2011

WAVE-INDUCED SEDIMENT TRANSPORT: SIMULATION OF TURBULENT WAVE BOUNDARY LAYERS

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WAVE-INDUCED SEDIMENT TRANSPORT: SIMULATION OF TURBULENT WAVE BOUNDARY LAYERS

BY

JEFFREY C. HARRIS

A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN OCEAN ENGINEERING

UNIVERSITY OF RHODE ISLAND

2011
DOCTOR OF PHILOSOPHY DISSERTATION

OF

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2011
ABSTRACT

Two manuscripts are presented which develop a numerical method for studying boundary layer flow and sediment transport on the seafloor. Inviscid flow, either through an analytic solution or a numerical wavetank (NWT) is used to force a previously developed three-dimensional Navier-Stokes model. The resulting hybrid model is able to simulate complex turbulent flows near the ocean bottom or around obstacles.

The first manuscript reports on developments of a perturbation approach to large-eddy simulations (LES) of wave-induced boundary layers. In the present formulation, the total velocity and pressure fields are expressed as the sum of irrotational and near-field viscous perturbation, where the irrotational field is known a priori. The LES equations are formulated and solved for the perturbation fields only, which are forced by the known incident fields. Results are presented for laminar oscillatory boundary layers, as well as for laminar steady streaming induced by small-amplitude waves, which show convergence to known analytic solutions. To demonstrate potential applications, forcing from a two-dimensional NWT is applied, showing the steady streaming that exists in a laminar boundary layer under large-amplitude water waves. Results are also shown for turbulent oscillatory boundary layers, which agree well with published experimental data.

The second manuscript presents LES results of sediment transport over vortex ripples. A conformal mapping is used to match the computational domain to an experimentally derived shape of vortex ripples formed in a large-scale oscillatory water tunnel. While the instantaneous velocity field and time-averaged velocity field agrees reasonably well with published experimental data, the time- and ripple-averaged velocity profile differs substantially. As well, the suspended sediment concentration above the ripple crest is substantially different than that observed
experimentally. These effects, likely the result of insufficient resolved turbulent intensity in the LES, result in poor predictions of suspended sediment transport rates.
ACKNOWLEDGMENTS

This work was made possible by the Department of Ocean Engineering at the University of Rhode Island (URI), particularly my advisor, Stèphan Grilli. The staff of the Pell library, particularly Roberta Doran, has been instrumental in processing interlibrary loan requests needed for the literature reviews in this dissertation.

Much of this work was supported by a three year National Defense Science and Engineering Graduate (NDSEG) fellowship from the Office of Naval Research.

The numerical results of this dissertation would not have been possible without the support of external computer time. Early on in this project it was provided by a grant of computer time from the DoD High Performance Computing Modernization Program at the Maui High Performance Computing Center and at the Naval Oceanographic Office Major Shared Resource Center. More recently, and for much of the final tests, computer time was provided by URI on a computer system overseen by David Freeman of the Chemistry department at URI.

The source code for the Navier-Stokes solver which was modified for this dissertation was provided by Robert Street and Oliver Fringer at the Environmental Fluid Mechanics Laboratory at Stanford University. This work was based on an earlier collaboration between their lab and Rick Gilbert, a former Master’s student at URI.

Finally, much thanks goes to those who provided data for comparison with these results, including Senthil Radhakrishnan, who provided a copy of the Jensen et al. data which was used in the first manuscript, and Jebbe van der Werf, who provided a copy of his data for comparison in the second manuscript.
PREFACE

This project, presented in Manuscript Format, started at the University of Rhode Island (URI) as a part of an Office of Naval Research effort to better understand mine burial prediction. For a few years, a collaboration existed between the Environmental Fluid Dynamics Laboratory at Stanford University headed by Robert Street and Stéphane Grilli’s research group in the Ocean Engineering department of URI. This work dealt with modeling the flow around a partially buried mine with a large-eddy simulation (LES). Rick Gilbert wrote numerous articles and a master’s thesis covering this implementation of the project. As described in the first manuscript, the research involved in this dissertation has diverged from the efforts at Stanford and focused on implementing a new perturbation method for boundary layer simulations. The earliest results of this new technique were published in the Proceedings of the 31st International Coastal Engineering Conference.

The first manuscript describes and validates the numerical methodology. A simple test case of Stokes flow is used to validate the model and gives results accurate to second-order in both space and time. In order to validate the convective terms of the momentum equation, which differ in this approach versus a typical Navier-Stokes solver, steady streaming within a wave-induced boundary layer is predicted. Both of these problems are for laminar flow, so theoretical expressions exist for the expected results. To demonstrate potential applications, forcing from a two-dimensional NWT is applied, showing the steady streaming that exists in a laminar boundary layer under large-amplitude water waves. Finally, two test cases of rough turbulent oscillatory flow are used to validate the turbulence models used against experimental data. Rough turbulent oscillatory flow is a contemporary research problem, and the results obtained are similar to other researchers.

The second manuscript is a validation of the sediment transport model. The
LES, which models suspended sediment as a passive tracer (with a constant settling velocity), is compared to experimental results for oscillatory flow over vortex ripples. The velocity field predicted by the coupled model compares well with the laboratory experiments for oscillatory flow over full-scale vortex ripples, but do not accurately predict the overall suspended sediment flux.

The five appendices cover: theoretical solutions to laminar boundary layer flows; general theory of wave-induced boundary layers; the setup of the LES simulations; a description of all changes to the LES source code; and a detailed description of the numerical methods used in the coupled LES code. A natural extension of this work would be an additional manuscript detailing wave-induced sediment transport around an obstacle. Model results on this difficult problem are not currently at a publishable stage.
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A perturbation approach to large-eddy simulation of wave-induced bottom boundary layer flows

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Published in *International Journal of Numerical Methods in Fluids*
Abstract

We present the development, validation, and application of a numerical model for the simulation of bottom boundary layer (BL) flows induced by arbitrary finite amplitude waves. Our approach is based on coupling a “near-field” local Navier-Stokes (NS) model with a “far-field” inviscid flow model, which simulates large scale incident wave propagation and transformations over a complex ocean bottom, to the near-field, by solving the Euler equations, in a fully nonlinear potential flow boundary element formalism. The inviscid velocity provided by this model is applied through a (one-way) coupling to a NS solver with Large Eddy Simulation (LES), to simulate near-field, wave-induced, turbulent bottom boundary layer flows (using an approximate wall boundary condition by assuming the existence of a log-sublayer). Although a three-dimensional version of the model exists, applications of the wave model in the present context have been limited to two-dimensional incident wave fields (i.e., long-crested swells), while the LES of near-field wave-induced turbulent flows is fully three-dimensional. Good agreement is obtained between the coupled model results and analytic solutions for both laminar oscillatory BL flow and the steady streaming velocities caused by a wave-induced BL, even when using open boundary conditions in the NS model. The coupled model is then used to simulate wave-induced BL flows under fully nonlinear swells, shoaling over a sloping bottom, close to the breaking point. Finally, good to reasonable agreement is obtained with results of well-controlled laboratory experiments for rough turbulent oscillatory BLs, for both mean and second-order turbulent statistics.

1.1 Introduction

Complex turbulent flows can be accurately modeled by solving Navier-Stokes (NS) equations, either by directly resolving all scales of turbulent motion (DNS;
e.g., Moin and Mahesh [1]) or in a time- or space-averaged sense, in combination with a turbulence closure scheme (e.g. Deardorff [2]). Many methods and algorithms have been proposed for doing so (which have been detailed elsewhere). Here, we present the integration and application of a previously proposed Large Eddy Simulation (LES; Zang et al. [3]) as a component of a new hybrid modeling approach for simulating wave-induced Boundary Layer (BL) flows. While more amenable to large size and high Reynolds number computations than DNS, the LES of complex three-dimensional (3D) flows over large and/or finely discretized domains still represents quite a formidable problem, despite the continual increase in computer performance. Hence, one must always try and limit the computational domain size to that necessary and sufficient for solving a given problem or physics, or even dimensionality (e.g., two-dimensional, 2D versus 3D). For coastal wave dynamics problems, which typically extend over multiple spatial and temporal scales (e.g., from deep water to the shoaling and surf zones), it is often sufficiently accurate to use a simpler approach for a large part of the domain, to propagate and transform waves to the region of specific interest, in which 3D-NS simulations can then be more realistically performed. Using a 3D-NS solver for the entire domain would not only be computationally prohibitive, but would likely yield less accurate results (due to under-discretization and excessive numerical diffusion), than for instance much less costly inviscid flow solvers (even fully nonlinear; e.g., Grilli and Subramanya [4]; Grilli and Horrillo [5]; Grilli et al. [6]) or higher-order Boussinesq equation models (e.g., FUNWAVE; Wei and Kirby [7]; Wei et al. [8]). Furthermore, for long-crested swell, nearshore wave transformations can often be assumed to be 2D.

This has provided a rationale for the development of hybrid modeling approaches, in which different types of models are coupled and used in various regions
of the fluid domain, where they are both more efficient and adapted to the dominant physics and scales in each given region (see, e.g., Grilli [9] for a review). Such models have already been applied to surfzone dynamics problems (e.g., Guignard et al. [10], Lachaume et al. [11], Biausser et al. [12]), wave structure interaction problems (e.g., Corte and Grilli [13]), and to model wave-induced flows and resulting sediment suspension over objects on the seabed (e.g., Gilbert et al. [14]). In the latter work, a so-called numerical wavetank (NWT) solving fully nonlinear potential flow (FNPF) equations was coupled to a 3D-LES in a somewhat heuristic manner.

As indicated above, the LES method used here is based on the approach of Zang et al. [3], who initially developed the NS solver and one of the subgrid-scale turbulence models being used here (dynamic mixed model) to study coastal upwellings [15, 16], and later modified the latter to study turbulent lid-driven cavity flows [3]; further modifications were done to study breaking interfacial waves [17] and suspended sediment transport [18, 19]. As discussed above, Gilbert et al. [14] coupled Zang et al.’s model to a 2D-NWT, to study wave-induced BL flows and sediment transport, through the addition to the NS model equations of the dynamic pressure gradient (equivalent to a body force) caused by waves, computed in the NWT. With this model, they were able to realistically (albeit quite qualitatively) simulate the suspended sediment transport over a partly buried circular obstacle, for a few periodic wave cycles. This implementation did not move beyond such simple cases, both because of the imperfect coupling between the LES and FNPF model equations and severe limitations of the LES grid size (as the code was not designed to take advantage of recent advances in distributed memory computing clusters).

We report here on more recent developments (in formalism, accuracy, and
efficiency) of the techniques used in Gilbert et al. [14]. Specifically, in a new proposed hybrid approach, a modified and extended version of Zang et al.'s [3] 3D-NS-LES model is used in a perturbation scheme to simulate near-field, fine scale, turbulent bottom BL flows induced by arbitrary finite amplitude waves (i.e., 2D swells), whose propagation and nearshore transformation over larger scale bottom features, are modeled from the far- to the near-field in an inviscid flow model (i.e., NWT), which solves Euler equations in a fully nonlinear potential flow (FNPF) formalism. The perturbation scheme consists in first dividing the total pressure and velocity fields into inviscid and viscous perturbation parts and then to rewrite NS equations for the perturbation fields only; this yields new forcing terms, which are function of inviscid flow fields representing incident wave forcing (e.g., similar to Kim et al. [20] and Alessandrini [21]). Moreover, in this approach, the computational domains for both NS-LES and FNPF models fully overlap, which makes it easy passing information from one domain to the other, although here we will just illustrate a one-way coupling, from large to fine scales flows. Additionally, this coupling method is very relevant to the physics of wave-induced flow problems since, for non-breaking waves and outside of BLs, the bulk of the flow is nearly inviscid.

It should be noted that developments of Zang’s LES also continued independently to those presented here in relation to the hybrid coupled modeling approach. Thus, Cui and Street [22] implemented a parallelized version of the code, which allowed for much larger computational domains. Grilli et al. [23] used this latter version to begin testing its suitability for wave-induced BLs, with the goal of again coupling it to a FNPF-NWT. A completely separate development of Cui and Street’s code for bedform evolution was done by Chou and Fringer [24, 25]. Other, unrelated research groups, have also been actively studying the application
of LES to turbulent oscillatory BLs (e.g., Salon et al. [26]; Radhakrishnan and Piomelli [27]). While the LES, subgrid-scale models, and perturbation method presented here have all been used in one form or another by previous researchers, the particular integration of these three components into an accurate and efficient parallelized implementation, well suited to coastal engineering problems, is new and unique. Additionally, the coupling to a 2D-FNPF-NWT, and potentially in future developments to a similar 3D-NWT (e.g., Grilli et al. [28]) makes it possible to use a variety of fully realistic nonlinear and irregular wave forcings, besides the commonly used simple oscillatory or linear wave flows (see e.g., Dean and Dalrymple [29]).

In summary, in this paper, we present recent improvements and validation of a new hybrid method applied to simulating oscillatory and wave-induced BL flows with a 3D-LES. For validation we compare simulation results to analytic solutions of laminar flows and to experimental results of rough turbulent oscillatory BLs. In our hybrid/perturbation approach, the total velocity and pressure fields are expressed as the sum of irrotational (thus kinematically inviscid) and near-field viscous perturbations above a rigid seafloor. The NS equations are formulated and solved for the perturbation fields only, which are forced by additional terms representing the incident fields. In the present applications, these are given either analytically or numerically obtained in a coupled 2D-FNPF-NWT.

1.2 Oscillatory BL flow physics and models

A wide range of approaches besides LES have been proposed for modeling turbulent oscillatory BLs, often in the context of wave-induced flow on the seafloor. The earliest approaches were merely empirical relationships or were based on a time-varying logarithmic BL assumption. Kajiura [30] considered a piecewise varying eddy viscosity distribution. Grant and Madsen [31] used a mixing-length ap-
proach where eddy viscosity was proportional to the height above the bed. These
and other similar works all reported good agreement with mean flow measure-
ments, but did not model turbulent statistics well if at all. Only later models,
like Trowbridge and Madsen’s [32] or Davies’s [33], considered a time-varying eddy
viscosity, which is experimentally observed. More recently, Reynolds averaged NS
models (RANS) of turbulent oscillatory BLs have been used extensively which
provided reasonable to good agreement with experiment for both mean flow and
second-order turbulent statistics (e.g., Blondeaux [34]; Aydin and Shuto [35]; Juste-
sen [36]; Justesen [37]; Thais et al. [38]; Mellor [39]; Tanaka and Sana [40]). In
those, many different turbulence models were used, from Saffman’s energy-vorticity
turbulence model, used by Blondeaux, to a high Reynolds number k-ε model used
by Justesen, or the two-equation turbulence closure of Chien, used by Thais et al.

The flow in a purely oscillatory boundary layer (BL) over a solid horizontal
wall is driven by a periodic pressure gradient. In the simplest case the forcing
flow is represented by a sinusoidal free-stream (inviscid) velocity given by \( u_i^f = \delta_{i1} U_0 \sin \omega t \), where \( U_0 \) is the amplitude and \( \omega \) the angular frequency. Far away from
the wall, water particles follow the free-stream and oscillate with an amplitude on
the order \( A = U_0/\omega \). In the BL, the flow additionally depends on the kinematic
viscosity, \( \nu \) and, for rough boundaries, on the Nikuradse roughness length, \( k_s \). The
BL flow regime is thus dependent on two nondimensional numbers: (i) a relative
roughness, \( A/k_s \); and (ii) the Reynolds number, \( U_0 A/\nu \). Fig. 1 shows various
regime regions identified based on values of those two parameters. Various authors
(e.g., Kamphuis [41]; Blondeaux [34]; Sleath [42]) have proposed slightly different
or additional regions, but in general the flow regime can either be described as
laminar, smooth turbulent, rough turbulent, or transitional. To a first-order, wave-
induced oscillatory BLs can be characterized in the same way. In this paper, we
Figure 1. Oscillatory BL flow regimes as a function of Reynolds number and relative roughness, as estimated by Kamphuis [41] and overview of conditions observed in selected experiments (• – Sleath [43]; ○ – Jensen et al. [44]; ♦ – Jonsson and Carlsen [45]).

will consider both laminar and rough turbulent conditions.

Many measurements of turbulent oscillatory BLs have been reported, usually made in an oscillatory water tunnel (e.g., Jonsson and Carlsen [45]), or a reciprocating wind tunnel (e.g., Hino et al. [46]), resulting in many advances in understanding oscillatory BLs. Measurements from wavetanks (e.g., Sleath [43]) are possible, but except in the largest wavetanks it is not usually possible to reproduce the high Reynolds number flows that are present in the ocean. Thus, Jonsson and Carlsen [45] measured mean flow velocities over rough walls in an oscillatory water tunnel for two different rough turbulent tests. They found that the velocity at points just above the rough bed could be well described by a log-layer assumption. Hino et al. [46] measured mean flow velocities, turbulent intensities,
Reynolds stresses and turbulent-energy production rates for oscillatory BLs over a smooth wall. Interestingly, they found that the spectral decay of the turbulent energy in the decelerating phase is steeper than the 5/3 power law of the Kolmogorov spectrum (see e.g., Pope [47] for a general description of spectral analysis of turbulence). Sleath [48] was one of the first to measure both turbulent intensity and mean flow velocity for oscillatory BLs over rough surfaces. Notably, Sleath found that the time-averaged eddy viscosity near the rough bed was negative, meaning that the turbulent momentum is transported against the mean velocity gradient, which implies that the turbulent kinetic energy production is negative. Sleath suggested that this was due to jets of fluid moving away from the wall near flow-reversals. Jensen et al. [44] measured mean flow velocity and turbulent intensity over both smooth and rough walls.

