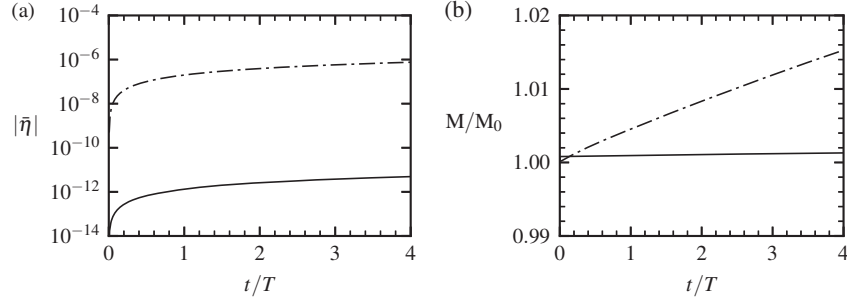


Figure 6: Comparison of mass and momentum conservation between the conservative scheme (—) and non-conservative scheme (— · —) for the simulation of linear viscous wave $Re = 500$. (a) Variation of mean surface elevation with time; the absolute value is taken in order to be plotted in logarithmic scale. (b) The total u -momentum normalized by the initial momentum M_0 . Time t is normalized by wave period T .

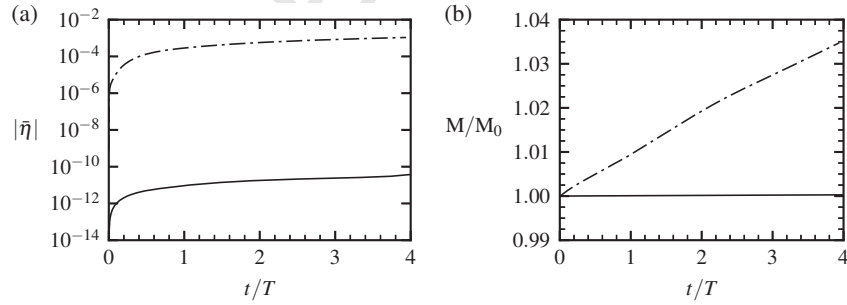


Figure 7: Comparison of mass and momentum conservation between the conservative scheme (—) and the non-conservative scheme (— · —) for the simulation of Stokes wave $Re = 500$. (a) Variation of mean surface elevation with time; the absolute value is taken in order to be plotted in logarithmic scale. (b) The total u -momentum normalized by the initial momentum M_0 . Time t is normalized by wave period T .

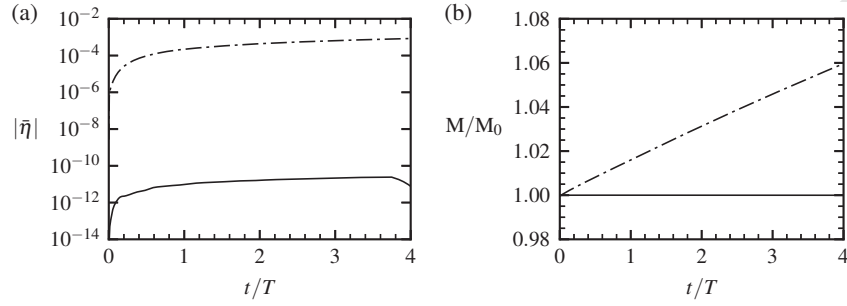


Figure 8: Comparison of mass and momentum conservation between the conservative scheme (—) and the non-conservative scheme (— · —) for the simulation of capillary wave $Re = 500$. (a) Variation of mean surface elevation with time; the absolute value is taken in order to be plotted in logarithmic scale. (b) The total u -momentum normalized by the initial momentum M_0 . Time t is normalized by wave period T .

	$\epsilon_{1,2}$	$\epsilon_{2,3}$	Convergence rate
Linear viscous wave			
L_∞	2.15e-4	5.42e-5	1.98
L_2	1.22e-4	3.07e-5	1.98
Stokes wave			
L_∞	3.22e-3	9.46e-4	1.77
L_2	1.37e-3	4.36e-4	1.65
Capillary wave			
L_∞	3.78e-2	1.05e-2	1.84
L_2	2.48e-2	7.06e-3	1.81

Table 3: L_∞ and L_2 errors of surface elevation η for the surface waves for different grid resolutions.

4.2.2. Crescent waves

The numerical capability of the present method to capture nonlinear waves is further tested with the crescent wave problem. This case also demonstrates the performance of the conservative scheme when waves are very steep (nearly breaking). The crescent wave evolves from a disturbed two-dimensional Stokes wave due to L_2 type instability [79].

The length and time in the problem setup is normalized by the characteristic wavenumber of the undisturbed Stokes wave k and the linear gravity-wave frequency $\omega = \sqrt{gk}$, respectively. The undisturbed Stokes wave has a steepness of $ak = 0.33$. The initial disturbance has surface elevation η^* and velocity potential ϕ^* given by

$$\begin{aligned}\eta^* &= \epsilon a \sin k_x x \cos k_y y, \\ \phi^* &= -\frac{\epsilon a}{(k_x^2 + k_y^2)^{1/4}} \cos k_x x \cos k_y y \exp[(k_x^2 + k_y^2)^{1/2} z],\end{aligned}\tag{52}$$

where $\epsilon = 0.16$, $k_x = 1.5$, and $k_y = 1.23$. Here, similar to the initialization method we use in section 4.2.1, we use the governing equation of velocity potential $\nabla^2 \phi = 0$ and the surface potential to determine the velocity potential ϕ , and then velocity $\mathbf{u}$. The simulation is carried out with $\text{Fr} = (\omega k^{-1})/\sqrt{gk^{-1}} = 1$ and $\text{Re} = \omega/\nu k^2 = 1000$ in a domain of size $L_x \times L_y \times \bar{H} = 4\pi \times 4\pi/1.23 \times 2\pi$. The domain is discretized by a $128 \times 128 \times 97$ grid. The grid is clustered near the surface with the minimum vertical grid spacing $\Delta z_{\min} = 0.025$. The computational parameters are consistent with those in [1].

Fig. 9 shows the surface elevation at different times during the growth of the crescent wave. It can be observed that the wave crests become steeper during the process. By $t/T = 3.17$ with T being the wave period of the initial Stokes wave, the edges of the crescent lines are well formed as shown in Fig. 9c. As the crests continue to grow sharper, the crescent lines extend into a semi-circular shape as shown in Fig. 9f. The crescent lines then grow into a triangular shape (Fig. 9h). The development process described above is consistent with the numerical experiment done using the mixed-Eulerian-Lagrangian (MEL) method [80].

Fig. 10 compares the surface profile along the center of the domain $y = 0$ at $t/T = 4.34$ (as in Fig. 9f) with results obtained by a perturbation method [79], the MEL method [80], and the previous non-conservative scheme [1]. Both the conservative and non-conservative schemes give results that are in agreement with other work. For comparison, we also show the result from a simulation case with a smaller Reynolds number $Re = 250$ in Fig. 10. It is clear that the larger viscous effect inhibits the growth of the crescent wave, and the resulting wave has decreased crest heights and a smoother profile.