Although far from the boundary wave-induced BLs tend toward an inviscid solution, wave-induced BLs differ from purely uniform oscillatory BLs in that weak vorticity is present at moderate distances from the seabed. While to a first-order this is typically insignificant, it does induce a steady streaming velocity. Longuet-Higgins derived a theory describing steady streaming velocity profiles for wave-induced laminar BL flows [49] or with time-invariant eddy viscosity distributions [50]. Trowbridge and Madsen [32] developed a model which instead considered a time-varying eddy viscosity distribution. Since then, Reynolds-averaged approaches have been commonly used for representing wave-induced BLs (e.g., Johns [51]; Jacobs [52]; Hsu and Ou [53]; Chowdhury et al. [54]; Deigaard et al. [55]). A more practical model of drift over very rough beds was developed by Davies and Villaret [56] where the dominant process is vortex shedding as opposed to random turbulence. Recently, Myrhaug and Holmedal [57] derived the steady streaming induced by random waves, in both laminar and turbulent conditions.
Others have focused on the effects of wave asymmetry. Scandura [58] numerically modeled steady streaming for a transitionally turbulent BL forced by a pressure gradient with two harmonics. Holmedal and Myrhaug [59] have considered the combination of Longuet-Higgins steady streaming and wave asymmetry, as well as their relative contributions to the overall steady streaming velocities for different parameters and for both sinusoidal and Stokes second-order waves. Note, in the present approach, the coupling of the 3D-LES to the fully nonlinear NWT, which also allows representing arbitrary bottom bathymetry, makes it possible to simulate the wave-induced forcing flow from fully realistic, strongly nonlinear (near-breaking), shoaling waves, which are both trough-crest and front-rear asymmetric.

When deriving a theory for wave-induced steady streaming over constant depth in a very thin BL (as compared to the wavelength), only the horizontal component of the inviscid forcing needs to be considered [60]. In this context, earlier theoretical and numerical research has focused on sinusoidal or second-order Stokes waves. Under sinusoidal waves, the steady streaming velocity is always in the direction of wave propagation [49], whereas under second-order Stokes waves, streaming is reduced or may be in the opposite direction [59]. Higher-order wave-forcing of course provides more realistic conditions, which, as indicated above, can be obtained from simulations in a FNPF-NWT, such as Grilli and Subramanya’s [4] 2D-NWT. In the latter, as in many similar NWTs, continuity is satisfied by solving Laplace’s equation for the velocity potential with a Boundary Element Method (BEM), and the nonlinear kinematic and dynamic free surface boundary conditions are integrated in time with a Mixed Eulerian-Lagrangian (MEL) scheme. The MEL scheme was first introduced in this context by Longuet-Higgins and Cokelet [61] and allowed for simulating overturning waves. [A similar 3D-NWT was developed
by Grilli et al. [28]. In the present work, we compare the effects of a variety of forcing functions on the oscillatory BL flow.

While Longuet-Higgins [49] validated his theory using earlier measurements, Russell and Osorio [62] and Collins [63] further confirmed that the drift velocity at the edge of the BL matched Longuet-Higgins’s theory for laminar flows over a flat bed. Because this velocity was independent of viscosity, Longuet-Higgins [50] suggested that, for a constant eddy viscosity, the same result would hold in turbulent conditions. Johns [64] extended this argument to vertically varying but time-independent eddy viscosity models, typical of the time. Collins’ [63] measurements suggested that this was not true at higher Reynolds numbers, which has since been confirmed by Brebner et al. [65], Bijker et al. [66], and van Doorn [67]. More recent studies have focused on other effects in the BL. The effect of wave asymmetry acts opposite to the effect of Longuet-Higgins steady streaming, as has been studied by Ribberink and Al-Salem [68] in an oscillating water tunnel. Many studies are focused on either flat seabeds or naturally occurring bedforms. Marin [69] studied Eulerian drift for progressive waves over a rippled bed in the transitionally turbulent regime, and found that the Davies and Villaret [56] model for turbulent flow could be adjusted to handle transitionally turbulent conditions.

1.3 Governing equations

Navier-Stokes (NS) equations for an incompressible, isothermal, Newtonian fluid read:

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{1}
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i u_j + \frac{p}{\rho} \delta_{ij} - \nu \frac{\partial u_i}{\partial x_j} \right) = 0 \tag{2}
\]

where \( u_i \) and \( p \) are the water velocity and dynamic pressure, respectively, in a fluid of density \( \rho \) and kinematic viscosity \( \nu \). We adopt the indicial tensor notation
convention, with $x_3$ denoting a vertical distance measured from some reference point.

Let us denote by $(u_I^i, p_I)$ the velocity and pressure fields of the ocean wave flow, considered to be inviscid outside of thin boundary layers (BLs). Such flows are well described by Euler equations:

$$\frac{\partial u_I^i}{\partial x_i} = 0 \quad (3)$$
$$\frac{\partial u_I^i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_I^i u_j^i + \frac{p_I}{\rho} \delta_{ij} \right) = 0. \quad (4)$$

Let us then introduce a decomposition of the total viscous flow into the sum of the latter inviscid free-stream flow and a defect or perturbation flow, of velocity $u_P^i$ and pressure $p_P$:

$$u_i = u_I^i + u_P^i \quad (5)$$
$$p = p_I + p_P. \quad (6)$$

Replacing Eqs. 5 and 6 into Eqs. 1 and 2, and subtracting Eqs. 3 and 4, we derive the governing equations for the perturbation fields as:

$$\frac{\partial u_P^i}{\partial x_i} = 0 \quad (7)$$
$$\frac{\partial u_P^i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_j^i = u_I^i u_j^i + \frac{p_P}{\rho} \delta_{ij} - \nu \frac{\partial u_i}{\partial x_j} \right) = 0. \quad (8)$$

Here the perturbation is defined in a region encompassing the near-field bottom boundary layer of interest.

Although formally different, for the range of problems studied here, these equations can be shown to be equivalent to the forcing of the total flow with the inviscid wave dynamic pressure gradient proposed by Gilbert et al. [14], expressed
as:

\[
\frac{\partial u_i}{\partial x_i} = 0 \quad (9)
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i u_j + \frac{p_P}{\rho} \delta_{ij} - \nu \frac{\partial u_i}{\partial x_j} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x_j}. \quad (10)
\]

There are two key advantages, however, to the current approach, as compared to this earlier work: (1) boundary conditions can be more clearly and accurately defined for the viscous perturbation (i.e., as vanishing or using a radiation condition away from the wall); and (2) only the inviscid velocity is needed in the NS forcing terms rather than the dynamic pressure gradient.

By applying a spatial-average operator (overbar) to the Navier-Stokes equations we obtain the momentum equation for the resolved perturbation as:

\[
\frac{\partial \bar{u}_P^i}{\partial x_i} = 0 \quad (11)
\]

\[
\frac{\partial \bar{u}_P^i}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j + \frac{p_P}{\rho} \delta_{ij} - \nu \frac{\partial \bar{u}_i}{\partial x_j} + \tau_{ij} \right) = 0. \quad (12)
\]

where \( \tau_{ij} \) is the subgrid scale (SGS) stress defined as:

\[
\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j. \quad (13)
\]

Note that, typically, SGS models only consider the deviatoric stress \( \tau_{ij} - \frac{\tau_{kk}}{3} \), because the resolved turbulent pressure, \( \bar{p}^* \), is different from the resolved hydrodynamic pressure with:

\[
\frac{\bar{p}^*}{\rho} = \frac{\bar{p}}{\rho} + \frac{1}{3} \tau_{kk}. \quad (14)
\]

For the SGS models considered here, we define:

\[
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2 \nu_T \tilde{S}_{ij} + C_r \left( L_{ij}^m - \frac{\delta_{ij}}{3} L_{kk}^m \right) \quad (15)
\]

where \( \nu_T \) is the eddy viscosity, \( \tilde{S}_{ij} \) is the resolved shear strain rate, \( L_{ij}^m \) is the modified Leonard term, and \( C_r \) is a constant coefficient (either one or zero, depending on the SGS decomposition used).
1.3.1 Discretization

The governing equations are discretized in three dimensions (3D) as in Cui and Street [22], i.e., using a finite-volume formulation with 2nd-order accuracy in both time and space on a non-staggered grid. Quadratic upstream interpolation for convective kinematics (QUICK) [70] is used to discretize the convective terms of the fluid flow, and 2nd-order centered differences are used for the remaining terms. The convective terms are time integrated using the 2nd-order Adams-Bashforth technique, and the diffusive terms with a 2nd-order implicit Crank-Nicolson scheme. The Poisson equation for the pressure field is solved with a multigrid technique. Note that in our hybrid approach, the inviscid velocity field is obtained directly from another model – in this paper, a theoretical solution or a 2D-NWT – and is not subject to the numerical errors of the NS solver.

For all of the test cases that are considered here, the computational domain is a box, $L_1$ long in the streamwise direction, $L_2$ wide in the spanwise direction, and $L_3$ high in the vertical direction. The corresponding number of gridpoints are $N_1$, $N_2$, and $N_3$, respectively.

For post-processing, it is useful to define variables in terms of integrals that, when discretized are sums, e.g., ensemble averages. Thus, for an arbitrary variable $q$ that is aperiodic, the average over a horizontal plane is:

$$\langle q \rangle(x_3) = \frac{1}{L_1 L_2} \int \int q \, dx_1 dx_3$$

(16) calculated as,

$$\langle q \rangle([x_3]_j) = \frac{1}{N_1 N_2} \sum_i \sum_k [q]_{i,j,k}$$

(17)

where here the additional subscripts $[i,j,k]$ are grid indices (with e.g., $i$ varying from 1 to $N_1$), whereas for periodic field variables, an ensemble average can be made more accurate by also averaging over several periods.
\[ \langle q \rangle(x_3) = \frac{1}{N} \frac{1}{L_1 L_2} \sum_{n=1}^{N} \int_{L_1}^{L_1} \int_{L_2}^{L_2} q(x_1, x_2, x_3, t + nT/2) dx_1 dx_2 \text{ or } \langle q \rangle(x_3) = \frac{1}{N} \frac{1}{L_1 L_2} \sum_{n=1}^{N} (-1)^n \int_{L_1}^{L_1} \int_{L_2}^{L_2} q(x_1, x_2, x_3, t + nT/2) dx_1 dx_2 \]

depending on whether the field variable is periodic or antiperiodic, such as the turbulent intensity or the mean velocity, respectively.

In theoretical models, oscillatory BLs are often considered to be “infinitely long”, which would correspond to a half-plane or half-space. This may represent physical circumstances quite well but is not practical in a numerical model where we want to limit the domain size to limit computational requirements. Hence, assuming the flow is statistically homogenous in a direction, we can apply periodic boundary conditions, with the premise that velocity fluctuations a half-domain away are completely uncorrelated with one another. Such space-periodicity conditions will be used for some of the applications presented here.

While the numerical method is designed to handle any structured 3D grid, here we limit our consideration to two types – regular grids in each direction, and regular grids with exponential stretching in the vertical direction. The latter is based on a stretching ratio based on the vertical distance between adjacent gridpoints (e.g., a 1.1 stretching ratio would correspond to a 10% increase in cell size with each step in the vertical direction).

Note that this vertical stretching induces a large aspect ratio for the cells near the boundary. Consider a grid with a seabed of height \( h(x_1, x_2) \), and vertical grid spacing \( \Delta x_3 \). From a vertical profile it may appear that eddies of \( O(\Delta x_3) \) are resolved, for e.g., an aspect ratio of 10:1 the grid-filter acts on a volume of approximately \( O(10^2 \Delta x_3^3) \), though near-wall eddies are expected to be \( O(2\kappa(x_3 - h)) \) across, so turbulent eddies near the surface are not resolved (e.g., when \( 2\kappa 10^{-2/3} \gtrsim \Delta x_3/(x_3-h) \)). These estimates are most accurate for flat seabeds, but analogous arguments can be made for complex bathymetry. Thus we expect
an underprediction of turbulent intensity near the wall, and a need to augment the subgrid scale stresses. The method used is described in the next section.

1.3.2 Bottom boundary condition

In all cases considered here, the bottom boundary condition is a no-flux condition with a shear stress applied depending on flow conditions, i.e.,

$$\tau_w = \rho \nu \left[ \frac{\partial \bar{u}_{tan}}{\partial n} \right]_{x_3 = h(x_1,x_2)}$$

(18)

where $n$ is the normal direction to the wall, $\bar{u}_{tan}$ is the resolved velocity tangential to the wall, and $\tau_w$ is the wall shear stress. In BL theory, the latter is typically defined as a function of the friction velocity $u_*$, as: $\tau_w = \rho u_*^2$, which yields,

$$\left[ \frac{\partial \bar{u}}{\partial n} \right]_{x_3 = h(x_1,x_2)} = \frac{1}{\nu} u_*^2.$$

(19)

Combining this with the condition that the eddy viscosity is zero along the bed, the boundary condition can be implemented as a purely viscous wall stress. Numerically, this velocity gradient condition is implemented through using layers of additional (ghost) cells, located outside of the domain. We apply one of two boundary friction velocity models, depending on the application. In each case we evaluate them for the gridpoints adjacent to the boundary (e.g., over a flat bed, at $x_3 = h(x_1,x_2) + \Delta x_3/2$). To be unambiguous for curved seabeds, we specify $z_1$ to be the distance of the center of the first grid cell to the boundary.

For laminar tests, we consider a no-slip condition such that:

$$u_* = \sqrt{\frac{\bar{u}_{tan} \nu}{z_1}}.$$ 

(20)

For rough turbulent cases, we assume that the von Karman-Prandtl equation (for a logarithmic sub-layer) can be applied at the first gridpoint above the bed. For hydraulically rough conditions, this reads:

$$\frac{\bar{u}_{tan}}{u_*} = \frac{1}{\kappa} \log \frac{z_1}{z_0}$$

(21)
where $\kappa$ is the von Karman constant, taken to be 0.41, and $z_0$ is the roughness length, which can be related to the Nikuradse roughness, $k_s = 30z_0$. Such a log-layer equation is known to be applicable in only a narrow regime of flows of engineering interest, but it is common practice to apply this in LES models of atmospheric flows [71]. For other approximate bottom boundary conditions see Cabot and Moin [72] and for a review of LES wall modeling see Piomelli and Balaras [73]. The use of the log-layer law is also supported by the experiments of Nakayama et al. [74]. Note that Nakayama et al.’s experiments considered a zero-pressure gradient, and did not include flow separation. These wall models may be unsuitable for situations with turbulent flow separation, but this is an issue to be considered in future work.

1.3.3 Subgrid scale models

Since no turbulence closure scheme has been found satisfactory for all situations, a variety of SGS models have been developed for large-eddy simulations. Most models are some variant of the Smagorinsky model, where the SGS stress is an algebraic function of the resolved shear stress rate. In this work, we consider several models for comparison, including the Smagorinsky model, the dynamic Smagorinsky model (DSM), and the dynamic mixed model (DMM). Note that, as in Cui and Street [22], the spatial gradient of eddy viscosity is neglected in the discretized governing equations.

**Smagorinsky model**

The Smagorinsky model [75] of the SGS stress,

$$
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_T \tilde{S}_{ij}
$$

(22)
is an algebraic function of the resolved shear strain rate tensor,

\[
\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]  

(23)

where \(|\bar{S}|\) is the magnitude of the shear strain rate tensor:

\[
|\bar{S}| = \sqrt{2 \bar{S}_{ij} \bar{S}_{ij}}.
\]  

(24)

The eddy viscosity, \(\nu_T\), is expressed as proportional to the magnitude of the local shear strain rate as:

\[
\nu_T = C_s \bar{\Delta}^2 |\bar{S}|
\]  

(25)

where \(C_s\) is the Smagorinsky model coefficient (the square of the Smagorinsky constant) and \(\bar{\Delta}\) is a grid-filter width that can be expressed from the Jacobian \(J\) of the coordinate transformation as: \(\bar{\Delta} = J^{1/3}\), or, for a Cartesian grid, as: \(\bar{\Delta} = (\Delta x_1 \Delta x_2 \Delta x_3)^{1/3}\). At a wall, the discretized shear strain rate tensor is calculated with one-sided finite differencing, since the shear imposed as a boundary condition is non-physical.

Lilly [76] found that for the Smagorinsky model to agree with the Kolmogorov turbulence spectrum for isotropic turbulence, the Smagorinsky constant must be approximately 0.16. It is well known that this overpredicts the amount of dissipation for wall-bounded flows. Here we use a Smagorinsky constant of 0.145 (i.e., model coefficient of 0.021), which is consistent with the earlier work of Gilbert et al. [14].

**Dynamic Smagorinsky model**

The next major advancement in SGS modeling was the dynamic Smagorinsky model (DSM) of Germano et al. [77], whereby the Smagorinsky coefficient in Eq. 25 is allowed to vary in time and space. At each point, following a procedure of Lilly [78] and Germano [79], the coefficient \(C_s\) is assumed to be scale-invariant. As
a result, Eqs. 22–25 can be defined for two different length scales (known as the filter widths), and then at each point the local $C_s$ can be chosen to be that which minimizes the least-squares error in the above equations.

In order to obtain the velocity fields at the appropriate length scales, the resolved velocity field is used, as well as a filtered version of the velocity field. Often a simple discrete filter (e.g., using the trapezoidal rule) is used, and typically the grid size ratio $\alpha$ is chosen as 2.0, based on the analysis of Germano et al. [77] (i.e., smaller values gave less accurate results while larger values provided no clear advantage). Lund [80] showed that often the filter-width is not properly determined, so while we use the same test-filter as Cui and Street [22], we use Lund’s more accurate filter-width definition of $\alpha \approx \sqrt{6} = 2.46$; see [80] for details.

While the dynamic Smagorinsky model requires fewer input parameters than a simple Smagorinsky model, and is typically more accurate, this least-squares procedure for finding the model coefficient can lead to numerical instabilities. Here, as in Zang [15], $C_s$ is local filtered, and a cutoff is implemented, preventing negative total viscosity (i.e., if the local eddy viscosity is calculated less than the kinematic molecular viscosity, it is set equal to $-\nu$).

**Dynamic mixed model**

Here, the SGS stresses are modeled using Zang et al.’s [3] dynamic mixed model (DMM), based on the stress decomposition proposed by Germano [81]:

$$\tau_{ij} = L_{ij}^m + C_{ij}^m + R_{ij}^m$$

(26)
which consists in a sum of the modified Leonard term, modified cross term, and modified SGS Reynolds stress, defined as:

\begin{align*}
L_{ij}^m &= \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \\
C_{ij}^m &= \bar{u}_i u'_j + u'_i \bar{u}_j + \bar{u}_i u'_j - u'_i \bar{u}_j \\
R_{ij}^m &= u'_i u'_j - \bar{u}'_i \bar{u}'_j,
\end{align*}

respectively. Then, by modeling the SGS stress as:

\begin{equation}
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2C_s \Delta^2 |S| S_{ij} + L_{ij}^m - \frac{\delta_{ij}}{3} L_{kk}^m
\end{equation}

and again assuming scale independence, the optimal model coefficient can similarly be found by applying Germano’s technique.

**Near-wall eddy viscosity**

One of the premises of SGS models is that the spatial filtering involved is over regions of small flow variations. This is not true, however, near a boundary when using an approximate boundary condition such as Eq. 21 (see e.g., Cabot and Moin [72]). Specifically, near a wall, the grid filter width is approximately \( x_3 - h \), but the largest eddies are only \( \kappa(x_3 - h) \) across. This affects the eddy viscosity in the near-wall region in a way which is model-specific. For the constant coefficient Smagorinsky model, for instance, it is well-known that the near-wall eddy viscosity is overpredicted. Because this behavior and limitations of the Smagorinsky model have been well documented in the literature, we do not modify this model, to use it as a “control” model in our work. The dynamic Smagorinsky models, by contrast, underpredict the near-wall eddy viscosity to the point that some modifications are necessary. The first change we make to the standard dynamic SGS models, to account for effects of the boundary, is to adjust the filtering operator. (i.e., a box-filter of the resolved velocity). Filtering at points near the wall will result
in a solution that depends on non-physical values at the ghost cells outside of the domain. Hence, near the boundary, we use instead the commutative filters of Vasilyev et al. [82] which are one-sided for points adjacent to a boundary. The resulting filtered velocity field is mathematically consistent throughout the domain, and only depends on points within the domain. Similarly, some care is taken to use one-sided finite differences in computing the shear strain rate at points near the boundary.

Additionally, following Chow and Street [83] and Chow et al. [84], the eddy viscosity at the wall in the SGS model is increased, in order to augment the near-wall shear stresses. Here we follow Zedler and Street [19], who by specifying the eddy viscosity as:

\[(\nu_T)_{total} = (\nu_T)_{SGS} + \kappa u_* (x_3 - h) \cos^2 \left( \frac{\pi (x_3 - h)}{4\Delta x_1} \right) \]  

(31)

for all points between the bed and a height \(2\Delta x_1\). This can also be expressed as:

\[(\nu_T)_{total} = (\nu_T)_{SGS} + \kappa u_* z \cos^2 \left( \frac{\pi z}{4\sqrt{J/2z_1}} \right) \]  

(32)

for \(z < 2\sqrt{J/2z_1}\), \(z\) is the distance from a point to the seabed, and as before, \(z_1\) is the distance of the center of the first grid cell to the boundary, and \(J\) is the Jacobian of the transformation used in deriving the discretized governing equations.

This scheme increases the near-wall stress and smoothly varies the eddy viscosity from that in the inner wall modeled region to the outer region in the LES domain. Note, this technique has similarities with both RANS modeling (since the filter width is horizontally large and the eddy viscosity is given from a mixing length theory) and wall models, since the eddy viscosity is dependent upon a height above the bed, which is not well defined for general surfaces. Preliminary tests, which will be detailed below as part of the turbulent BL application, confirmed that when an augmented near-wall stress term such as Eq. 32 is not included,
results are qualitatively similar, but the wall stress is underpredicted by as much as 50%. See Piomelli et al. [85] and Chow et al. [84] for recent advances in using even more sophisticated techniques for augmenting near-wall stresses in a LES.

1.3.4 Fully nonlinear potential flow

In this work we use different unsteady inviscid flow solutions to force the large-eddy simulations of the BL flow. Some are simple analytical solutions (such as a uniform oscillatory flow) but, to simulate realistic wave forcing, we use results of a 2D numerical wavetank based on fully nonlinear potential flow theory (i.e., in which fully nonlinear kinematic and dynamic free surface boundary conditions are kept in a MEL formalism; Grilli and Subramanya [4]; Grilli and Horrillo [5]; Grilli et al. [6]). Governing equations and numerical methods for this 2D-NWT are briefly summarized below, in the context of the perturbation approach introduced before.

For incompressible irrotational flows, we define $u^I_k = \partial\Phi/\partial x_k$, with $\Phi$ the velocity potential. With this definition, mass conservation becomes Laplace’s equation:

$$\nabla^2 \Phi = 0$$

(33)

which is efficiently and accurately solved using a higher-order Boundary Element Method (BEM) based on Green’s second identity:

$$\alpha(x_j)\Phi(x_j) = \int_{\Gamma} \left\{ \frac{\partial\Phi(x_i)}{\partial n} G_{ij} - \Phi(x_i) \frac{\partial G_{ij}}{\partial n} \right\} d\Gamma(x_i)$$

(34)

where $\Gamma(x_i)$ denotes the NWT boundary, $n_i$ is the outwards unit normal vector to the boundary (Fig. 2), $G_{ij}$ is the free-space Green’s function given in 2D by:

$$G(x_i, x_j) = -\frac{1}{2\pi} \log |x_i - x_j|$$

(35)
where \( x_i \) and \( x_j \) are both points on the boundary, with the latter referred to as collocation node, and \( \alpha \) is a coefficient function of the angle of the boundary at \( x_j \).

On the free surface \( \Gamma_f \) (Fig. 2), the fully nonlinear kinematic and dynamic boundary conditions,

\[
\frac{D r_i}{Dt} = \frac{\partial \Phi}{\partial x_i}
\]

\[
\frac{D \Phi}{Dt} = -g x_3 + \frac{1}{2} \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_i} - \frac{p_a}{\rho}
\]

respectively (where \( x_3 \) is the vertical coordinate), are time integrated using second-order Lagrangian Taylor series expansions, for the free surface position \( r_i \) and potential \( \Phi(r_i) \) (i.e., using both \( \Phi \) and \( \partial \Phi / \partial t \), and their normal and tangential derivatives), and an explicit time stepping scheme. A (Neumann) no-flow or specified normal velocity condition is specified on the other NWT boundaries, including a wavemaker and the seabed.

The above boundary integral equations are discretized, as detailed in Grilli and Subramanya [4], for a series of collocation nodes \( x_j, j = 1, ..., N \) on the boundary, and using higher-order elements to interpolate between the nodes. The resulting linear system of equations is solved at each time step to provide boundary values of \( \Phi \) and its normal and time derivatives, which in turn are used in the time updating of free surface solution.

Wave generation in the NWT can be accomplished in several ways. For the application presented here, generation using a flap wavemaker is simulated at the leftward boundary of the NWT, \( \Gamma_w \), by specifying a (horizontal) stroke motion, \( x_w(t) \), similar to that of a physical wavetank (Fig. 2). With this method, regular waves can be easily generated (e.g., Grilli and Horrillo [5]; Grilli et al. [6]), as well as more complex wave climates.

In the far-field wave domain, incident waves propagate, transform, and shoal over the specified sloping bottom topography, as simulated in the NWT. In the
near-field, waves would eventually overturn and break, and dissipate their energy. To prevent breaking in the NWT, which would interrupt FNPF computations, following Grilli and Horrillo [5], incident wave energy is gradually dissipated in an absorbing beach (AB) at the far shallower end of the NWT and using an actively absorbing lateral piston (AP) boundary (Fig. 2). In the AB, energy dissipation results from the (negative) work against waves of an absorbing surface pressure $p_a$, specified in the dynamic free surface boundary condition, proportional to the normal particle velocity as:

$$p_a(x_1, t) = \nu_a(x_1) \frac{\partial \Phi}{\partial n}$$ \hspace{1cm} (38)

where $\nu_a$ denotes a smoothly varying AB absorption function in the long NWT horizontal direction $x_1$ (see [5] for detail).

The NS model grid is finely discretized and thus may have millions of grid-points; so it could be computationally expensive to calculate the BIE solution in the NWT for every such internal point. For turbulent cases considered by Gilbert et al. [14], assuming fairly long and regular incident waves, this was tackled by computing the inviscid wave velocities only at a subset of the NS gridpoints and then interpolating over the entire NS grid. Internal velocities were computed in the NWT using a boundary integral equation (note this is also a mathematically
exact equation):

\[ u_k(x_j) = \int_{\Gamma} \left\{ \frac{\partial \Phi(x_i)}{\partial n} (\nabla_k G_{ij}) - \Phi(x_i) \left( \nabla_k \frac{\partial G_{ij}}{\partial n} \right) \right\} d\Gamma(x_i). \]  

(39)

Because the present applications of the coupled NWT-NS-LES are only for wave-induced flows within a very thin BL, the vertical variation of the inviscid velocity can be neglected within the BL. Accordingly, the inviscid forcing velocity in the BL is computed for a series of grid cell horizontal abscissa \( x_{g_1} \) at seabed points, as:

\[ u^I_1(x_{g_1}, t) \approx \left( \frac{\partial \Phi}{\partial x_1} \right)_{(x_{g_1}, h(x_{g_1}))} \]  

(40)

\[ u^I_2(x_{g_1}, t) = 0. d0 \]  

(41)

\[ u^I_3(x_{g_1}, t) \approx \left( \frac{\partial \Phi}{\partial x_3} \right)_{(x_{g_1}, h(x_{g_1}))} . \]  

(42)

This assumption is reasonable because for the application on a sloping bed shown below, the bed slope \( m \) is very small, and because the simulation domain is very thin. This approximation is further justified below in the presented application, where it is used when the incident wavelength is very large with respect to the BL thickness. These internal velocities are then used to force the NS-LES model, as detailed above.

1.4 Applications

1.4.1 Laminar wave-induced boundary layers

Stokes boundary layer

Stokes’ second problem [86] provides an exact solution for the horizontal velocity profile in a laminar BL of thickness \( \delta_S = \sqrt{2 \nu / \omega} \) (known as the Stokes-layer thickness), forced by an oscillatory flow of angular frequency \( \omega = 2\pi/T \) or period \( T \). A major feature of laminar oscillatory BLs is that the phase lag between the
Table 1. Parameters for laminar oscillatory BL simulations in NS-LES model. Note, results are independent of horizontal parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain height</td>
<td>$16\delta_S$</td>
</tr>
<tr>
<td>Upper boundary condition</td>
<td>Zero-gradient</td>
</tr>
<tr>
<td>Wall boundary condition</td>
<td>No-slip</td>
</tr>
<tr>
<td>Initial conditions</td>
<td>$u^I_i(x_i, t = 0) = 0$</td>
</tr>
<tr>
<td>Simulation spin-up time</td>
<td>$100T$</td>
</tr>
<tr>
<td>Forcing</td>
<td>$u^I_1(t) = U_0 \sin \omega t; u^I_2 = u^I_3 = 0$</td>
</tr>
<tr>
<td>Free-stream velocity</td>
<td>$U_0 = \pi$</td>
</tr>
<tr>
<td>Forcing period</td>
<td>$T = 1$</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>$\nu = \pi$</td>
</tr>
<tr>
<td>Stokes length</td>
<td>$\delta_S = 1$</td>
</tr>
<tr>
<td>Reynolds number</td>
<td>$Re\delta = 1$</td>
</tr>
</tbody>
</table>

wall shear stress, $\tau_w$, and the free-stream velocity is $45^\circ$. For other regimes, however, this angle varies. In the following test case, the inviscid flow forcing is simply a spatially uniform horizontal, sinusoidal flow:

$$u^I_i = \delta_i U_0 \sin \omega t \quad (44)$$

where $U_0$ is the amplitude of the free-stream velocity. The analytical solution of Stokes' second problem yields the following horizontal velocity:

$$u_{a1} = U_0 (1 - \exp[-(x_3 - h)/\delta_S]) \sin(\omega t - (x_3 - h)/\delta_S). \quad (45)$$

Fig. 3 shows vertical profiles of horizontal velocity at a few phases of the flow, based on this solution.

As a numerical a first validation test of the implementation of the perturbation approach in the NS model, we computed such laminar oscillatory BL flows for a variety of grid sizes and time steps, setting the Reynolds number based on Stokes layer thickness to: $Re\delta = U_0\delta_S/\nu = 1$ (note, here, of course, the LES is not called upon and the eddy viscosity is set to zero). Spatial periodicity was assumed in the horizontal direction and a no-slip boundary condition was specified on the bed. The grid is 16 Stokes thicknesses high, and 1 Stokes thickness wide in both horizontal
Figure 3. Stokes second problem for an oscillatory laminar BL flow. Analytical solution for the vertical variation of the horizontal velocity, $u_{a1}$, for different phases of oscillations.

directions. For each test case, four points in each horizontal directions are used (though for a 2D laminar case, the streamwise and spanwise discretizations are irrelevant since those terms cancel out in the governing equations). At the vertical boundary, a zero-gradient condition is applied (i.e., $\partial u_1 / \partial x_3 = 0$).

Each simulation was run for 100 periods $T$ until a quasi-steady state was reached. We assume that the size of the domain and this spin-up time are both sufficiently large as to have negligible effects on the results (for high resolutions these assumptions may be less valid). Table 1 gives a summary of the numerical parameters. The maximum error in the horizontal velocity after 100 periods of oscillation, as compared to the above analytical solution, was calculated as a measure of the numerical accuracy of the NS-LES simulations:

$$
\epsilon = \max \left[ u_1(x_3, t = 100T) - u_{a1}(\omega t = 0) \right].
$$

(46)

While there are many numerical parameters affecting NS-LES simulations, for this idealized laminar oscillatory BL problem, all other things being equal, only
two are significant: the vertical grid spacing $\Delta x_3$ and time step $\Delta t$. Indeed, for this case, the governing equations reduce to a one-dimensional problem where the viscous term (computed with second-order center differencing) is integrated in time (with the second-order Adams-Moulton method). Thus, we expect that as long as we use a small enough time step and/or the BL is sufficiently (vertically) resolved, the numerical error $\epsilon$ should show a second-order reduction with either grid size or time step. This is verified in Fig. 4, for computations performed using a very small time step, $\Delta t = 0.001T$, and grid size $\Delta x_3 = \delta_S/32$ to $\delta_S$, and in Fig. 5 where a small grid size, $\Delta x_3 = \delta_S/64$, is used and time step varies from $\Delta t = 0.01T$ to $0.2T$. The expected second-order convergence is obtained when neither of the governing parameters is too small or too large. When time step or grid size was very large, the model did not resolve the BL oscillations well, and when the time step was very small, errors were dependent mostly on grid size. For (unnecessarily) very small time step and grid size, the error increased slightly as compared to the expected convergence, likely due to round-off and truncation errors.