The conservation properties of the conservative and non-conservative schemes are quite different, as shown in Fig. 11. When the non-conservative scheme is used, the mean surface first fluctuates in the first two wave periods, and then keeps increasing as shown in Fig. 11a. By $t/T = 5$, the mean surface is elevated by 1.4×10^{-3} . Comparatively, the deviation of mean surface does not exceeds 10^{-10} when the conservative scheme is used. Fig. 11b compares the variation of the total u -momentum M , which should be constant theoretically because there is no shear stress at the upper and lower boundaries. However, M decreases by 5% at $t/T = 5$ when the non-conservative scheme is used. Such large an error is intolerable. On the other hand, the change of M with the conservative scheme is controlled within 0.01%.

4.2.3. Sideband waves carried by a wave train

The ability of the present method to capture long-term nonlinear wave interactions is shown in this section using the simulation of sideband waves carried by a Stokes wave train [81]. The amplitudes of the fundamental Stokes wave and sideband waves change with time due to nonlinear interaction, and form modulation-demodulation cycles. The energy is transferred from the fundamental wave to the sidebands during the modulation, and the energy returns to the original component during the demodulation. It is also found that when the initial steepness of the fundamental wave is large enough, the energy is transferred to the lower sideband permanently after the demodulation, resulting in a frequency downshift. The shift of the energy peak is considered to be caused by

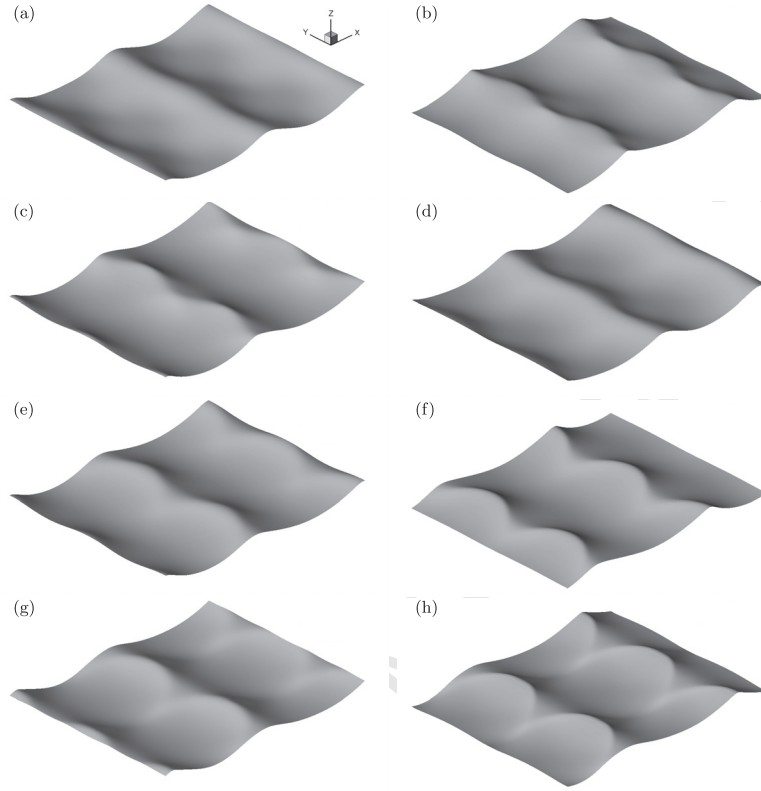


Figure 9: Free-surface patterns during the development of crescent wave. (a) $t/T = 0$, (b) 0.64, (c) 1.08, (d) 2.00, (e) 3.17, (f) 4.34, (g) 5.15, (h) 6.61. Here, T is the wave period of the undisturbed Stokes wave.

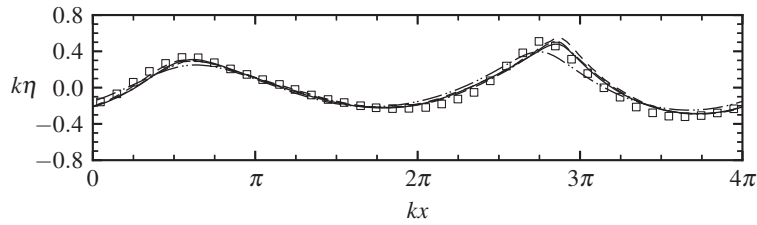


Figure 10: Surface elevation along the centerline $y = 0$ at $t/T = 4.34$: —, numerical solution obtained by the present conservative scheme at $Re = 1000$; $\square$, prediction by a perturbation method [79]; — —, numerical solution obtained by the previous non-conservative scheme [1]; — · —, numerical solution obtained by the MEL simulation [80]; · · ·, numerical solution obtained by the present conservative scheme at $Re = 250$. Here, T is the wave period of the undisturbed Stokes wave.

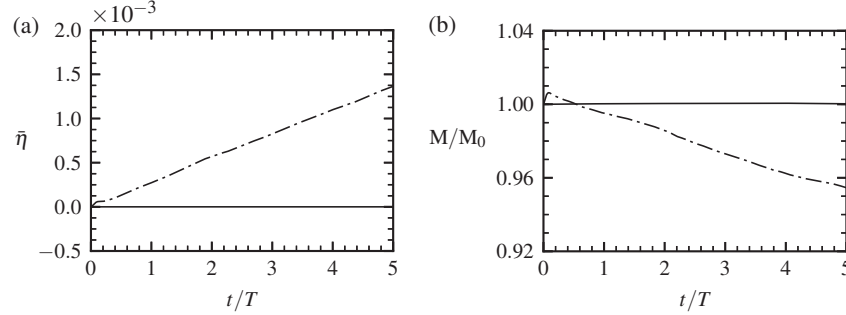


Figure 11: Comparison of mass and momentum conservation between the conservative scheme (—) and non-conservative scheme (---) for the simulation of crescent wave. (a) Variation of mean surface elevation with time. (b) The u -momentum normalized by the initial momentum M_0 . Time t is normalized by the wave period of the undisturbed Stokes wave T .

the dissipation [82, 83]. This case shows the ability of the present scheme to capture the effects of viscous dissipation in the wave evolution. Different from the instability of crescent waves, in the present problem, the evolution of different wave components through nonlinear interactions occurs on a longer time scale, which poses a higher requirement on the numerical conservation performance.