**Steady streaming**

The next validation test of the implementation of the perturbation approach in the NS-LES solver is also for a laminar wave-induced BL, which unlike the previous application is forced by a time- and space-varying inviscid velocity, representing an incident linear Stokes wave. This results in an additional test of the convection terms in the model. The inviscid forcing is analytically defined from linear wave theory as (Dean and Dalrymple [29]):

\begin{align*}
  u'_1 &= \frac{Hgk \cosh(k(x_3 - h))}{2\omega \cosh kh} \cos(kx_1 - \omega t) \\
  u'_2 &= 0 \\
  u'_3 &= \frac{Hgk \sinh(k(x_3 - h))}{2\omega \cosh kh} \sin(kx_1 - \omega t)
\end{align*}

\begin{align*}
  (47) \\
  (48) \\
  (49)
\end{align*}
Figure 4. Maximum numerical error of NS-LES for velocity in an oscillatory laminar BL (with $Re_\delta = 1$), as a function of grid size for $\Delta t/T = 0.001$.

Figure 5. Maximum numerical error of NS-LES for velocity in an oscillatory laminar BL (with $Re_\delta = 1$), as a function of time step for $\Delta x_3 = \delta_S/64$. 
for a wave height $H$ and angular frequency $\omega$, in depth $h$, and wavenumber $k$ given by the dispersion relationship: $\omega^2/g = k \tanh kh$. In this case, rather than solving for the perturbation pressure to enforce mass conservation, we note that near the bottom, $u_3(x_1, x_3, t) << u_1(x_1, x_3, t)$, so that we can ignore the vertical momentum equation in the BL and instead compute the vertical velocity from the mean mass conservation (note, here again the turbulent fluctuations are zero so: $\bar{u}^P_3 = u^P_1$):

$$\bar{u}^P_3(x_1, x_3) = -\int_0^{x_3} \frac{\partial \bar{u}^P_1}{\partial x_1}(x_1, x'_3) \, dx'_3$$

Because this bypasses the Poisson equation solver, that is normally used in the NS code to calculate pressure, the computational speed is dramatically increased. However, the solution produced here would be equivalent to that found using the full NS equation solver, assuming a correct pressure boundary condition is specified.

Longuet-Higgins [49] was the first to show the occurrence of and calculate the mean (i.e., period-averaged) mass transport velocity $\langle u \rangle$ (i.e., steady streaming) induced in the oscillatory BL under progressive waves, in the direction of wave propagation. This velocity occurs even when the forcing is specified from linear wave theory (note, additional contributions to the steady streaming velocity can also be result from nonlinear effects such as Stokes drift or from wave asymmetry). Thus, Longuet-Higgins found the linear Eulerian drift as:

$$\langle u \rangle = \frac{k\omega H^2}{4 \sinh^2 kh} \left[ \frac{3}{4} - e^{-\xi} \cos \xi + \frac{1}{2} e^{-\xi} \sin \xi + \frac{1}{4} e^{-2\xi} \right.$$  

$$\left. - \frac{1}{2} \xi e^{-\xi} \cos \xi - \frac{1}{2} \xi e^{-\xi} \sin \xi \right]$$

where $\xi = (x_3 - h)/\delta_S$ [50, 87].

In this application, we computed the steady streaming in the laminar regime, i.e., using the LES with no eddy viscosity, starting with waves of height $H = 0.46$ m, period $T = 6$ s, in depth $h = 5$ m (which is incidentally the conditions from an example used by Myrhaug and Holmedal [57]). We initially used a grid of
Figure 6. Vertical profile of non-dimensional Eulerian drift velocity, in a laminar oscillatory BL forced by linear Stokes waves, computed in NS-LES model (·) using a 128 x 128 grid, versus Longuet-Higgins [50] theory (—).

128 points in both streamwise (horizontal) and vertical directions (again, for this 2D laminar case, the spanwise direction is irrelevant), and a time step $\Delta t = T/256$. With this data, the spatial grid covered one wavelength $\lambda = 2\pi/k$ in horizontal by $16\delta_S$ in vertical direction. Periodic boundary conditions were specified in the horizontal directions and a no slip condition on the bed. Results in Fig. 6 for this case show that the calculated vertical profile of the Eulerian drift velocity agrees very well with the theoretical Eq. (51).

Convergence of the numerical solution is further assessed for this case, by varying the vertical grid size and calculating the difference between the steady streaming velocity for the highest point in the domain over the bed, $u_\infty$ versus the theoretical solution of $(3k\omega H^2)/(16 \sinh^2 kh)$, obtained by setting $x_3 \to \infty$ in Eq. (51). Fig. 7 shows that this error significantly and linearly reduces when the number of vertical grid points is varied from 16 to 128. Additional numerical accuracy and convergence tests are performed for oscillatory BL flows under different types of waves in the following sections.
Figure 7. Same application and physical data as in Fig. 6. Error (relative to the theoretical solution) of far-field \((x_3 \to \infty)\) Eulerian streaming velocity as a function of vertical grid size.

Figure 8. Same application and physical data as in Fig. 6. Non-dimensional far field Eulerian streaming velocity, in a laminar oscillatory BL forced by linear Stokes waves, computed in NS-LES model (various lines) versus theory (converged value of nearly 1), using open boundary conditions, for domains of length \(8\lambda\) (—), \(4\lambda\) (–), \(2\lambda\) (– · · ·), and \(\lambda\) (· · ·).
Open boundary conditions

In earlier simulations of near-bed wave-induced flows (e.g., Gilbert et al. [14]), a boundary condition of the type $\partial u_i/\partial n = 0$ was used to simulate open boundary conditions on the lateral boundaries of the NS domain. Although not needed for the present periodic forcing, such conditions are tested in the present application, rather than periodic conditions as done so far, as these will allow simulating arbitrary rather than idealized incident waves in later applications. Additionally, correctly predicting steady streaming is key in wave-induced BLs, and thus we investigate the effect of this boundary condition on the simulated streaming velocities.

In the present perturbation approach, the open boundary condition for the horizontal velocity reads: $\partial u_{1i}^P/\partial n = 0$, which is exact for a spatially uniform oscillatory BL, but not for a wave-induced BL. We test the effect of this condition by running a test similar to that in the previous section, but varying the domain length with respect to the incident wavelength: $L_1/\lambda$. In order to keep $\Delta x_1$ constant and thus not to affect the discretization error, the number of grid points is adjusted at the same time. Because we want to consider several orders of magni-
nitude, we will separately consider the case where \( L_1 > \lambda \) (Fig. 8) and \( L_1 < \lambda \) (Fig. 9). For the larger domains, we use \( \Delta x_1 = \lambda/32 \), and \( L_1 = \lambda, 2\lambda, ..., 2^4\lambda \), and for the smaller domains, \( \Delta x_1 = \lambda/256 \), and \( L_1 = \lambda, \lambda/2, ..., \lambda/2^4 \).

Results in the figures show that, when applying a simple free gradient boundary condition for the horizontal velocity, we achieve similarly good results for steady streaming velocities, as when using a periodic condition, a quarter-wavelength from the edge of the domain. This condition is thus reasonably successful, as long as the NS domain is about a wavelength across. Simulating steady streaming in smaller domains would most likely require more sophisticated boundary conditions.

**Eulerian drift in near-breaking waves**

While we have so far only considered BL forcing from linear waves, with one set of parameters, a variety of more realistic forcings can be used in the coupled model. This is illustrated by calculating the Eulerian BL drift for FNPF waves shoaling over a sloping bed, in a setup similar to that of Fig. 2.

To reduce the computational cost, laminar flow conditions were selected in these simulations. Indeed, the number of grid points required in the model, in each direction (i.e., \( N_1, N_2, N_3 \)), is a function of flow conditions. For the laminar wave-induced BL case, one only needs to resolve a single wavelength (e.g., \( N_1 = O(10^2) \)), the lateral direction is unimportant (e.g., \( N_2 = O(10^0) \)), and the BL needs to be resolved (e.g., \( N_3 = O(10^2) \)); hence, the total number of points is \( O(10^4) \). By contrast, for a turbulent oscillatory BL (such as in the last application in the next section), the lateral direction is important for resolving three-dimensional eddies (e.g., \( N_2 = O(10^2) \)), and in the streamwise direction it is the eddies which must be resolved, not the wavelength of a wave, but again, \( N_1 = O(10^2) \), so the total number of grid points is \( O(10^6) \). The present wave-induced BL case is more computationally intensive than the idealized oscillatory flow specified in the last
Table 2. NWT parameters for example of steady streaming of near-breaking waves on a sloping bed.

<table>
<thead>
<tr>
<th>Domain</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wave period ( (T) )</td>
<td>2.5 s</td>
</tr>
<tr>
<td>Initial wave height ( (H_0) )</td>
<td>0.175 m</td>
</tr>
<tr>
<td>Forcing</td>
<td>Streamfunction wave</td>
</tr>
<tr>
<td>Timestep ( (\Delta t) )</td>
<td>0.025 s</td>
</tr>
<tr>
<td>Slope ( (m) )</td>
<td>1/24</td>
</tr>
<tr>
<td>Simulation time</td>
<td>( 25T )</td>
</tr>
<tr>
<td>Number of wave gages</td>
<td>38</td>
</tr>
<tr>
<td>Wave gage locations ( x_{g1} )</td>
<td>From 10.375 to 19.625 m, spaced evenly</td>
</tr>
</tbody>
</table>

application, because hundreds of wave periods are needed in order for the steady streaming velocity to converge (a second-order effect), whereas for the oscillatory BL, only ten oscillations or so are used. Because of the vast difference in the size of eddies in the BL and a typical wavelength, the computational domain required for a turbulent wave-induced BL would be larger than both (e.g., \( N_1 = O(10^4) \); \( N_2 = O(10^2) \); \( N_3 = O(10^2) \)), resulting in a domain with perhaps \( O(10^8) \) grid points. Additionally, the simulation would have to be run for hundreds of periods as well, resulting in a computational time several orders of magnitude longer than for results shown here.

Another feature of the present simulations (Table 2) is that “numerically exact” FNPF periodic waves are generated in the NWT, instead of approximate periodic waves, such as generated by a sinusoidally moving piston or flap wave-maker (as in laboratory wave generation). Specifically, we use the zero mean-flux streamfunction wave generation proposed by Grilli and Horrillo [5], to generate a wave of period \( T = 2.5 \) s and height \( H = 0.175 \) m in a NWT of “offshore” depth \( h_o = 1 \) m, which extends over 40 m (Fig. 2). This method was developed to generate nonlinear waves in a NWT, whose nonlinear Stokes drift is cancelled by specifying a current equal and opposite to the wave mean mass flux. This both
prevents the tank mean water level from artificially increasing and allows for the undertow current generated in the nearshore part of the tank to “exit” through the tank offshore boundary.

To cause wave shoaling, a slope $s = 1/24$ is specified in the NWT starting at 5 m from the wavemaking boundary. To prevent wave overturning and breaking (which would interrupt FNPF computations), the water depth levels off at 20 m from the wavemaker, at a depth of 0.375 m, and then increases to $h_1 = 0.5$ m in the absorbing beach (AB), following a hyperbolic tangent similar to the increase of the damping coefficient in the AB; this causes wave de-shoaling and makes it easier for the AB to absorb the incident wave energy. The NWT boundary is discretized with 513 nodes, with a grid spacing on all boundaries of approximately 0.16 m. Along the surface, the boundary is discretized with 249 Mixed Cubic Interpolation (MCI; [4]) elements. On the wavemaker, bottom, and absorbing piston of the NWT, the boundary is discretized with 3, 125, and 2 three node cubic elements, respectively. In order to force the oscillatory BL to be laminar (see Fig. 1), a kinematic viscosity of $1 \times 10^{-5}$ m/s$^2$ is assumed.

In order to obtain highly nonlinear physics related to shoaling (e.g., with both trough/crest and rear/front wave-asymmetry), the coupled NS-LES domain had to be located very close to the theoretical breaking point for the selected sloping bed geometry. Even with the AB starting at the end of the sloping bed, it was observed that the absorption distance was not sufficient to prevent large nonlinear waves from forming a small scale overturning jet, due to the Lagrangian motion of the NWT nodes/water particles that caused node convergence in the wave crest area. The act of regridding free-surface nodes at equal arclength intervals at every time step in combination with the AB, appeared sufficient to prevent hydrodynamic instabilities from causing waves to overturn.
Figure 10. Example of surface elevation, and horizontal/vertical velocity components simulated at the NWT seabed (—), 15 m from the wavemaker (averaging the results at adjacent wave gages at 14.875 and 15.125 m).
Figure 11. Free-surface elevation predicted by NWT around the area of interest (from 11 to 19 m from the wavemaker, with overlapping data from 5T to 21T every two periods. [Vertical exaggeration is 2x.] The NS-LES domain is sketched for information.

The inviscid flow forcing for the NS-LES domain, encompassing the BL, is obtained using the approximation from Eqs. 40 to 42, from velocities computed at 32 wave gages (Fig. 10). Note that the Stokes BL thickness is several orders of magnitude smaller than the water depth in the NWT, so the approximation using inviscid seabed velocities seems quite reasonable. [Note, inviscid velocities could be calculated at internal points within the NS-LES domain; however because the BL is so thin in this application, any vertical variation in such velocities would be more likely caused by numerical errors than any physical variation; similarly, the velocity gradient is computed with finite-differences but this could be made more accurate using the NWT boundary integral equation.]

The inviscid forcing is ramp-up by running the NWT for an initial 25 wave periods, and is then used to force the NS solver. To do so, the final wave period of NWT simulations is repeated from then on, to provide a quasi-periodic forcing. This assumes that the NWT has reached a quasi-periodic state by then, which is demonstrated, e.g., in Fig. 11.

For each test, we use a moderately coarse NS grid of 32x32 (LxH) points, with 100 timesteps per period (Table 3). The NS domain is 8 m long (from 11 to 19 m from the wavemaker; Fig. 11), 4.5 cm thick, and the simulations are run for 1000 wave periods. [The domain was specified with two points in the lateral direction,
Table 3. NS-LES solver parameters for the steady streaming of near-breaking waves on a sloping bed.

<table>
<thead>
<tr>
<th>Domain</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_1 \times L_2 \times L_3$</td>
<td>$8 \text{ m} \times 0.1 \text{ m} \times 0.045 \text{ m}$</td>
</tr>
<tr>
<td>$N_1 \times N_2 \times N_3$</td>
<td>$32 \times 2 \times 32$</td>
</tr>
<tr>
<td>Upper boundary condition</td>
<td>Zero-gradient</td>
</tr>
<tr>
<td>Wall boundary condition</td>
<td>No-slip</td>
</tr>
<tr>
<td>Initial conditions</td>
<td>$u(x_i, t = 0) = 0$</td>
</tr>
<tr>
<td>Timestep ($\Delta t$)</td>
<td>0.025 s</td>
</tr>
<tr>
<td>Viscosity ($\nu$)</td>
<td>$10^{-5} \text{ m}^2/\text{s}$</td>
</tr>
<tr>
<td>Simulation time</td>
<td>2502.5 s</td>
</tr>
</tbody>
</table>

with a width of 10 cm, although this is presumed to be unimportant for this laminar case.] In general, a streaming velocity away from the beach was observed (Fig. 12), with significant variation across the domain. Interestingly, the trend of larger offshore mean current in deeper water just outside the BL is reversed very near the seabed (Fig. 13). Note that others (e.g., Myrhaug and Holmedal [57]) have also found that adding the second-order component of a Stokes wave results in a weaker mean onshore than that predicted by Longuet-Higgins theory or even an offshore Eulerian steady streaming, as shown here. [One possible mechanism for the reversal of the drift velocity direction is the generation of an offshore undertow current, due to the impermeable boundary condition on the right side of the NWT.]

While these results show that the coupled numerical model works as intended and can produce relevant results for realistic incident waves, applicable to actual wave-induced BLs, a final demonstration is required to show that the SGS models implemented in the LES are adequate to reproduce the desired turbulent flow properties. This is done in the next section.

1.4.2 Turbulent oscillatory boundary layers

We next validate the LES for turbulent oscillatory oscillatory BLs. We choose a uniform oscillatory flow because of the lack of sufficiently detailed experimental
Figure 12. Eulerian drift at the edge of the boundary layer predicted by Navier-Stokes solver for fully-nonlinear potential flow forcing.

Figure 13. Time-averaged Eulerian drift profiles (versus distance off seabed) predicted by Navier-Stokes solver for fully-nonlinear potential flow forcing at $x = 13.125$ m (—), $x = 15.125$ m (−−), and $x = 17.125$ m (···).
Table 4. Parameters (period $T$, free-stream maximum velocity $U_0$, viscosity $\nu$, Nikuradse roughness $k_s$, and free-stream amplitude $A$) for selected laboratory experiments of turbulent oscillatory BLs (Jensen et al.’s [44]) used for comparison with numerical simulations.

<table>
<thead>
<tr>
<th>Test no.</th>
<th>$T$ (s)</th>
<th>$U_0$ (m/s)</th>
<th>$\nu$ (m$^2$/s)</th>
<th>$Re$</th>
<th>$k_s$ (mm)</th>
<th>$A/k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>9.72</td>
<td>1.02</td>
<td>$1.14 \times 10^{-6}$</td>
<td>$1.6 \times 10^6$</td>
<td>0.84</td>
<td>1800</td>
</tr>
<tr>
<td>13</td>
<td>9.72</td>
<td>2.00</td>
<td>$1.14 \times 10^{-6}$</td>
<td>$6.0 \times 10^6$</td>
<td>0.84</td>
<td>3700</td>
</tr>
</tbody>
</table>

data for more complex wave-induced flows. To compare results with the laboratory experiments of Jensen et al.’s [44], which were performed in an oscillatory flume (U-tube), the model inviscid forcing was selected similarly to the initial laminar BL test cases, as a vertically uniform oscillatory flow (see Eq. 44), with velocity amplitude $U_o$ and period $T$ ($\omega = 2\pi/T$). Jensen et al.’s experiments consisted in 15 different test cases, of which we selected for comparison two cases with a rough bed: no. 12, and 13 (see physical data in Table 4). In each case, the mean velocity and Reynolds stresses were measured as a function of time and elevation over the rough bed in the BL.

To achieve good accuracy and resolution in simulated results and also ensure that the number of “samples” used for ensemble averaging is large enough, a NS grid size of 128x32x64 is used in simulations (see numerical parameters in Table 5), slightly larger than that used by Radhakrishnan and Piomelli [27] who recently reported on similar comparisons. Note, for very simple flows such as considered here, this need for performing averaging operations is one disadvantage of NS-LES models as compared to a RANS models, which directly compute mean quantities.

**Wall stress and mean velocity**

Jensen et al. did not measure wall stress $\langle \tau_w \rangle$, but rather (for test #13 only) they did measure a time-series of the mean streamwise velocity at a very small height over the wall, $x_3 = 0.0006A$ (relative to the amplitude of oscillation $A =$
Table 5. Parameters for numerical simulations of turbulent oscillatory BLs.

<table>
<thead>
<tr>
<th>Domain</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_1 \times L_2 \times L_3$</td>
<td>$636.3 \delta_S \times 318.2 \delta_S \times 100 \delta_S$</td>
</tr>
<tr>
<td>$N_1 \times N_2 \times N_3$</td>
<td>$128 \times 64 \times 32$</td>
</tr>
<tr>
<td>Grid (Smagorinsky SGS model)</td>
<td>Uniform grid spacing</td>
</tr>
<tr>
<td>Grid (dynamic SGS models)</td>
<td>Vertical exponential stretching with ratio 1.1</td>
</tr>
<tr>
<td></td>
<td>Minimum grid height: 0.93 mm</td>
</tr>
<tr>
<td></td>
<td>Aspect ratio at wall: 10:1:10</td>
</tr>
<tr>
<td>Upper boundary condition</td>
<td>Zero-gradient</td>
</tr>
<tr>
<td>Wall boundary condition</td>
<td>Log-layer approximation</td>
</tr>
<tr>
<td>Wall roughness</td>
<td>$z_0 = 2.8 \times 10^{-5}$ m</td>
</tr>
<tr>
<td>Initial conditions</td>
<td>$u(x_i, t = 0) = 0$</td>
</tr>
<tr>
<td>Simulation spin-up time</td>
<td>$5T$</td>
</tr>
<tr>
<td>Forcing</td>
<td>$u_1^I(t) = U_0 \sin \omega t$</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>$T/4860$ (test 12) or $T/9720$ (test 13)</td>
</tr>
<tr>
<td>Simulation time</td>
<td>$10T$</td>
</tr>
<tr>
<td>Output sampling frequency</td>
<td>Every $T/12$</td>
</tr>
</tbody>
</table>

$U_0/\omega$; equivalent to a height $x_3$ of 1.86 mm), which we used together with a log-law assumption, to predict wall stress. Figs. 14 and 15 show wall stress computed for tests #12 and #13, using the three sub-grid scale models in the NS-LES; in the latter test, this is compared with experimental values inferred from near-wall velocity measurements.

Wall stress is qualitatively consistent among the three SGS turbulence models used. Additionally, for test #13, numerical results with the DSM and DMM approaches agree well both with each other and with experiments, while these are underpredicted by the Smagorinsky model; a better agreement for the latter could probably be achieved by calibrating the Smagorinsky coefficient. Note that while of the DSM and DMM approaches show a good performance, they rely on the enhanced eddy viscosity near the wall, which tends towards the mixing-length approximation. A time-invariant eddy viscosity distribution proportional to the height above the wall was found by Grant and Madsen [31] to produce good results.
Figure 14. Numerical simulations of turbulent oscillatory BL: mean wall stress, \( \langle \tau_w \rangle \) (determined by log-law) as a function of phase angle for conditions of test #12 (Jensen et al’s [44]) with different SGS models: (—) Smagorinsky; (— —) dynamic Smagorinsky; (···) dynamic mixed model.

for both wall stress and mean flow, so it is reasonable to expect that the DSM and DMM approaches would also be successful.

Results in Figs. 16 and 17 show that model results for the mean flow velocity, \( \langle u_1 \rangle \), are again qualitatively consistent among the three SGS turbulence models used, with the Smagorinsky approach underestimating the BL thickness. Numerical results using DSM or DMM agree well with experiments, for both the #12 and 13 test cases, at six selected phases of the flow, over half a period of oscillation.

**Turbulent intensity and Reynolds stress**

For both test cases #12 and 13, we calculated the streamwise turbulent intensity \( \langle u_1^2 \rangle^{1/2} \) (Figs. 18 and 19), the vertical (wall normal) turbulent intensity \( \langle u_3^2 \rangle^{1/2} \) (Figs. 20 and 21), and the Reynolds stresses \( \langle u'_1 u'_3 \rangle \) (Figs. 22 and 23), and compared those to experiments. The figures show a good agreement of all model results with experiments when using DSM or DMM, but not so with the Smagorinsky model. In particular, for test #12, at the lower Reynolds number, the Smagorinsky approach fails to produce much resolved turbulence. This high-
Figure 15. Same case as Fig. 14, for test #13, with comparison to experiments (●).

Figure 16. Same case as Fig. 14. Mean streamwise velocity profiles, $\langle u_1 \rangle$, for test #12.
lights the significance of having to tune this model’s coefficient to different flow conditions.

Near the wall, all simulation results underpredict the experimental turbulence intensity. For the constant coefficient Smagorinsky model, this is expected because this model is known to overpredict near-wall dissipation. For the dynamic models, the underpredicted turbulent intensity is more likely due to the grid aspect ratio near the wall. The vertical stretching of the grid results in “pancake”-like grid cells, which are significantly wider in the streamwise and spanwise directions than in the wall-normal direction. The typical eddy size, however, is of similar size in all directions, and so the implicit grid-scale filter averages over many eddies in a way similar to a RANS ensemble average. The most similar numerical study to the present one is the LES work of Radhakrishnan and Piomelli [27], which studied test case #13. Their results for the near-wall turbulent intensity are similar to ours for most phases of the oscillation, although Radhakrishnan and Piomelli did
obtain a better agreement with experiments at $\omega t = 60^\circ$ and $\omega t = 90^\circ$, albeit using different SGS models, and without having the large aspect ratio for the grid cells near the wall.

Far from the wall, there is an occasional underprediction of the turbulent intensity. Other numerical studies have reported this problem as well, which Meller [39] suggests is an experimental artifact. The amplitude of the oscillation for test #13 is 3.1 m, so a fluid particle can move as far as 6.2 m over the course of each oscillation. Hence, at the end of each period (i.e., around 0°), some of the fluid being measured may have a half-period earlier been outside of the 10 m straight test section of the oscillatory water tunnel used in experiments. Although Jensen et al. took some additional measurements to attempt to show that this would have no effect, it does seem to explain the outlier seen at the 0 degree phase angle (e.g., Fig. 18). The results far from the wall are similar to others (e.g., Radhakrishnan and Piomelli), although our turbulent intensities match experiment somewhat better far from the wall at phases 0° and 30°.

In some cases, the size of the discretization may prove to be the limiting factor. For case #13, for instance, the Reynolds stress at 90° was experimentally measured to be maximum at 2.6 $\delta_S$ over the bed (Fig. 23), whereas the first grid cell is 3 $\delta_S$ high. Important physics may not be properly modeled as a result. Note that Sleath [48] found that the Reynolds stress is a minor contributor to the shear stress. As a result, one would expect that the vertical momentum flux would be governed more by the periodic velocity components than the turbulent momentum flux, and so more study would be required to verify whether resolving this peak in Reynolds stress is important for the numerical simulations.
Figure 18. Streamwise turbulent intensity, $\langle u'^2 \rangle^{1/2}$, for test #12.

Figure 19. Streamwise turbulent intensity, $\langle u'^2 \rangle^{1/2}$, for test #13.
Figure 20. Wall normal turbulent intensity, \( \langle u_3'^2 \rangle^{1/2} \), for test #12.

Figure 21. Wall normal turbulent intensity, \( \langle u_3'^2 \rangle^{1/2} \), for test #13.
Figure 22. Reynolds stress, $\langle u_1' u_3' \rangle$, for test #12.

Figure 23. Reynolds stress, $\langle u_1' u_3' \rangle$, for test #13.
Velocity spectra

In addition to examining second-order turbulence statistics, we analyzed velocity spectra, such as the streamwise velocity fluctuation spectrum, which can be defined as the discrete Fourier transform:

$$E_{11}(k_1) = \left| \sum_{n=1}^{N_i} [u_1]_{n,j,k} e^{-2\pi ink_x/N_i} \right|$$

and can also be phase-averaged. Note, such spectra are computed directly from the resolved velocities at each grid point, and thus develop as a result of simulations. It should be stressed that the numerical method is not a spectral method and, hence, spectra are not a priori assumed in the SGS models used here.

Fig. 24, for instance, shows the phase-averaged spatial velocity power spectra for the DSM test #13 run at 0°. We are able to see at least what appears to be the inertial subrange in the spectral results (slope 5/3). Note that the spectra are not smooth lines, but somewhat stochastic. This indicates that the scale of the largest vortex structures is not well-resolved, which is somewhat expected because particles in the free-stream oscillate horizontally over $2A = 2U_0/\omega \approx 6.2$ m, whereas the computational domain is approximately an eighth of that size. A similar problem was encountered by Costamagna et al. [88], but because the Jensen et al. data is for fully turbulent conditions, we may use phase-averaging (i.e., averaging the data for the same phase from different oscillations) in order to smooth results, as we have done above. Because the dynamics is mostly controlled by the near-wall behavior (where the eddies are smaller), the largest scales are unlikely to be particularly important, but future studies should consider using larger computational domains to verify this claim.

Two-point spatial correlation

One premise of the modeling of turbulent flows in “infinitely long” oscillatory BLs, using a finite length spatially periodic domain, is that there is no correlation
Figure 24. Nondimensional velocity spectra for the resolved streamwise velocity field.

between the velocity fluctuations a half-domain away (see, e.g., Moin and Mahesh [1]). This will be achieved provided the domain size is large enough, which can be a posteriori verified in numerical results by calculating and verifying that the two-point spatial autocorrelation of the perturbation velocity field is nearly zero, between points half a domain away in the horizontal direction.

Fig. 25 shows the autocorrelation of each of the three components of the velocity fluctuations in both the streamwise and spanwise directions at a given height for the DSM run of test 13. The autocorrelation function is very small for much of the domain, in both streamwise and spanwise directions, indicating that the domain is large enough.
Figure 25. Two-point spatial autocorrelation functions for the component velocity fluctuations, $u'_1$ (—), $u'_2$ (– –), $u'_3$ (···), at the first gridpoint above the rough bed, as a function of distance for test case #13, in both the streamwise direction (averaged over the spanwise direction; upper panel) and spanwise direction (averaged over the streamwise direction; lower panel).
1.5 Conclusions

A perturbation approach to the Navier-Stokes (NS) equations was developed for simulating wave-induced Boundary Layer (BL) flows, in a coupled model implementation, in which the NS domain is embedded within a fully nonlinear inviscid Numerical Wave Tank (NWT). The NS equations are solved using a Large-Eddy Simulation (LES) with a variety of subgrid scale (SGS) turbulence models. For many coastal engineering problems, the physics of waves is such that the flow is nearly irrotational in most of the fluid domain, except for thin free surface and bottom BLs. Hence, the region of the seafloor requiring full NS modeling may be relatively small, which justifies the coupled/hybrid approach and allows using efficient and relevant models for various parts or regions of the solution, based on the corresponding salient physics. Another advantage of the perturbation method is that the inviscid component of the flow fields (which is either analytical or obtained in the NWT) is not subject to the numerical errors of the NS solver.

The NS solver is first validated for simple laminar or turbulent oscillatory BL flows (for the former, the eddy viscosity was zero and the LES was bypassed). For laminar cases, results are very close to theoretical closed-form solutions for oscillatory BLs, both in simple periodic flows or under linear wave forcing. Moreover, simulations demonstrate the expected rates of convergence to the exact solution, with both spatial and temporal discretizations. The hybrid NWT-NS model is then used to compute the steady streaming current due to fully nonlinear periodic waves, shoaling on a slope near the breaking point, which demonstrates the possibilities of the approach to simulate realistic nearshore wave processes. Simulations for rough turbulent oscillatory BL flows are finally performed, which favorably compare to experimental data, for both mean and turbulent fields.

More specifically, results for one-dimensional (i.e., forced by spatially uniform
horizontal flows) laminar oscillatory BLs over a flat boundary showed the expected second-order convergence of numerical errors to the Stokes solution [86], in both space and time. This was to be expected from published results, as all of the modified terms in the new perturbed NS equations, as compared to the original Cui and Street work [22], were zero for this very simple test case. Similarly good results were obtained for laminar oscillatory BLs induced by linear Stokes waves, which yield non-spatially uniform forcing flows. This case further tested the application of the inviscid forcing terms in the perturbation form of the momentum equations (i.e., nonlinear convective terms). In these simulations, we first used spatially periodic boundary conditions in both lateral directions of the NS domain and found that the computed steady streaming velocities in the BL closely matched those theoretically predicted by Longuet-Higgins [50]. Effects of using more general (gradient free) open boundary conditions were then tested in the case of wave forcing, and results were shown to be accurate within half a wavelength of the lateral boundaries of the NS domain.

Preliminary numerical tests of the fully coupled NWT-NS model were performed, for simple “numerically exact” nonlinear periodic incident waves shoaling over a 1:24 slope. Specifically, we calculated fully nonlinear inviscid flow fields near the breaking point in the NWT, for periodic waves shoaling over a plane slope, and used those to force BL flows (limited to laminar cases) in a small embedded near-bottom NS-LES domain. Results show that for the selected parameters, unlike with the flat-bottom linear wave forcing case, the steady streaming in the BL is both stronger and directed offshore, with significant spatial variation.

Finally, for rough turbulent oscillatory BL flows, the LES model, with various SGS, was able to accurately predict measured mean flow fields, wall stress, and second-order turbulent statistics. Specifically, all results favorably compared
with the experimental data of Jensen et al.’s test #12 and 13 [44] (except over small regions for the turbulent fields). Our simulations with dynamic SGS showed somewhat better agreement with the measured turbulent intensity far from the wall than the recent results of Radhakrishnan and Piomelli [27]. This may be partly due to using a gradient-free boundary condition, as opposed to setting the wall-normal velocity to zero in the free-stream, and to increased model accuracy when using the perturbation method.

While these experiments show that a hybrid NWT-LES can accurately determine turbulent characteristics of coastal flows, note that for turbulent boundary layers over complex 3D bathymetry, this technique may still be computationally demanding depending on the size of the domain. A LES of turbulent flow needs to simulate eddies which may be several orders of magnitude smaller than the size of the domain, in three-dimensions (regardless of whether the driving force is uniform, or varies in one or more dimensions), and perhaps over several hundreds of wave periods to determine e.g., the induced steady streaming velocity. Limitations have existed for high-Reynolds laboratory measurements as well, however, and only recently has the wave-induced steady streaming velocity of a fully turbulent boundary layer over sloping bed been made [89]. More complex applications should be made possible as computer performance increases.

In future work, we will build on the model capabilities demonstrated in these initial somewhat idealized numerical applications, by simulating more general wave-induced turbulent BL flows. We will finally add a sub-model for sediment suspension and transport, with the eventual goal of being able to simulate wave-induced bed form development around objects on the seabed.
Acknowledgements

Both authors gratefully acknowledge support of grant Nb. N000140510068 from the US Office of Naval Research (ONR) Coastal Geosciences Division (code 321CG). In addition, the first author acknowledges support from an ONR-NDSEG fellowship. R. Street and O. Fringer are thanked for providing the initial LES code, and Dr. Senthil Radhakrishnan is gratefully acknowledged for providing us with a copy of the Jensen et al. data.