The wave train is simulated in a domain of length $2\pi/L$, and L is used as the characteristic length. The characteristic velocity is $U = \sqrt{gL}$. The fundamental wave train is a Stokes wave with steepness $a_0 k_0 = 0.2$ and wavenumber $k_0 L = 9$, i.e., nine wave periods in the domain. The fundamental wave is perturbed by two sideband waves at the most unstable modes, $k_0 L = 6$ and $k_0 L = 12$. The amplitudes of the sideband waves are 10% of that of the fundamental wave, such that the initial condition for surface elevation and surface potential is [84]

$$\begin{aligned} \eta(x, 0) &= \eta_0 + 0.1a_0 \cos(6x - \pi/4) + 0.1a_0 \cos(12x - \pi/4), \\ \Phi^S(x, 0) &= \Phi_0^S + 0.1 \frac{a_0}{\sqrt{6}} e^{6\eta} \sin(6x - \pi/4) + 0.1 \frac{a_0}{\sqrt{12}} e^{12\eta} \sin(12x - \pi/4), \end{aligned} \quad (53)$$

where η_0 and Φ_0^S are the surface elevation and potential function of the fundamental wave [76], respectively. Using η and Φ^S , we initialize the velocity field using $\nabla^2 \phi = 0$ and $\mathbf{u} = \nabla \phi$ as detailed in section 4.2.1. Dimensionless parameters in this problem include the Reynolds number $\text{Re} = \sqrt{gL^3}/\nu$ and

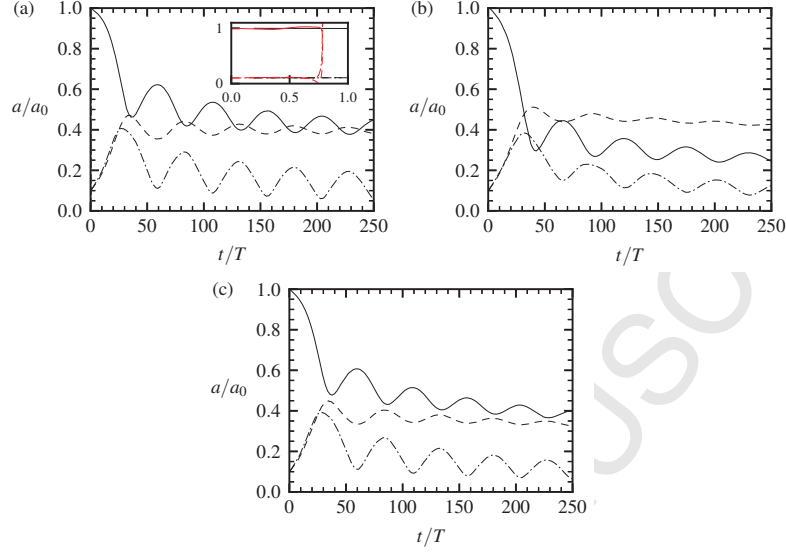


Figure 12: Evolution of the normalized amplitudes of the fundamental wave ($k = 9$, —) and sideband waves ($k = 6$, ---, $k = 12$, - · -) obtained using the conservative scheme for (a) $\text{Re} = 5.37 \times 10^6$, $\text{We} = 2.7 \times 10^5$; (b) $\text{Re} = 1.45 \times 10^5$, $\text{We} = 2.2 \times 10^3$; (c) $\text{Re} = 1.45 \times 10^5$, $\text{We} = \infty$. Also in the small window of (a) are the results from the non-conservative scheme (red). Time t is normalized by the wave period of fundamental wave T .

Weber number $\text{We} = \rho g L^2 / \gamma$, while the Froude number $\text{Fr} = U / \sqrt{g L}$ is 1 by the choice of characteristic velocity. We consider a case with $\text{Re} = 5.37 \times 10^6$ and $\text{We} = 2.7 \times 10^5$, which correspond to a fundamental wave with wavelength 1 m for $\rho = 10^3 \text{ kg/m}^3$, $\nu = 10^{-6} \text{ m}^2/\text{s}$ and $\gamma = 0.074 \text{ N/m}$. A shorter wave train of wavelength 0.09 m is also simulated, corresponding to $\text{Re} = 1.45 \times 10^5$ and $\text{We} = 2.2 \times 10^3$. For comparison, a case of the short wave train without the surface tension effect, i.e., $\text{Re} = 1.45 \times 10^5$ and $\text{We} = \infty$, is simulated to show the effects of surface tension. The simulation is carried out in a domain of size $L_x \times \bar{H} = 2\pi \times 4.0$, with grid number 80×129 . The grid is clustered near the surface with the minimum vertical grid spacing $\Delta z_{\min} = 0.013$.

Fig. 12a shows the temporal evolution of the amplitude of the fundamental waves and sideband waves for the long wave train. As the wave train starts evolving, the amplitudes of the sideband waves increase at the expense of the

fundamental wave. After the fundamental wave reaches the first minimum, energy is transferred back to the fundamental component from the sidebands. Some energy is retained by the subharmonic mode, and the fundamental wave does not return to its initial amplitude. The cycles of energy exchanges between the fundamental and sideband waves continue with damped amplitudes. Some temporary frequency downshifts occur when the fundamental wave reaches local minima in a cycle, but no permanent shift is observed during the simulation period. The non-conservative scheme breaks down shortly after the simulation begins. As shown in the small window of Fig. 12, a nonphysical sharp jump of the wave amplitude occurs right before the breakdown, indicating a numerical instability. This suggests that the conservative scheme has better performance in numerical stability than the non-conservative scheme.

Fig. 12b shows the evolution of the short wave train, which has lower Reynolds and Weber numbers. The simulation using the non-conservative scheme is still unstable, therefore we only show the results from the conservative scheme. After the first modulation-demodulation cycle, the subharmonic wave becomes the dominant mode, and remains to be the dominant component during the evolution of the wave train. Compared to the long wave train, the fundamental wave loses more energy in the first modulation process. The loss of energy is due to the damping of the higher harmonic waves generated from the nonlinear interactions between the fundamental and the upper sideband waves [83, 81]. The energy loss to the viscosity ultimately leads to the frequency downshift. On the other hand, in Fig. 12c, without the surface tension, only a series of decaying modulation-demodulation cycles without frequency downshift is observed. This suggests that the surface tension plays a crucial role in enhancing the generation of short waves, which are damped by the viscous effect. The above results indicate that the conservative scheme can simulate the recurring modulation phenomenon in the long-term evolution of the wave train, and also capture the dissipation effects that can lead to the frequency downshift of the surface waves.

4.2.4. Decay of the broadband wave

In this section, we use a broadband wave field to show the capability of the present numerical scheme to simulate a complex three-dimensional wave field. We initialize the wave field using a JONSWAP spectrum [85], of which the energy density function is given by

$$S(k) = \frac{\alpha}{2k^3} \exp \left[-\frac{5}{4} \left(\frac{k_p}{k} \right)^2 \right] \gamma^{\exp \left[-\frac{(\sqrt{k} - \sqrt{k_p})^2}{2\sigma^2 k_p} \right]},$$

$$\gamma = 3.3,$$

$$\sigma = \begin{cases} 0.07 & k \leq k_p, \\ 0.09 & k > k_p. \end{cases}$$
(54)

Here, $S(k)$ is a one-dimensional spectrum given in the wavenumber space, and the constant α and peak wavenumber k_p are the parameters of the spectrum. For a three-dimensional wave field, the directional wave spectrum is

$$\tilde{S}(k, \theta) = S(k)\chi(k, \theta),$$
(55)

where the directional function $\chi(k, \theta)$ is given by

$$\chi(k, \theta) = \begin{cases} \frac{2}{\pi} \cos^2 \theta & |\theta| \leq \frac{\pi}{2}, \\ 0 & |\theta| > \frac{\pi}{2}, \end{cases}$$
(56)

such that the wave components spread over an angle of π . Both the JONSWAP spectrum and the directional function used here are representative of the broadband wave field. While the JONSWAP spectrum is an empirical model for wind waves, we do not include wind inputs in the present setup. Without any input of the energy, the waves are expected to decay due to the viscous dissipation. For the simulation, we choose the parameters $\alpha = 0.047$ and $k_p = 12.4 \text{ m}^{-1}$ for the initial spectrum $S_0(k)$, and we only consider the gravity effects with $g = 9.8 \text{ m} \cdot \text{s}^{-1}$. The initial wave field is obtained using the superposition of linear wave components at random phases. The amplitudes of each wave components are calculated using Eqs. (54-56). The simulation is performed in a domain of size $16 \text{ m} \times 9 \text{ m} \times 3 \text{ m}$, discretized by a grid having $640 \times 480 \times 201$

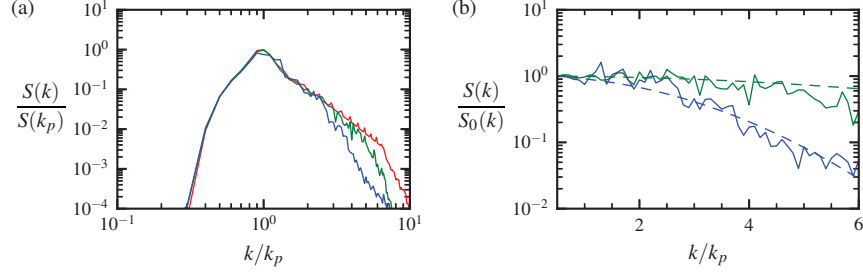


Figure 13: Evolution of the wave spectrum: $t/T_p = 0$ (red), $t/T_p = 35$ (green) and $t/T_p = 250$ (blue). (a) Wave spectrum $S(k)$. (b) Relative wave spectrum S/S_0 : —, solution obtained using the conservative scheme; - - -, $\exp(-4\nu k^2 t)$. The wavenumber k is normalized by the peak wavenumber k_p .

points. The grid is clustered near the surface with a minimum vertical spacing of $\Delta z_{min} = 0.8$ mm.

Fig. 13 shows the evolution of the one-dimensional wave spectrum $S(k)$ obtained from the present conservative scheme, while the non-conservative scheme fails to simulate the broadband waves. It is shown in Fig. 13a that the wave energy decays with time. The wave energy in the high wavenumber region decays faster than that in the low wavenumber region. The ratio of the wave spectrum to the initial spectrum $S(k)/S_0(k)$ is shown in Fig. 13b, which also shows that the shorter waves decay faster than the longer waves. The decay of the spectrum generally follows a rate of $\exp(-4\nu k^2 t)$ [75], i.e., the spectrum decays exponentially with time t , and the decay rate increases quadratically with wavenumber k . The decay of the short waves results in the change of the surface patterns, as shown in Fig. 14. Initially, there exist many short waves, leading to a rough surface (Fig. 14a). By contrast, at a later time $t/T_p = 250$, the surface appears smoother due to the decay of the short waves (Fig. 14b). The above results indicate that the present numerical scheme is able to simulate complex three-dimensional broadband waves, and directly capture the viscous effect in wave evolution.

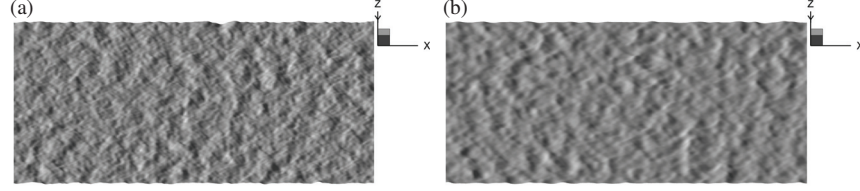


Figure 14: Free-surface elevation of the broadband waves. (a) $t/T_p = 0$, (b) $t/T_p = 250$. Here T_p is the wave period of the peak wave. To show the details of the short waves, only an area of $6\text{ m} \times 5\text{ m}$ at the center of the domain is shown, and the elevation is amplified by three times.

4.3. Vortex pair interacting with free surface

Next, we consider the interaction between the free surface and a pair of vortices in viscous fluid [86] to show the ability of the present scheme for rotational, viscous, free-surface flows. In this problem, two counter-rotating two-dimensional vortices of the same strength initially located far below the surface rise towards the free surface through self-induced motion. The vortices induce surface disturbance as they approach the free surface. Meanwhile, the two vortices depart from each other horizontally due to the blocking effect of the boundary before they move away from the surface.

The problem is non-dimensionalized by the initial distance of the vortices l_0 , and the translational velocity of the vortex pair $V = \kappa/l_0$ with κ being the vortex strength. Therefore, the Froude number and the Reynolds number are defined as $\text{Fr} = V/\sqrt{gl_0} = \kappa/\sqrt{gl_0^3}$ and $\text{Re} = Vl_0/\nu = \kappa/\nu$, respectively. The simulation is carried out in a domain of size $L_x \times \bar{H} = 6 \times 6$. The undisturbed free surface is at $z = 0$. The vortices are initially located at $z = -3$, and are symmetric about axis $x = 0$. The dimensionless velocity inside the vortex core $r \leq r_L$ is initialized by a Lamb vortex model [75] as

$$v_\theta = -\frac{1}{r} \left[1 - \exp\left(-\frac{r^2 \text{Re}}{4t_0}\right) \right], \quad r \leq r_L, \quad (57)$$

where v_θ is the azimuthal velocity; and r is the distance from the vortex center. Outside the vortex $r > r_L$, velocity is given by an irrotational point vortex model. The calculations are performed for $r_L = 0.25$, $t_0 = 0.25$, $\text{Re} = 100$,

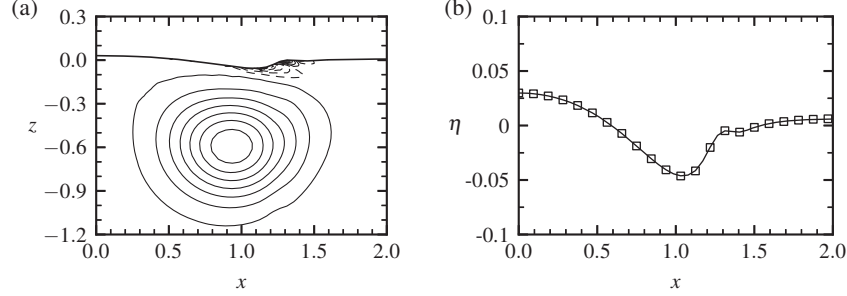


Figure 15: Interaction of a vortex pair with a free surface for $Re = 100$: (a) contours of vorticity ω_y at $t = 3.5$; (b) surface profile in (a) predicted by the conservative scheme (—) and the non-conservative scheme ($\square$). All figures show only the positive x -plane due to symmetry.

and $Fr^2 = 0.02$. This pair of Reynolds number and Froude number yields moderate deformations of the free surface [86], which can generate rich surface flow features while preventing the deformations to be too large. Another case of $Re = 20$ is simulated to show the influence of the viscous effect. To capture the near-surface dynamics accurately, a grid clustered vertically near the surface is used, with the minimum grid spacing $\Delta z_{min} = 0.0042$.