List of References


MANUSCRIPT 2

Large eddy simulation of sediment transport over rippled beds

Jeffrey C. Harris and Stéphan T. Grilli

In preparation for Coastal Engineering
Abstract

We present the application of a numerical model for the simulation of bottom boundary (BL) flows and sediment transport. Our approach is based on coupling a “near-field” local Navier-Stokes (NS) model with a “far-field” inviscid flow model, which provides the large-scale incident forcing. The inviscid velocity provided by this forcing is applied through a (one-way) coupling to a Large Eddy Simulation (LES), to simulate near-field, wave-induced, turbulent bottom boundary layer flows. The velocity field predicted by the coupled model compares well with the laboratory experiments for oscillatory flow over full-scale vortex ripples, but do not accurately predict the overall suspended sediment flux.

2.1 Introduction

Rippled seabeds are a common feature in coastal waters, and strongly affect wave-induced bottom boundary layer flow. Many methods have been proposed for modeling rippled beds, from modeling individual particles (i.e., discrete particle models; [1]) to simply adjusting the effective bottom roughness [2]. Here, we present the application of a previously validated large eddy simulation (LES [3, 4]) to modeling these vortex ripples. While much simpler than a discrete particle model, the LES of three-dimensional (3D) flows over a complex boundary still requires significant computational time, despite the continual increase in computer performance. For this reason, one must limit the computational domain to that necessary and sufficient for solving a given problem. For example, periodic boundary conditions may be suitable for modeling oscillatory boundary layers inside water tunnels, as long as the turbulence is sufficiently resolved (e.g., [4]). This type of simplification allows for simulations on simple, small domains that represent much larger experimental

Similarly, only the largest wavetanks can produce the flow conditions neces-
sary to form vortex ripples on the scale observed in coastal waters. To a first
order, though, vortex ripples are forced by the horizontal oscillation of water over
the seabed. Instead of using a wavetank, then, experiments can be done in an
oscillatory water tunnel (e.g., [5]), which is simply forced by a piston at one end.
This is a vastly simpler laboratory setup, but still captures much of the dynamics
of the wave boundary layer, including the shedding of vortices from the ripple
crests. It does not allow the measurement of Longuet-Higgins steady streaming [6]
or Stokes drift to nonlinear wave asymmetry, but these are second-order effects.

The present LES work is an extension of that by Harris and Grilli [4]. The
method used is a modification of the LES of Cui and Fringer [7], and an advance-
ment of earlier work done by Gilbert et al. [8]. The turbulent bottom boundary
layer is considered as perturbation of an inviscid flow over the same domain. The
perturbation scheme consists in first dividing the total pressure and velocity fields
into inviscid and viscous perturbation parts and then to rewrite NS equations for
the perturbation fields only; this yields new forcing terms, which are function of
inviscid flow fields representing the incident wave forcing (e.g., similar to [9, 10]).
The coupling approach used here makes it possible to use a variety of fully re-
alistic nonlinear and irregular wave forcings, besides the commonly used simple
oscillatory or linear wave flows (see e.g., [11]). While this coupled version has been
validated against turbulent bottom boundary layers [4], this particular version of
the code has not been validated for complex boundaries, or used for modeling
sediment transport.

A completely separate development of Gilbert et al.’s [8] LES work on sus-
pended sediment transport has continued independently to those presented here
[12, 13], and as well Cui and Street’s[7] LES has been further developed to study
bedform evolution by Chou et al. [14, 15]. Chou et al. [16] were able to extend
the model to consider an evolving bed, and with sufficient computer time were able to simulate the formation of vortex ripples on a sandy bed. Note, however, that Chou et al.’s work has only considered limited comparisons with experimental data. They did not make direct comparisons of velocity fields, suspended sediment concentrations, or sediment transport rates with observations.

Beyond simply increasing knowledge about the bottom boundary layer, models of sediment transport as sophisticated as an LES have the potential to provide predictions of sediment transport around objects, an important problem in scour around pipelines (e.g., [17, 18]) and burial of bottom sea mines (e.g., [19, 20, 21, 22, 23, 24, 25]). Many, even recent, bed morphology models are limited to 2D (e.g., [26, 27]), and 3D models which are able of simulating three-dimensional scour on a bed have only recently been developed (e.g., [28]). The coupled LES formulation used here, if validated, could be applied on larger scales to these problems while including fully nonlinear effects of waves, as opposed to only considering uniform oscillatory flow.

In summary, we present new applications of a hybrid method to simulating sediment transport over vortex ripples with a 3D-LES. For validation we compare simulation results to laboratory data including measured velocity and suspended sediment concentration fields. In our hybrid/perturbation approach, the total velocity and pressure fields are expressed as the sum of irrotational (thus kinematically inviscid) and near-field viscous perturbations above a rigid seabed. The NS equations are formulated and solved for the perturbation fields only, which are forced by additional terms representing the incident fields. While there are few differences between this and any other LES method in current applications, it serves as a test case for a method which could be easily be adapted for much more complicated scenarios (e.g., sediment transport caused by irregular waves around
2.2 Measurements and models of vortex ripples

There are many types of models for simulating flow over ripples. Some of the earliest models of flow over ripples considered inviscid flow (e.g., [29]). One-dimensional eddy viscosity models (e.g., [30]), though simple, are a practical method of modeling suspended sediment concentrations and flux. Because the dynamics of the flow over ripples is dominated by the coherent eddies formed at the ripple crests, with stochastic turbulence a secondary process, discrete vortex models (e.g., [31, 32]) have seen some success. Reynolds averaged approaches (RANS; e.g., [33]) are another common technique, and Chang and Scotti [34] has compared RANS techniques with LES for modeling flow over ripples. It is also possible to compute a direct numerical simulation (DNS) of flow over ripples (e.g., [35, 36]), but there are stringent limits on the Reynolds number of the flow that are computationally feasible.

Seabed ripples can be found in a variety of height and lengths, from several centimeters to several meters. Vortex ripples are characterized by flow separation...
in the lee of the ripple crest (Fig. 26). This flow separation results in a recirculation eddy being formed, which is ejected away or released from the ripple crest at flow reversal. The wave flow over the ripple geometry induces sheet vortices over the ripple crests every half wave-period, which dominate momentum and sediment transport in the boundary layer (BL). Bagnold [37] was the first to study vortex ripple shapes and the flow above them. Since that time, the formation of these ripples have been studied extensively, both for the more commonly considered long-crested ripples (e.g., [38, 39, 20, 40]), as well as for three-dimensional ripples that can be formed when waves approach the coast at an angle (e.g., [41]). In addition, the relationships between ripple geometry and the oscillatory flow parameters are well established (see e.g., [42]).

Since modeling ripple formation with 3D Navier-Stokes solvers such as an LES require substantial computational effort (such as [16]), and because these ripples rather quickly become quasi-steady state, we limit our focus to the velocity field, suspended sediment concentration, and sediment transport rates over rippled beds. A large variety of field experiments have looked at sediment ripples, including comparing suspended sediment concentration over rippled beds with existing models of ripple characteristics (e.g., [43, 44, 45]). Several experiments have looked at the evolution of sand ripples over time as wave-conditions change (e.g., [46, 47]), as well as considering the effective roughness or wave friction factor of the ripple-covered bed [48]. Traykovski et al. [49] made detailed measurements from a multi-instrument tripod of current, vertical profiles of suspended sediment concentration, and sidescan sonar measurements of bedform geometry over six weeks of observations, which included the passage of several tropical storms. Even more detailed field measurements and analysis of mean and turbulent flow fields have been conducted by Williams et al. [50], considering hydrodynamic conditions, bed
forms, and suspended sediment concentration. Detailed particle-image velocimetry (PIV) measurements in the coastal bottom boundary layer have been made (e.g., [51]), are not presently as well suited for numerical simulations as laboratory observations.

Laboratory experiments often provide more controlled conditions for studying flows over ripples, but few measure both the entire flow field and suspended sediment concentration field, while also obtaining the same types of flow conditions seen in the field. Ribberink and Al-Salem [5] made detailed time-dependent measurements of flow velocity and suspended sediment concentration, but in sheet flow conditions over a flat bed. Faraci and Foti [52] studied the evolution and migration of rolling grain ripples over a seabed, which are on a smaller scale than vortex ripples, and are characterized not by the lee vortex that appears each half-cycle, but due to the motion of sediment along the seabed. Thorne et al. [53] made measurements of ripples in a large wave flume, including measurements of bedform morphology and suspended sediment concentration. These experiments were limited, though, by including few flow measurements, and only from electromagnetic current meters, which do not resolve the vortices that dominate the momentum transfer in the boundary layer. Marin [54] considered both the flow field and Eulerian drift over ripples with progressive waves, but at low Reynolds number, and with a fixed bed. Only recently have full-scale vortex ripples been studied in the lab. van der Werf et al. [40] conducted the first field-scale measurements in the lab over a mobile bed which involved measuring both the velocity field and suspended sediment concentration. We use this dataset for validating the LES in this paper.

There are several recent modeling approaches similar to that presented here. The laboratory test case from van der Werf et al. [40] considered here has been modeled by van der Werf et al. [55] with both $k - \omega$ and discrete vortex parti-
cle tracking models. They show reasonable agreement with measurements both in terms of the velocity field and the sediment transport. Models of suspended sediment transport over ripples using similar numerical methods (though developed independently) have been considered by Zedler and Street [13] and Chou and Fringer [16]. Chou and Fringer have been able to use the same type of LES to model the evolution of ripples on the seabed, but with less detailed comparison with experimental results than presented here.

2.3 Governing equations
2.3.1 Large-eddy simulation

Navier-Stokes (NS) equations for an incompressible, isothermal, Newtonian fluid with the Boussinesq approximation are given by:

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{53}
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i u_j + \frac{p}{\rho_0} \delta_{ij} - \nu \frac{\partial u_i}{\partial x_j} \right) = -\frac{\rho - \rho_0}{\rho_0} g \delta_{i3} \tag{54}
\]

where \( u_i \) and \( p \) are the water velocity and dynamic pressure, respectively, in a fluid of density \( \rho \) with background density \( \rho_0 \) and kinematic viscosity \( \nu \), and \( \delta_{ij} \) is the Kronecker delta:

\[
\delta_{ij} = \begin{cases} 
1 & i = j \\
0 & i \neq j
\end{cases}
\tag{55}
\]

We adopt the indicial tensor notation convention, with \( x_3 \) denoting a vertical distance measured from some reference point. Here the density \( \rho_0 \) is the density of water, with \( \rho - \rho_0 = \rho_0 (s - 1)C \), where \( C \) is the suspended sediment concentration (i.e., SSC), and \( s \) is the relative density of the sediment. Note that the dimensionless units of SSC here are a volume fraction.

Similar to Zedler and Street [12] and Gilbert [56], the suspended sediment concentration is governed by an advection-diffusion equation with a constant settling
velocity \( w_s \):

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} \left( u_j C - w_s \delta_{i3} C - \kappa \frac{\partial C}{\partial x_j} \right) = 0
\] (56)

where the diffusivity, \( \kappa = \nu / \sigma \) with \( \sigma \) the Schmidt number (assumed to be 1.0).

This formulation of the sediment concentration equation assumes that the sand concentration is low enough to avoid particle-fluid and particle-particle interactions beyond a constant settling velocity; the validity of this assumption is discussed by Villaret and Davies [57] and Elghobashi [58]. Elghobashi states that a sediment suspension can be considered dilute if the volume fraction of sediment is less than \( 10^{-3} \), and that the physical coupling between the fluid and particles can be considered to be truly one-way for volume fractions of sediment less than \( 10^{-6} \). Using these criteria, in the experiments considered here, only points directly next to the sand ripples would be considered to be a dense suspension, although there may be some effect on the turbulence that is not included in our model. We note, however, that previous simulations using similar approaches to ours have been successful in predicting the sediment transport in the same experiments [55].

Let us denote by \((u^I_i, p_I)\) the velocity and pressure fields of the ocean wave flow, considered to be inviscid outside of thin boundary layers (BLs) near the seabed. Such flows are well described by Euler equations:

\[
\frac{\partial u^I_i}{\partial x_i} = 0
\] (57)

\[
\frac{\partial u^I_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u^I_i u^I_j + \frac{p_I}{\rho_0} \delta_{ij} \right) = 0.
\] (58)

Let us then introduce a decomposition of the total viscous flow into the sum of the latter inviscid free-stream flow and a defect or perturbation flow, of velocity \( u^P_i \) and pressure \( p_P \):

\[
 u_i = u^I_i + u^P_i
\] (59)

\[
 p = p_I + p_P.
\] (60)
Replacing Eqs. 59 and 60 into Eqs. 53 and 54, and subtracting Eqs. 57 and 58, we derive the governing equations for the perturbation fields as:

\[
\frac{\partial u^P_i}{\partial x_i} = 0 \quad (61)
\]

\[
\frac{\partial u^P_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i u_j - \frac{u_i u_j}{\rho_0} + \frac{p_F}{\rho_0} \delta_{ij} - \nu \frac{\partial u_i}{\partial x_j} \right) = -\frac{\bar{\rho} - \rho_0}{\rho_0} g \delta_{ij}. \quad (62)
\]

Here the perturbation is defined in a region encompassing the near-field bottom boundary layer of interest, which becomes the computational domain.

Although formally different, for the range of problems studied here, these equations can be shown to be equivalent to the forcing of the total flow with the inviscid wave dynamic pressure gradient proposed by Gilbert et al. [8] (with the exception of the inclusion of density variations), expressed as:

\[
\frac{\partial u_i}{\partial x_i} = 0 \quad (63)
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i u_j + \frac{p_F}{\rho_0} \delta_{ij} - \nu \frac{\partial u_i}{\partial x_j} \right) = -\frac{1}{\rho_0} \frac{\partial p_L}{\partial x_j}. \quad (64)
\]

There are two key advantages, however, to the current approach, as compared to this earlier work: (1) boundary conditions can be more clearly and accurately defined for the viscous perturbation (i.e., as vanishing or using a radiation condition away from the wall); and (2) only the inviscid velocity is needed in the NS forcing terms rather than the dynamic pressure gradient.

By applying a spatial-average operator (overbar) to the governing equations we obtain the momentum equation for the resolved perturbation as:

\[
\frac{\partial \bar{u}^P_i}{\partial x_i} = 0 \quad (65)
\]

\[
\frac{\partial \bar{u}^P_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{u}_j - \frac{\bar{u}_i \bar{u}_j}{\bar{\rho}} + \frac{p_F}{\bar{\rho}} \delta_{ij} - \nu \frac{\partial \bar{u}_i}{\partial x_j} + \tau_{ij} \right) = -g(s-1) \bar{C} \delta_{i3} \quad (66)
\]

\[
\frac{\partial \bar{C}}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_j \bar{C} - w_s \delta_{i2} \bar{C} - \frac{\nu}{\sigma} \frac{\partial \bar{C}}{\partial x_j} + \chi_j \right) = 0 \quad (67)
\]

where \( \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \) is the subgrid scale (SGS) stress, and \( \chi_j = \bar{u}_j \bar{C} - \bar{u}_j \bar{C} \) is the subgrid scale sediment flux. Note that, typically, SGS models only consider
the deviatoric stress $\tau_{ij} - \tau_{kk}/3$, because the resolved turbulent pressure, $\bar{p^*}$, is different from the resolved hydrodynamic pressure with $\bar{p^*}/\rho = \bar{p}/\rho + \tau_{kk}/3$.

The governing equations are discretized in three dimensions (3D) as in Cui and Fringer [7], i.e., using a finite-volume formulation with 2nd-order accuracy in both time and space on a non-staggered grid. Quadratic upstream interpolation (QUICK; [59]) is used for convective terms. Second-order centered differences are used for the remaining terms. The convective terms are time integrated using the second-order Adams-Bashforth technique, and the diffusive terms with a second-order implicit Crank-Nicolson scheme. The Poisson equation for the pressure field is solved with a multigrid technique. In order to use sufficiently fine discretization in the simulations, the LES was implemented in parallel using Fortran and MPI, for use on large computer clusters.

2.3.2 Experimental post-processing

The Mr5b63 experiment of van der Werf et al. [40] is used for comparison with the LES. The experiment was conducted in an oscillatory flow tunnel, starting with a flat bed on sand with a median grainsize of 0.44 mm. The flow velocity was asymmetric, and well-described by:

$$u_\infty(t) = U_1 \cos(\omega t - \gamma) + U_2 \cos(2\omega t - 2\gamma)$$

$$\gamma = \arccos \left( \frac{\sqrt{U_1^2 + 8U_2^2} - U_1}{4U_2} \right).$$

where $U_1 = 0.54$ m/s, an $U_2 = 0.095$ m/s, with a fundamental period of oscillation of 5.0 s. Such a flow corresponds to an asymmetric wave, where a negative velocity corresponds to an “offshore” flow, compared to a positive (or “onshore”) flow. Eventually the flat bed evolved into a bed of ripples with a wavelength of 0.41 m, and a ripple height of 0.076 m which stayed relatively constant (with a migration rate of 18 mm/min.). Upon reaching a quasi-steady state, measurements were
made of the velocity field (with particle image velocimetry; PIV) and suspended sediment concentration field (with an acoustic backscatter system; ABS).

Both the PIV and ABS measurements are statistical averages over several oscillations. The PIV measurements were phase-averaged over five oscillations. The ABS measurements were compiled while six ripples migrated past the instrument. As well, the PIV measurements were based on using the suspended sand as a seeding agent, which does not quite follow the path of the water. The settling effect of the sediment was removed by van der Werf et al. by forcing the velocity data to be horizontally periodic and removing the horizontally-averaged vertical velocity (which must be true from continuity). Note that the ABS concentration measurements are accurate only within a factor of two, which limits the degree to which the suspended sediment transport rates can be expected to agree with the LES results, though van der Werf et al. did calibrate the data against other measurements of suspended sediment.

Once the flow is stopped, high-resolution measurements of the ripple profile were made with a laser displacement sensor (LDS). Six parallel profiles were measured, 40 mm apart across the oscillatory tunnel width, with each profile measured every 5 mm, with a vertical resolution of the LDS of 0.05 mm. For many early
Table 6. Coefficients used in defining ripple shape.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$a_n$</th>
<th>$b_n$</th>
<th>$n$</th>
<th>$a_n$</th>
<th>$b_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.745562</td>
<td>-0.063282</td>
<td>8</td>
<td>-0.007931</td>
<td>-0.004064</td>
</tr>
<tr>
<td>1</td>
<td>0.485113</td>
<td>-0.078410</td>
<td>9</td>
<td>0.005202</td>
<td>0.002373</td>
</tr>
<tr>
<td>2</td>
<td>-0.091539</td>
<td>0.004472</td>
<td>10</td>
<td>-0.004025</td>
<td>-0.002684</td>
</tr>
<tr>
<td>3</td>
<td>0.048834</td>
<td>-0.011970</td>
<td>11</td>
<td>0.002636</td>
<td>0.001718</td>
</tr>
<tr>
<td>4</td>
<td>-0.30707</td>
<td>-0.003163</td>
<td>12</td>
<td>-0.003081</td>
<td>-0.001059</td>
</tr>
<tr>
<td>5</td>
<td>0.020498</td>
<td>0.002812</td>
<td>13</td>
<td>0.001901</td>
<td>0.001005</td>
</tr>
<tr>
<td>6</td>
<td>-0.013989</td>
<td>-0.005800</td>
<td>14</td>
<td>-0.001752</td>
<td>-0.001307</td>
</tr>
<tr>
<td>7</td>
<td>0.009962</td>
<td>0.003686</td>
<td>15</td>
<td>0.001166</td>
<td>0.001898</td>
</tr>
</tbody>
</table>

Theoretical models of flow over ripples (e.g., [60, 61, 62, 63]), the ripple profile was specified with a conformal mapping. A series approach such as that used by Shum [64] can provide a reasonably accurate match to any given profile:

$$x_1 = \xi + \sum_{n=0}^{N} \left[ -\frac{b_n}{k} \cos nk\xi + \frac{a_n}{k} \sin nk\xi \right]$$  \hspace{1cm} (70)

$$x_3 = \sum_{n=0}^{N} \left[ \frac{a_n}{k} \cos nk\xi + \frac{-b_n}{k} \sin nk\xi \right].$$  \hspace{1cm} (71)

The coefficients needed to reproduce the ripple shape (Fig. 27) have been previously computed by van der Werf et al. [55], and used here (Table 6).

The PIV measurements (Fig. 28) clearly show the lee vortex that forms each half-cycle of the oscillation, and suspended sediment concentration measured by ABS (Fig. 29) show that sediment is being suspended by these vortices. One important feature of the PIV data is that the lee vortices never completely detach from the boundary, which often happens with vortex ripples. Also, at times when there is very clearly high velocities on the leading edge of the ripple (e.g., at $\omega t = 60^\circ$; Fig. 28), when one would assume the sand bed stress is very high, local sediment sediment concentrations are not particularly high relative to the rest of the ripple (though it is possible that it is, but limited to a thin layer that is not resolved by the observations). This has implications for the forcing and boundary conditions that are applied to the LES, described next.
Figure 28. Velocity field of the suspended sand measured by PIV for $\omega t = 0^\circ, 60^\circ, 120^\circ, 180^\circ, 240^\circ, 300^\circ$, interpolated onto computational grid (for consistency with the LES results later), and plotting every other point (for clarity).

Note that the PIV measurements presented in this section (Fig. 28) have not been corrected for the fall velocity of the sediment and are only for qualitative comparison. Also, note that (particularly clear in Fig. 29) that the ripple shape measured by the LDS does not correspond perfectly to the shape of the ripples observed during the PIV and ABS measurements. Some of the gaps between the ABS measurements and the ripple profile measured, however, could be due to such high concentrations of suspended sediment that no measurements could be recorded.
Figure 29. Suspended sediment concentration field ($\log_{10}(c)$) measured by ABS for $\omega t = 0^\circ, 60^\circ, 120^\circ, 180^\circ, 240^\circ, 300^\circ$. 

2.3.3 Boundary conditions and forcing

The hybrid LES used here is forced by specifying the inviscid velocity used in Eq. 5. Harris and Grilli [4] was able to use the flexibility of this method to couple the LES to a numerical wavetank. In the present case, it is less useful. At the upper edge of the oscillatory flow tunnel, while the flow may be essentially inviscid, because both the far-field velocity and ripple shape are asymmetrical, if the ripples were in the open ocean a non-zero Eulerian drift would be induced at the edge of the boundary layer. In an oscillatory flow tunnel, though, a pressure gradient would form to prevent any net water flux. In order to include this effect without having to model the entire tunnel, we use a technique similar to van der Werf et al. [55], whereby at each timestep we determine what the inviscid velocity magnitude \( u_\infty(t) \) should be to force the flow at \( x_3 = 0.8\lambda \) to be equal to Eq. 3.

One can easily use the conformal mapping that describes the ripple shape (Eq. 70, 71) to also describe the computational domain:

\[
x_1 = \xi + \sum_{n=0}^{N} \left[ \frac{-b_n}{k} \cos nk\xi + \frac{a_n}{k} \sin nk\xi \right] e^{-nk\chi} \tag{72}
\]

\[
x_3 = \chi + \sum_{n=0}^{N} \left[ \frac{a_n}{k} \cos nk\xi + \frac{-b_n}{k} \sin nk\xi \right] e^{-nk\chi}. \tag{73}
\]

In order to vertically stretch the grid, as in Harris [4], with a stretching ratio \( \alpha = 1.05 \), the grid is defined by:

\[
\xi(n_1, n_3) = L_1 \frac{n_1 - N_1/2}{N_1} \tag{74}
\]

\[
\chi(n_1, n_3) = L_3 \frac{\exp[n_3 \log \alpha] - 1}{\exp[N_3 \log \alpha] - 1}. \tag{75}
\]

We then use the conformal mapping to find an analytic expression for the inviscid
velocity:

\[ u_1 = u_\alpha(t) \Re \left\{ \frac{1}{1 - \sum_{n=0}^{N} (a_n + ib_n)n \exp[ni(k(\xi + i\chi))] } \right\} \] (76)

\[ u_3 = u_\alpha(t) \Im \left\{ \frac{-1}{1 - \sum_{n=0}^{N} (a_n + ib_n)n \exp[ni(k(\xi + i\chi))] } \right\} . \] (77)

This is very similar to the approach taken by Longuet-Higgins \cite{62}, who modeled flow over ripples by a combination of inviscid flow (found by conformal mapping) and discrete vortices.

Here \( u_\alpha(t) \) is slightly different than the \( u_\infty(t) \) mentioned earlier. In an oscillatory water tunnel there can be no net flow, unlike the open ocean. As such, a steady pressure gradient may form to counteract any steady drift currents that would otherwise exist. This pressure gradient is added by correcting the inviscid velocity. We apply a scheme at each timestep which forces the average horizontal velocity to \( u_\infty \):

\[ u_\alpha(t_{n+1}) = u_\infty(t_{n+1}) - \langle u \rangle(t_n)|_{x_1=-\lambda/2} + u_\alpha(t_n) \] (78)

A similar technique has been used by Holmedal and Myrhaug \cite{65}.

At the upper boundary, in contrast with the zero-gradient boundary conditions of Harris \cite{4}, the normal (i.e., vertical) gradient of the horizontal velocity is set to zero, and the vertical velocity is set to zero (i.e., a free-slip boundary condition). In the free-stream direction, periodic boundary conditions are used to approximate an infinitely long oscillatory water tunnel. On the other lateral boundaries (the span-wise direction), a no-slip condition is applied, similar to that induced by the edges of the water tunnel.

For the bottom boundary, we apply a log-layer condition. The local friction velocity, \( u_\ast \), is then defined as:

\[ \frac{\bar{u}_{\tan}}{u_\ast} = \frac{1}{\kappa} \log \frac{z_1}{z_0} \] (79)
where $\kappa$ is the von Karman constant, taken to be 0.41, and $\bar{u}_s$ is the local resolved velocity tangential to the wall (i.e., the resolved velocity at a gridpoint next to the boundary, with the normal velocity subtracted), and $z_1$ is the distance from the wall to the center of the nearest grid cell. Like Chou and Fringer [16], we find that the roughness length $z_0$ needs to be around the median grain diameter, $d_{50}$, larger than that typically used for a fixed bed, because saltating sand grains increase the local roughness.

The motion of the sediment at the seabed is governed by bedload transport, the settling of suspended sediment, and sediment pickup. These processes can be described by nondimensional parameters, including the density ratio $s$ and the Shields parameter $\theta$,

$$\theta = \frac{u_*^2}{(s - 1)gd_{50}}$$

with $\theta_{cr}$ the critical Shields parameter. The onset of sediment motion on the seabed is defined by comparing the Shields parameter to its critical value. The latter is obtained from van Rijn [66], with a critical Shields parameter of 0.0314. Note, the effect of the bed slope is neglected.

The sediment pickup, $P$, is modeled using the empirical relationship proposed by van Rijn [67] for noncohesive sediments with grain sizes between 0.2 mm and 2 mm, where $T = \frac{\theta - \theta_{cr}}{\theta_{cr}}$ is the transport stage parameter:

$$P = \begin{cases} 0.00033T^{1.5} & \text{if } \theta > \theta_{cr} \\ 0 & \text{if } \theta \leq \theta_{cr} \end{cases}$$

for a Shields parameter greater than the critical value as suggested by Nielsen [2]. Alternate pickup functions are discussed by van Rijn [66]. The pickup function is used to apply a boundary condition for the SSC.

Since both the eddy viscosity and diffusivity are zero at the bed, the bottom
boundary conditions are applied as:

\[ u_2^* = -\nu \frac{\partial \bar{u}}{\partial n} \]  

\[ P = -\kappa \frac{\partial \bar{C}}{\partial n} \]  

similar to Harris and Grilli [4].

2.3.4 Subgrid scale model

The governing equations for the LES contain subgrid scale terms \( \tau_{ij} \) and \( \xi_j \) which are modeled with the dynamic mixed model of Zang et al. [68], which is based on the stress decomposition proposed by Germano [69]. Note that, as in Cui and Fringer [7], the spatial gradient of eddy viscosity is neglected in the discretized governing equations. A complete description of the SGS model as applied to this numerical technique is given by Harris and Grilli [4]. Sediment concentration is not explicitly included in the SGS closure, although Chou and Fringer [16] argue that the effects of SSC on subgrid-scale physics are implicitly modeled through their effects on the resolved fields of an LES to some degree. While the SSC is often high enough to affect turbulence, above the \( 10^{-6} \) limit given by Elghobashi [58], it is a dilute suspension, except extremely close to the ripple surface. For dilute suspensions (an SSC below \( 10^{-3} \)), particle-particle interactions are negligible, so we consider the dynamic mixed model suitable.

As in Harris and Grilli [4] and following Chow and Street [70] and Chow et al. [71], the eddy viscosity at the wall in the SGS model is increased in order to augment the near-wall shear stresses. Under the assumption that near the wall the flow can be approximated by a log-layer and that the eddy viscosity determined by the SGS model is negligible, we augment the eddy viscosity by:

\[ (\nu_T)_{total} = (\nu_T)_{SGS} + \kappa u_* z \cos^2 \left( \frac{\pi z}{4 \sqrt{J/2z_1}} \right) \]  

(84)
for \( z < 2\sqrt{J/2z} \), \( z \) is the distance from a point to the seabed, and as before, \( z_1 \) is the distance of the center of the first grid cell to the boundary, and \( J \) is the Jacobian of the transformation used in deriving the discretized governing equations. For a Cartesian grid, the near-wall thickness of \( 2\sqrt{J/2z} \) reduces to \( 2\Delta x_1 \). This is an extension of the technique used by Harris and Grilli [4] to curvilinear boundaries.

2.4 Results and Discussion

2.4.1 LES Setup

We use the model described above with a modest grid that has 64x32x32 (LxWxH) points, spanning a length 41 cm (one ripple wavelength), on average 50 cm high, and with a width of 30 cm. The suspended sediment concentration computations are done using the median grain diameter of 0.44 mm – unlike van der Werf et al. [55], who uses an estimated median suspended sediment diameter. This is done in part because our method was not intended for a specific experimental validation, but for a more general model of wave-induced sediment transport, and it may not always be feasible to estimate the median suspended sediment diameter a priori. Note that eventually the simulations could be improved using \( n \) tracers, by solving \( n \) advection-diffusion equations. Similar to Harris [4], the simulation runs for 10 periods of oscillation (i.e., 50 s), using a timestep of 0.5 ms (i.e., 100,000 timesteps). Checks on the validity of the model discretization (e.g., that the correlation length is less than the size of the domain) is left for future work.

For processing results, we are interested in four types of averages: the phase-averaged results (i.e., the results at a set \( \omega t \)); the period-average results (i.e., the time-average); the period- and ripple-averaged results (i.e., the results at a given vertical height – from a reference level, not from the seabed height); and finally the cumulative average. For each, we are interested in the velocity, the suspended sediment concentration, and the sediment fluxes. For simplicity, we will denote the
Figure 30. Contour plot of SSC at $t = 26.625 \ (\omega t \approx 120^\circ)$ showing significant three-dimensional turbulence. Lack of contours close to the ripple surface indicate extremely high SSC values.

average of e.g., $q$, by $\langle q \rangle(\omega t, x_1, x_3)$, $\langle q \rangle(x_1, x_3)$, $\langle q \rangle(x_3)$, and $\langle g \rangle$, respectively, we will ignore the subgrid scale effects (e.g., the differences between $\langle q \rangle$ and $\langle \bar{q} \rangle$), and compute the horizontal averages by re interpolating the results onto a uniform grid. For comparison with experimental data, we use the same data post-processing as van der Werf et al. [40].

2.4.2 Convergence

The LES simulations predict that three-dimensional turbulence is developed quickly (Fig. 30). As such, spanwise averaging is applied to all of the results in order to compare with the two-dimensional laboratory observations.

We can observe that the model seems to converge quickly to a solution. This can most easily be observed in the spatially-averaged wall stress (Fig. 31). Convergence is further demonstrated below in terms of vertical profiles of horizontal
Figure 31. Spatially averaged wall stress in the streamwise direction. Note the quick convergence to a quasi-steady solution.

velocity, as well as in the overall suspended sediment flux.

We can also compare $u_\infty$ and $u_\alpha$ (Eq. 78). The time-varying difference (lower panel) indicates a pressure gradient that builds up as a result of the boundary layer, important for ensuring mass conservation in the simulated water tunnel is zero.

2.4.3 Velocity field

In order to show the relationship between the LES results and the experimental results, we plot the vector field of each for each 60°, applying spanwise averaging for the LES results (Fig. 33), for the last (tenth) oscillation of the simulation. By comparing to the PIV measurements (Fig. 28), we see that the two agree quite well in all regards. At 0°, when there is no flow in the far-field, there is a strong offshore vortex, although in the LES results, the vortex is not as well formed. At 60°, flow is in the onshore direction, with lower velocities near the bed. At 120°, there is a large lee (onshore) vortex. At 180°, flow in the far-field is weak, but near the bed, there is a moderate offshore flow. By 300°, there is a clear lee (offshore)
Figure 32. Far-field velocity, $u_\infty$ (solid line), and forcing velocity, $u_\alpha$ (dashed line). The difference between the two is the result of a quasi-steady pressure gradient that builds up in the oscillatory water tunnel.
Figure 33. Spanwise-averaged velocity field predicted by LES, for six different phases of the oscillation, in the tenth oscillation.
vortex.