Fig. 15 shows the surface elevation and vorticity ω_y as the vortices approach the surface for $Re = 100$. Only the positive- x half of the domain is shown due to the symmetry. At the center of the domain, the free surface is slightly pushed up by the vortex pair, and a relatively sharp depression is created on the other side of the vortex. Surface vorticity is generated associated with the deformation of the surface to the right of the depression. As shown in Fig. 15b, the surface profile predicted by the present method is in a good agreement with the previous method.

We further examine the conservation of mass and momentum in this case. As shown in Fig. 16a, for the non-conservative scheme, the mean surface is elevated rapidly when the vortex pair interacts with the free surface. Even after the vortices leave the surface, the mean surface does not return to its initial location. In contrast, the mean surface deviation in the conservative scheme is controlled

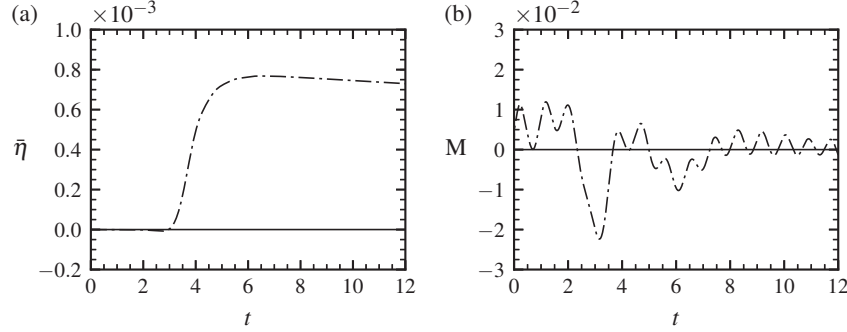


Figure 16: Comparison of mass and momentum conservation between the conservative scheme (—) and non-conservative scheme (---) for the simulation of the interaction of a vortex pair with a free surface, $Re = 100$. (a) Variation of mean surface elevation with time. (b) Variation of the total u -momentum with time; the momentum is only integrated in the positive x -plane due to symmetry.

within 10^{-14} . The difference between the two schemes in the momentum conservation is also obvious in Fig. 16b. The surface deformation causes spurious momentum change in the fluid with the non-conservative scheme, whereas the momentum in the conservative scheme barely changes. We would like to point out that in free-surface turbulent flows, turbulent vortices constantly interact with the surface, therefore the numerical error in conservation observed here can accumulate over the course of the simulation.

For the case with a smaller Reynolds number $Re = 20$, the surface deformation and vorticity distribution are shown in Fig. 17. Due to the strong viscous effect, the vortex is more diffused compared with that in Fig. 15. The strength of the vortex also diminishes fast so that the surface deformation is damped, and no sharp depression is observed. Correspondingly, the surface vorticity associated with the surface deformation is also weak. Due to the negligible surface elevation in this case, we do not show the comparison of the conservation properties for conciseness.

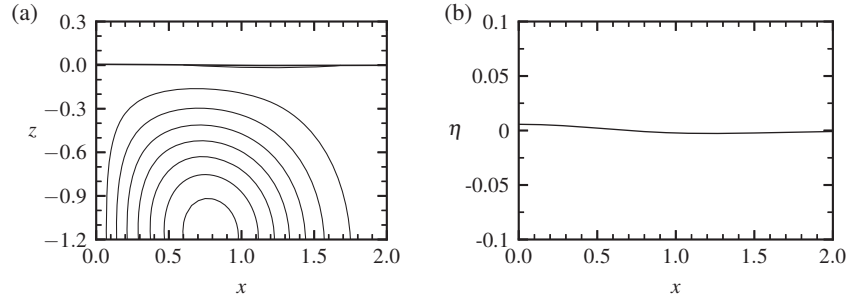


Figure 17: Interaction of a vortex pair with a free surface for $Re = 20$: (a) contours of vorticity ω_y at $t = 3.5$; (b) surface profile in (a) predicted by the conservative scheme (—). All figures show only the positive x -plane due to symmetry.

4.4. Langmuir circulation

One of the major applications of the present numerical scheme is the simulation of wave-current-turbulence interaction problems. We use the case of Langmuir circulation to show this capability. Langmuir circulation is a phenomenon that frequently occurs in upper oceans and lakes as a result of the interactions among surface gravity waves, wind-driven current, and turbulence [2]. The circulations are pairs of counter-rotating vortices, roughly aligned with the wind direction. The convergence zones between the circulating structures are manifested by the amalgamation of buoyant materials, known as windrows. Langmuir circulations are now considered as turbulent coherent structures (thus the turbulence therein is called Langmuir turbulence) associated with the distortion of surface waves. The effects of surface waves on the current and turbulence beneath are traditionally modeled through the Craik–Leibovich (C-L) equations [87, 88]. In the C-L equations, the fluid motions are averaged over waves, and the instantaneous wave motions are not directly included in the model (i.e., the water surface is flat). Instead, a vortex force $\mathbf{u}_s \times \boldsymbol{\omega}$, where $\mathbf{u}_s$ is the Stokes drift of surface waves and $\boldsymbol{\omega}$ is the vorticity, models the accumulative distortion effects of waves on turbulence. Although the C-L equations are only a wave-phase-averaged description of the turbulent flow below surface waves, they are used with LES in most of the existing numerical studies of Langmuir circulation

(see e.g. [8, 89, 90, 91]). With the present method, it is possible to perform simulation of Langmuir circulation with waves explicitly resolved such that flow physics can be directly captured without the use of the vortex force modeling and flat-surface approximation.

However, the wave-resolved simulation of Langmuir circulation is challenging because the fluid motions span a wide range of spatial and temporal scales. The magnitude of the Langmuir circulation, mean current, and turbulent fluctuations is typically one order smaller than that of the wave motions. Meanwhile, the eddy turnover timescale of the Langmuir circulation is substantially longer than the wave period. A more detailed order-of-magnitude analysis for our simulation case is shown later. The above disparate scales pose great challenges to the simulation in that the turbulent flow needs to take at least several eddy turnover time and thousands of wave periods to reach fully developed state, but at the same time the secondary circulations and turbulence can be contaminated by numerical error. The test cases presented in preceding sections show that the non-conservative scheme yields numerical error in a short period of time, and in the case of Langmuir circulation, the error is found to substantially accumulate over time. We find that when the non-conservative scheme is used in simulations of Langmuir circulation, the total volume increases by 1.1% after only one eddy turnover time. The error in momentum balance is even worse, reaching 11% over the same period of time. Such large numerical errors render the simulation results obtained with the non-conservative scheme unacceptable. In contrast, the change of volume is negligible when the conservative scheme is used. An integration of the momentum also shows that the conservative scheme has much smaller momentum error, only about 1.7%. This result shows that the conservative scheme is more accurate, and is necessary for capturing the complex interactions among waves, current, and turbulent flows, especially when the physical problem involves multiple time and velocity scales.

The simulations are performed in a domain of size $L_x \times L_y \times \bar{H} = 16\pi/7 \times 16\pi/7 \times 1$ when normalized by the mean depth $\bar{H}$. A surface wave with wavelength $\lambda = 4\pi/7$ and steepness $ak = 0.084$ propagates in the x -direction. The

current and turbulence is driven by a constant shear force τ aligned with the x -direction and tangent to the wave surface. The velocity is normalized by the friction velocity $u_* = \sqrt{\tau/\rho}$. We set the Reynolds number $\text{Re} = u_* \bar{H}/\nu = 2000$, and Froude number $\text{Fr} = u_*/\sqrt{g\bar{H}} = 4.62 \times 10^{-4}$. With the absence of a turbulent wall-layer model at the wavy free surface, this moderate Reynolds number allows us to perform wall-resolved LES, where the grid is refined near the surface to resolve the inner boundary layer directly. The Froude number is directly related to the wave properties, which affect the turbulent Langmuir number $\text{La}_t = (u_*/U_s)^{1/2}$ with U_s being the surface Stokes drift of the wave. Here, La_t is used to evaluate the relative importance of the shear forcing and wave forcing [89], and is an important dimensionless number in determining the flow features of Langmuir circulation. Using the estimation from the linear wave theory, the surface Stokes drift is $U_s = (ak)^2 \sqrt{g/k}$, and the Froude number corresponds to a turbulent Langmuir number $\text{La}_t = 0.35$. It is reported that a turbulent Langmuir number $\text{La}_t < 0.7$ indicates a wave forcing strong enough for the generation of Langmuir circulations and for the Langmuir turbulence to be dominant [90]. Using the turbulent Langmuir number Fr and wave steepness ak , we can estimate the range of velocity scales in the problem. The orbital velocity of wave $\mathbf{u}_w$ is estimated by the linear wave theory to be $O(U_s/ak)$, therefore we have

$$\mathbf{u}_w \sim O(U_s/ak) = O\left(\frac{u_*}{ak\text{La}_t^2}\right) \approx O(10^2 u_*).$$

On the other hand, the current speed and turbulent motions are $O(u_*)$, which are thus much weaker than the wave motions. We can also estimate the time scales. The wave period T_w is

$$T_w = \frac{2\pi}{\sqrt{gk}} = \frac{2\pi\text{Fr}}{\sqrt{k\bar{H}}} \frac{\bar{H}}{u_*} = \text{Fr} \sqrt{\frac{2\pi\lambda}{\bar{H}}} \frac{\bar{H}}{u_*} \approx 1.56 \times 10^{-3} \frac{\bar{H}}{u_*},$$

where $\bar{H}/u_*$ is the eddy turnover time of turbulent motions. This means that there are about 640 wave periods in one eddy turn over time. The above analysis again confirms the wide range of scales in the problem of Langmuir circulation, which requires a conservative scheme for accurate simulations.

The simulations are initiated with a linear wave with no mean current. The surface wave is dynamically imposed and maintained using a pressure-forcing method [78]. Small disturbances are added near the surface to initiate the turbulence generation. Another case without surface wave is set up for comparison.

For the analysis of the results, we introduce a triple velocity decomposition $\mathbf{u} = \mathbf{u}_c + \mathbf{u}_w + \mathbf{u}'$. The sum of mean current $\mathbf{u}_c$ and wave-induced orbital velocity $\mathbf{u}_w$ is assumed to be spanwise-independent, and is therefore obtained by phase-averaging as

$$\mathbf{u}_c + \mathbf{u}_w = \langle \mathbf{u} \rangle(x, z, t) = \frac{1}{T} \frac{1}{L_y} \int_t^{t+T} \int_0^{L_y} \mathbf{u}(x + ct, y, z, \tau) dy d\tau. \quad (58)$$

The remaining part $\mathbf{u}'$ is turbulence fluctuation. To separate the current and wave velocity, we use the definitions in generalized Lagrangian mean [92]. The total Lagrangian transport $\bar{\mathbf{u}}^L$, contributed by the Eulerian current transport and wave-induced Lagrangian transport, is obtained with a Lagrangian average of velocity $\langle \mathbf{u} \rangle$,

$$\bar{\mathbf{u}}^L(\mathbf{x}, t) = \frac{1}{T_L} \int_0^{T_L} \langle \mathbf{u} \rangle(\mathbf{x} + \boldsymbol{\xi}(\mathbf{x}, \tau), \tau) d\tau. \quad (59)$$

Here, T_L is the Lagrangian wave period [93]; $\mathbf{x} + \boldsymbol{\xi}$ is the trajectory of a fluid particle convected by $\langle \mathbf{u} \rangle$. The wave-induced Lagrangian transport is approximated by wave pseudomomentum $\mathbf{P}_i = -\overline{\xi_{j,i}(\langle \mathbf{u} \rangle - \bar{\mathbf{u}}^L)_j}$. The mean current is therefore $\mathbf{u}_c = \langle \mathbf{u} \rangle - \mathbf{P}$.

A snapshot of the instantaneous turbulent vortex structures in the Langmuir circulation flow obtained from the simulation is shown in Fig. 18. The vortex structures are identified by the λ_2 -criterion, where the vortex core is associated with negative λ_2 [94]. Here, λ_2 is the second largest eigenvalues of the tensor $\mathbf{S}^2 + \boldsymbol{\Omega}^2$, where $\mathbf{S} = (\nabla \mathbf{u}' + \nabla \mathbf{u}'^T)/2$ and $\boldsymbol{\Omega} = (\nabla \mathbf{u}' - \nabla \mathbf{u}'^T)/2$. Strong vortices are confined near the wave surface, and are mostly aligned in the streamwise direction. These quasi-streamwise vortices alternate in signs and result in local upwelling and downwelling mixing. The downwelling zone corresponds to a surface convergence region. The vortices have different strength, streamwise length, and spanwise spacing. The irregular patterns of the vortices is a manifestation

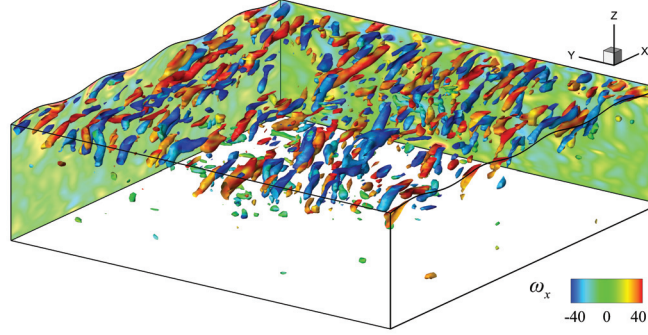


Figure 18: Instantaneous vortex structures in Langmuir turbulence identified by iso-surfaces of negative λ_2 [94]. The iso-surfaces are colored by the streamwise vorticity ω_x .

of the turbulence randomness.

The surface flow structures are visualized through tracking the distribution of floating particles as shown in Fig. 19. Initially, 10^4 particles are released randomly on the surface (Fig. 19a). The particles are then transported by the flow, but are restricted to the surface. After $tu_*/\bar{H} = 0.125$ (Fig. 19b), which is about 80 wave periods, most particles amalgamate into several narrow bands that are oriented into the streamwise direction, and only a few particles scatter between the bands. We also note that the spacing between the bands is irregular, and bands join and split in the process. Overall, the number of bands decrease, as shown in Fig. 19c when $tu_*/\bar{H} = 0.25$ (about 161 wave periods). The irregular patterns of the bands and the change of patterns over time indicates that there are unsteady local circulations with multiple scales and different strengths, as one observes from the instantaneous vortex structures. Small circulations tend to merge into larger and steadier ones. These observations are consistent with the features of Langmuir circulations obtained in previous studies [2, 89].

Two pairs of counter-rotating structures are revealed when we perform averaging of $\mathbf{u}'$ over time and the streamwise direction, as shown in Fig. 20. The averaging operation removes the instantaneous, unsteady vortices observed in Fig. 18, and retain the large-scale structures with long lifetime. These rotating structures, which we call the mean Langmuir circulations, are the steady

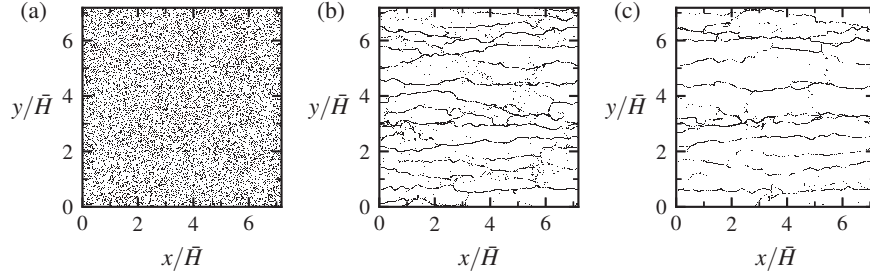


Figure 19: Distribution of particles after being released randomly on the surface. (a) Initial distribution at $t = 0$; (b) at $tu_*/\bar{H} = 0.125$ (about 80 wave periods after releasing); (c) at $tu_*/\bar{H} = 0.25$ (about 161 wave periods after releasing).

secondary flows induced by the wave-current interactions. The vortices extend to the bottom, with the spanwise width slightly larger than the depth. The alternating spanwise velocity at the surface generates converging and diverging zones. Below the converging zones are the downwelling regions, which are narrower than the upwelling ones. The downwelling flow is stronger than the upwelling flow. These asymmetric features of vortices are consistent with the descriptions of Langmuir circulations [87]. Also shown in the figure is the deviation of the mean streamwise velocity from the mean current. The flow in the downwelling regions is faster than the surroundings, which is the result of high momentum flow near the surface brought down by the downwelling motions. On the other hand, the low momentum fluid is transported upward by the upwelling motions. These imply that the vortices enhance the vertical momentum transport.

Fig. 21 shows the mean current profiles in the Langmuir circulation flow and purely shear-driven flow. The mean current in Langmuir circulations is much weaker than that in the shear turbulence. In addition, the current in the Langmuir turbulence is almost uniform as the depth changes except in the vicinity of the surface, indicating an enhanced vertical mixing by Langmuir circulations compared to shear turbulence.

The turbulence statistics of the Langmuir circulation flow and shear tur-

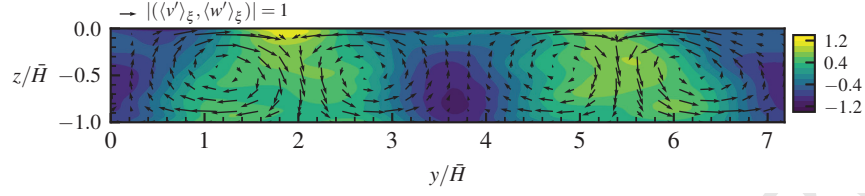


Figure 20: Mean Langmuir circulation structures shown by the vectors $(\langle v' \rangle_\xi, \langle w' \rangle_\xi)$ and the contours of $\langle u' \rangle_\xi$. The vectors show the direction of rotation, and the lengths of vectors indicate the velocity magnitude of circulation. The contours of $\langle u' \rangle_\xi$ indicate the deviation of streamwise velocity from the mean current. The velocities are normalized by u_* .

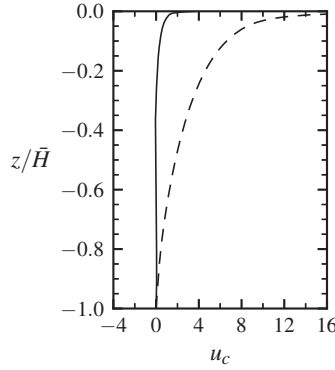


Figure 21: Mean current profiles in Langmuir circulation flow with $La_t = 0.35$ (—) and shear turbulence (---). The velocity is normalized by u_* .

bulence are compared in Fig. 22. As shown, spanwise and vertical fluctuations are intensified in Langmuir circulation flow, consistent with the presence of streamwise vortices. Meanwhile, streamwise velocity fluctuations are suppressed in Langmuir circulation. Comparing the fluctuation intensities in three directions, we find that $\langle v'^2 \rangle > \langle w'^2 \rangle > \langle u'^2 \rangle$ for Langmuir circulation, and $\langle u'^2 \rangle > \langle v'^2 \rangle > \langle w'^2 \rangle$ in shear turbulence. This result agrees with previous studies [89, 90]. Reynolds shear stress, an indicator of vertical momentum flux, is also increased near the surface, indicating the intensified vertical mixing by Langmuir circulation. The results shown above confirm that our wave-resolved simulation successfully captures the features of Langmuir circulation.

The present method is a useful tool for studying wave-current-turbulence

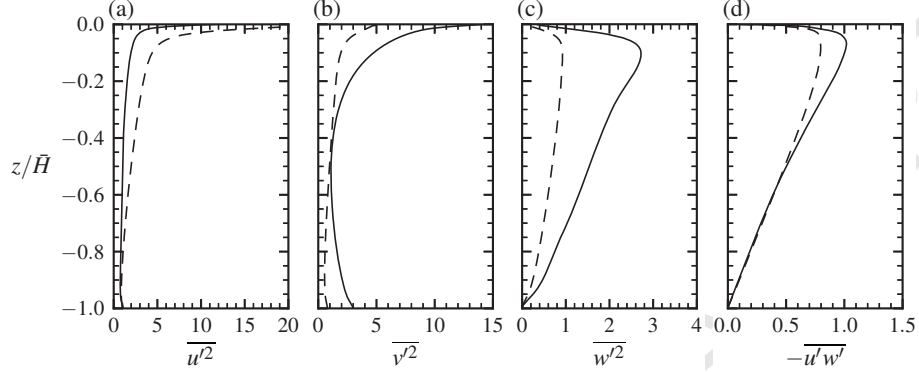


Figure 22: Vertical profiles of Reynolds stresses in Langmuir circulation and shear turbulence: —, Langmuir circulation with $\text{La}_t = 0.35$; ---, shear turbulence. (a) $\overline{u'^2}$; (b) $\overline{v'^2}$; (c) $\overline{w'^2}$; (d) $-\overline{u'w'}$. The Reynolds stresses are normalized by u_*^2 .

interactions in Langmuir circulation, especially the wave-phase-dependent flow quantities that cannot be obtained from the traditional approach using the C-L equations. An example is shown by the distribution of Reynolds stresses in Fig. 23. As shown in Fig. 23a, streamwise fluctuations $\langle u'^2 \rangle$ are confined to the near-surface region, consistent with Fig. 22a. For $\langle v'^2 \rangle$, Fig. 23b shows that its contours roughly follow the wave geometry, indicating its strong dependence on the vertical distance from the surface. Fig. 23c shows that the vertical turbulence fluctuations $\langle w'^2 \rangle$ are enhanced under the wave crest. The increased vertical fluctuations also correspond to the intensified Reynolds shear stress $-\langle u'w' \rangle$ under the wave crest, as shown in Fig. 23d. The latter two results indicate that the vertical mixing is enhanced as the wave crest passes by.

5. Conclusions

In this paper, we present a conservative numerical scheme designed for the simulation of free-surface viscous wave and turbulent flows on a curvilinear wave-surface-fitted grid. Good conservation properties of the new scheme are obtained with the use of strong conservative formulations of the continuity equation and Navier–Stokes equations. The numerical implementation is consistent

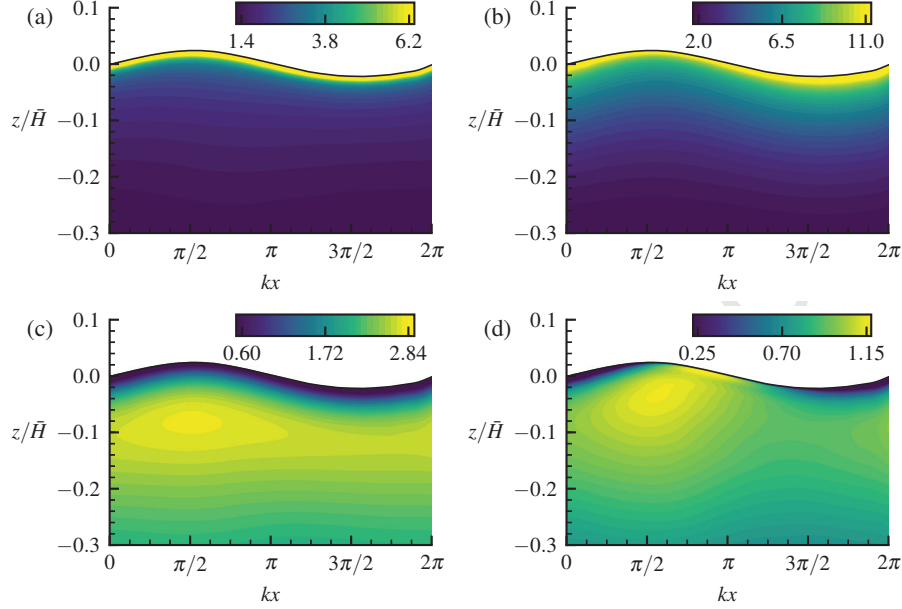


Figure 23: Contours of phase-averaged Reynolds stresses in the Langmuir circulation flow: (a) $\langle u'^2 \rangle$; (b) $\langle v'^2 \rangle$; (c) $\langle w'^2 \rangle$; (d) $-\langle u'w' \rangle$. The Reynolds stresses are normalized by u_*^2 .

with the conservative formulation and ensures that the conservation properties are preserved. A Fourier-series-based pseudo-spectral method is employed for the discretization in the horizontal directions, and a finite-difference method is used in the vertical direction. The incompressibility condition is satisfied by using a fractional-step method and the iterative solution of a nonlinear pressure Poisson equation. The free surface elevation is integrated in time with a Runge–Kutta scheme.

We have also developed LES for free-surface turbulent flows in the framework of the conservative scheme. The SGS stress terms are also written in a conservative form. A Lagrangian-average based scale-dependent dynamic model is used to account for the inhomogeneity in the turbulent flows of interest. Such SGS modeling avoids ad-hoc parameterization, and allows the applications to more complex turbulent flows.

The solutions of the present method are validated against several existing

analytical and numerical solutions. It is found that the present method can simulate canonical waves and complex nonlinear wave interactions accurately. Good agreement is found in all comparisons. Specifically, the comparison with the previous non-conservative scheme shows that the conservative scheme has substantial improvement in the conservation of mass and momentum, especially when the wave steepness increases. The conservative scheme also predicts the long-term nonlinear wave interactions between fundamental and sideband modes, for which the non-conservative scheme fails to simulate. The frequency downshift due to the viscous dissipation and the surface tension is also captured in the simulations. The simulation of the decay of broadband waves indicates that the present conservative scheme has the ability to simulate viscous effects in a complex wave field.

As a demonstration of the strength of the new scheme, it is applied to the simulation of Langmuir circulation, a problem with complex wave-current-turbulence interactions. The simulation is carried out with the surface waves resolved explicitly. The conservative scheme is found necessary for reliable numerical predictions of the long-term evolution of free-surface turbulence flows, because significant errors in mass and momentum conservation can accumulate and contaminate the results when a non-conservative scheme is used. The statistical results show that the interactions between surface waves and shear-driven turbulence result in a more uniform current and intensified spanwise and vertical turbulence fluctuations, which are consistent with the characteristics of the Langmuir circulation flows. Meanwhile, the present method also successfully captures the circulations of different scales and surface flow structures. We have demonstrated the ability of the present method to capture both the mean and instantaneous distortion effects of waves on the current and turbulent flows underneath.

The numerical scheme presented in this paper has the capability for high-fidelity simulation of a variety of complex turbulent flows with surface waves. Conservative scheme is not only shown to produce more accurate results, but also proven to be necessary for physical problems involving nonlinear wave in-

teraction and complex wave-current-turbulence interaction. The present scheme can also be used for studies of the viscous effect in the nonlinear wave dynamics. Furthermore, LES extends the ability of the method to high Reynolds number turbulent flows. To further improve the simulation ability, more experimental data and DNS data need to be analyzed to investigate SGS modeling of the free-surface kinematics and dynamics. The effect of waves on SGS stresses is also an important factor in the LES. These research topics will be studied in our future research.

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