It is also useful to consider the period-averaged behavior of the velocity, which drives much of the transport in the coastal bottom boundary layer. Our present LES results are similar to the PIV measurements (Fig. 34). The largest difference is that the offshore (left-side) vortex is slightly different in the LES results. This is a rather remarkable agreement, and better than that shown by van der Werf et al. [55]. In their results with a RANS \((k-\omega)\) model, they had no period-averaged vortex on the offshore side, and in their discrete vortex model they had more symmetric period-averaged flow.

We can also consider the vertical profile of the period- and ripple-averaged horizontal velocity (Fig. 35). This result does not quite match the data, but is within the range of results reported by van der Werf et al. [55] with other models. The LES does seem to predict some of the features well, such as a maximum offshore velocity at the ripple crest and a significant drop-off in mean velocity by \(x_3 = 0.5\lambda\). This further demonstrates convergence of the model towards a solution within ten oscillations (Fig. 36).

2.4.4 Suspended sediment

The phase-averaged suspended sediment field (Fig. 37) does not show as good agreement as the velocity field, although the major features are qualitatively predicted. Primarily, there is a layer of very high SSC close to the ripple surface which moves with the flow above. The major difference from the ABS measurements (Fig. 29) is an underprediction of SSC above the ripple crest. The transition between the onshore and offshore flow, seen at 120° and 180° also shows a significant difference in the location of the maximum SSC – there is a “cloud” of SSC in the LES which is always farther offshore (in the figures, on the left) than the similar feature in the ABS measurements. Similarly, the thickness of the high SSC
Figure 34. Cycle-averaged velocity measured by experiment (upper panel); predicted by LES (center panel); and the difference (lower panel).
Figure 35. Vertical profiles of period- and ripple-averaged horizontal velocity, including the experimental measurements (dots), and the LES predictions (solid line) for the tenth oscillation.

Figure 36. Vertical profiles of period- and ripple-averaged horizontal velocity, for each of the ten simulated oscillations (solid lines) compared to the experimental measurements (dots).
Figure 37. Suspended sediment concentration field predicted by LES ($\log_{10}(C)$), for six different phases of the oscillation, in the tenth oscillation.
Figure 38. Vertical profiles of period- and ripple-averaged suspended sediment concentration for the tenth oscillation of the LES (solid line), compared to the experimental data (ABS – dots; measured by a transverse suction system – circles).

layer onshore (in the figures, on the right), at $60^\circ$ is underpredicted by the model. These differences may be attributed to how the bottom boundary condition, and the near-wall eddy viscosity, are determined with a log-layer assumption, which does not take into consideration the adverse pressure gradient which exists at that point. The results are qualitatively similar at other times.

If we consider the vertical profile of suspended sediment (Fig. 38), the SSC is overpredicted below the ripple crest, and underpredicted above the ripple crest. Notably the decay with height of the SSC above the ripple crest is reasonable, although the value is around seven times too low to match experiment.

2.4.5 Sediment flux

The goal in simulating vortex ripples, naturally, is to obtain accurate suspended transport rates. If we sum the total suspended sediment transport, $q_s = \langle uC \rangle$, we can then compare the LES result to the experimental data.

The suspended sediment flux profile (Fig. 39) obtained from LES does not
match experimental results very well. We do see that the maximum period- and ripple-averaged suspended sediment flux is at the ripple crest, but the transport is onshore, as opposed to the observed offshore transport.

If we look at the total suspended sediment transport in any given period of oscillation instead we find (Table 7) that there is a substantial mismatch between the LES and the experimental results, even though the solution appears to converge to a solution. This is in contrast to van der Werf et al. [55] who with their k-ω model were able to obtain a suspended sediment transport rate only 26% percent lower than that observed.

If we compare the instantaneous sediment fluxes, both observed (Fig. 40) and predicted (Fig. 41), the issue is primarily driven by an exceedingly high predicted suspended sediment flux onshore at $\omega t = 60^\circ$. As the predicted and observed velocity fields are similar, this indicates that near the ripple surface, the predicted suspended sediment concentration is significantly higher than that observed. This
Table 7. Period- and ripple-averaged sediment fluxes.

<table>
<thead>
<tr>
<th>Oscillation</th>
<th>$q_s$ (mm$^2$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>64.4</td>
</tr>
<tr>
<td>2</td>
<td>178.1</td>
</tr>
<tr>
<td>3</td>
<td>159.3</td>
</tr>
<tr>
<td>4</td>
<td>159.8</td>
</tr>
<tr>
<td>5</td>
<td>175.4</td>
</tr>
<tr>
<td>6</td>
<td>162.0</td>
</tr>
<tr>
<td>7</td>
<td>161.5</td>
</tr>
<tr>
<td>8</td>
<td>149.1</td>
</tr>
<tr>
<td>9</td>
<td>163.9</td>
</tr>
<tr>
<td>10</td>
<td>166.4</td>
</tr>
</tbody>
</table>

Exp. results $-10.6 \pm 1.7$

Figure 40. Observed suspended sand fluxes at six different phases of the oscillation.
Figure 41. Spanwise-averaged suspended sediment flux predicted by LES, for six different phases of the oscillation, in the tenth oscillation.
highlights a need for more sophisticated models, like the bedform evolution model of Chou and Fringer [16], to be well validated before use in general applications. While they were able to obtain ripples of length similar to that found in some experiments, they did not have direct comparisons of important parameters, such as sediment transport rates.

2.4.6 Future improvements

Without a substantial change in the grid resolution, forcing, or boundary conditions, LES results are primarily affected by the subgrid-scale model. For a model to be a true LES, there needs to be resolved three-dimensional turbulent fluctuations in the velocity field. Near the seabed, where these fluctuations cannot be practically resolved at high Reynolds numbers, a wall model must be used. Here, this is handled by the near-wall eddy viscosity enhancement, which essentially is a RANS mixing-length model, assuming the eddy viscosity is proportional to the height above the bed and the friction velocity.

The largest error seen in the above analysis is a low SSC above the ripple crest. This, in turn, contributes to a different suspended sediment flux than is observed. There is a corresponding above-expected SSC near the ripple surface. This is likely due to the fact that the turbulent eddy viscosity in the outer layer is much less than that within the RANS-like layer (Fig. 42). (A better comparison might be the turbulent eddy diffusivity, but their values are similar.) It seems reasonable to conclude that the subgrid-scale turbulent flux of suspended sediment is important, and is being underpredicted. SGS flux of momentum may also be underpredicted, but dissipation to a large degree is occurring in the near-wall layer where eddy viscosity is being enhanced, since no vortex is reaching completely outside of this near-wall layer.

This transition between a smooth RANS solution to a well-resolved turbulent
Figure 42. Comparison of SSC ($\log_{10}(c)$) and eddy viscosity ($\log_{10}(\nu_T)$) after two oscillations (i.e., at $t=10$ s). Note that near the eddy viscosity varies significantly near the bed as well, but the axis was chosen to highlight the issues in the outer layer of the flow.
velocity field for an LES is actually a significant problem with hybrid RANS/LES schemes. This can be fixed with techniques such as controlled forcing, or applying synthetic turbulence (see e.g., Keating et al. [72]). Actually, in the results presented here, the turbulent fluctuations above the ripple crest are mostly due to the lateral no-slip boundary conditions. In preliminary testing with periodic boundary conditions, no turbulent eddies were resolved. While others have used turbulent initial conditions to trigger turbulence in similar simulations (e.g., Zedler and Street [13]), an improved interface condition would provide a more general solution.

There are other ways that the RANS-like near-wall layer could be improved. It is presently not grid independent. The scaling function for the enhanced eddy viscosity is not a function of the local grid aspect ratio, so a different grid-stretching ratio would presumably give different results. More importantly, it does not take into account the effects of pressure gradients, which are extremely important for separated flows, such as that seen here. Such a wall model would be different than a log-layer assumption. A modified log-layer assumption, derived by Fourriere [73], could be applied, where both the local pressure gradient and the surface roughness is considered in deriving the mean velocity profile. A similar equation has been found by [74] and [75] to be experimentally correct.

2.5 Summary

A hybrid LES approach to modeling the Navier-Stokes equations is applied to the simulation of sediment transport over sand ripples. This hybrid technique is likely to be particularly useful for complex coastal engineering problems near the seafloor. In that case, the full Navier-Stokes equations may only be needed in a relatively small region. Harris and Grilli [4] have already shown this approach to be accurate for modeling turbulent oscillatory boundary layers over flat beds, and practical for coupling to numerical wavetanks. In this paper, we compared our
model with the experimental data of van der Werf et al. [40] in order to study the velocity field and suspended sediment concentration.

We obtain good agreement for the velocity field, including the instantaneous velocity and the period-averaged velocity, as well as obtaining reasonable agreement for the vertical profiles of period- and ripple-averaged horizontal velocity. We obtain reasonable agreement of suspended sediment concentration, although the SSC above the ripple crest is lower than observations. As a result, the overall suspended sediment flux is substantially different from what is observed, and could possibly be improved with some minor changes to the model setup.

Future work may extend upon these results, in particular, by improving the turbulence model used to produce better predictions of suspended sediment transport, and perhaps eventually considering a moving seabed similar to Chou and Fringer [16], allowing the shape of the ripples to evolve over the course of the simulation.

Acknowledgements

Prof. R. Street and Prof. O. Fringer are thanked for providing the initial LES code, and Dr. J. van der Werf and Dr. J. Malarkey are gratefully acknowledged for providing us with a copy of the experimental data used.

List of References


APPENDIX A

Theoretical solutions to laminar test cases

A.1 Exact solution of laminar oscillating boundary layer

The classic laminar solution to the oscillating boundary layer is given by the second problem of Stokes [1]. When the flow is horizontally uniform, the equation of motion can be written as:

\[
\frac{\partial}{\partial t}(u(z, t) - u^I(t)) = \nu \frac{\partial^2 u(z, t)}{\partial z^2} \tag{A.1}
\]

where \(u\) is the horizontal velocity, \(u^I\) is the horizontal free-stream velocity, \(\nu\) is the kinematic viscosity of the fluid, and \(z\) is the vertical coordinate. The boundary conditions are given as no-slip at the wall, and that the velocity tends to the free-stream velocity far from the boundary:

\[
u = 0 \quad z = 0 \tag{A.2}
\]

\[
u = u^I \quad z \to \infty \tag{A.3}
\]

where the horizontal free-stream velocity as sinusoidal, with an amplitude \(U_0\) and angular frequency \(\omega\),

\[
u^I = U_0 \sin \omega t. \tag{A.4}
\]

This form is chosen so that the inviscid velocity is zero when time is zero, which is the same forcing chosen for the first manuscript. To integrate the momentum equation, we express the free-stream velocity in complex phasor notation instead:

\[
u^I = \Re\{-iU_0 e^{i\omega t}\} \tag{A.5}
\]

because it simplifies the manipulations shown below.
Typically this problem is solved by introducing a defect velocity which is the difference between the free-stream and local velocity. In the notation of the manuscript, this is the perturbation velocity, $u^P$:

$$u = u^I + u^P. \quad (A.6)$$

The equation of motion for this defect velocity is:

$$\frac{\partial u^P}{\partial t} = \nu \frac{\partial^2 u^P}{\partial z^2}. \quad (A.7)$$

By applying separation of variables, the solution is given by:

$$u^P = U_0 \Re \left[ e^{i\omega t} D(z) \right] \quad (A.8)$$

$$D(z) = \frac{\nu}{i\omega} \frac{\partial^2 D(z)}{\partial z^2} \quad (A.9)$$

and by applying the boundary conditions,

$$D(z) = i e^{-(i+1)z/\sqrt{2\nu/\omega}} \quad (A.10)$$

so,

$$u^P = -U_0 \exp \left[ -z/\sqrt{2\nu/\omega} \right] \sin \left( \omega t - z/\sqrt{2\nu/\omega} \right). \quad (A.11)$$

Defining $\delta_S = \sqrt{2\nu/\omega}$ as the Stokes-layer thickness, the final solution is:

$$u = U_0 \left( 1 - \exp[-z/\delta_S] \right) \sin(\omega t - z/\delta_S). \quad (A.12)$$

One can additionally show that since the shear stress is given by:

$$\tau(z, t) = \rho \nu \frac{\partial u}{\partial z} \quad (A.13)$$

that the wall shear stress, $\tau_w(t) = \tau(0, t)$ is given by:

$$\tau_w(t) = \rho U_0 \sqrt{\nu \omega} \sin(\omega t - \pi/4) \quad (A.14)$$
so one clearly sees that the wall stress leads the free-stream velocity by 45°.

Despite the theoretical solution, the thinness of the Stokes layer has meant that experimental verification of the Stokes layer velocity profiles did not become practical until laser Doppler velocimetry was introduced. Beech [2], and Hwung et al. [3], and Liu et al. [4] all presented LDV measurements of the Stokes layer.

A.2 Steady streaming in a progressive water wave

For monochromatic forcing, the fundamental difference between the Stokes boundary layer and a wave-induced boundary layer is the time-average transport. This steady streaming is only present when either multiple frequencies or a spatial variation exists in the free-stream oscillation. It was first described by Rayleigh [5] in the context of acoustic streaming. Many have expanded upon the original result, notably Longuet-Higgins [6] who derived the Lagrangian drift under a progressive wave. The formula for Eulerian drift is derived below, following the technique used by Mei [7]. We cover the derivation briefly more for the purposes of demonstration than rigor.

First we consider a progressive wave under the assumption that $1 \gg kA >\gg (k\delta)^2$. The velocity can be expanded as a perturbation series with $kA$ the small parameter:

$$u = u_1 + u_2 + \ldots$$ \hspace{1cm} (A.15)

where $u_1 = O(\omega A)$ and $u_2 = O(\omega kA^2)$.

The first order momentum equation for the horizontal velocity is:

$$\frac{\partial u_1}{\partial t} = \frac{\partial U_I}{\partial t} + \nu \frac{\partial^2 u_1}{\partial z^2}$$ \hspace{1cm} (A.16)
with boundary conditions

\[ u_1 = 0 \quad z = 0 \quad (A.17) \]

\[ u_1 \to U_I \quad z >> \delta. \quad (A.18) \]

We can define the inviscid velocity as:

\[ U_I(x, t) = \Re(U_0(x)e^{-i\omega t}) \quad (A.19) \]

so the solution is given by the earlier Stokes boundary layer solution:

\[ u_1 = \Re(U_0f(\xi)e^{-i\omega t}) \quad (A.20) \]

\[ f(\xi) = 1 - e^{-(1-i)\xi} \quad (A.21) \]

From continuity, the vertical velocity is:

\[ w_1 = \Re\left[\delta \frac{\partial U_0}{\partial x} e^{-i\omega t} \frac{1+i}{2} \left(1 - e^{-(1-i)\xi} - \xi\right)\right] \quad (A.22) \]

which is significant in the second-order momentum equation:

\[ \frac{\partial u_2}{\partial t} - \nu \frac{\partial^2 u_2}{\partial z^2} = U_I \frac{\partial U_I}{\partial x} - u_1 \frac{\partial u_1}{\partial x} - w_1 \frac{\partial u_1}{\partial z} \quad (A.23) \]

The time- or ensemble-average (denoted here by \( \langle \cdot \rangle \)) of the second-order velocities is given by:

\[ -\nu \frac{\partial^2 \langle u_2 \rangle}{\partial z^2} = \langle U_I \frac{\partial U_I}{\partial x} \rangle - \langle u_1 \frac{\partial u_1}{\partial x} \rangle - \langle w_1 \frac{\partial u_1}{\partial z} \rangle \quad (A.24) \]

with boundary conditions:

\[ u_2 = 0 \quad z = 0 \quad (A.25) \]

\[ \frac{\partial u_2}{\partial z} \to 0 \quad z >> \delta \quad (A.26) \]

then we end up with the solution of:

\[ \langle u \rangle = -\frac{1}{\omega} \Re g(\xi) U_0 \frac{\partial U_0}{\partial x} \quad (A.27) \]

\[ g(\xi) = -\frac{1}{2} (1 - 3i)e^{(-1+i)\xi} - \frac{i}{2} e^{-(1+i)\xi} - \frac{1+i}{4} e^{-2\xi} \]

\[ + \frac{1}{2} (1 + i)\xi e^{(-1+i)\xi} + \frac{3}{4}(1 - i) \quad (A.28) \]
For a progressive wave we can approximate $U_0$ as

$$U_0 = \frac{\omega A}{\sinh kh} e^{ikx} \quad \text{(A.29)}$$

so our final solution is

$$\langle u \rangle = \frac{k\omega A^2}{\sinh^2 kh} \Re [ig(\xi)] \quad \text{(A.30)}$$

which expands to

$$\langle u \rangle = \frac{k\omega A^2}{\sinh^2 kh} \left[ -\frac{3}{2} e^{-\xi} \cos \xi - \frac{1}{2} e^{-\xi} \sin \xi + \frac{1}{2} e^{-\xi} \cos \xi + \frac{1}{4} e^{-2\xi} \right.$$

$$\left. - \frac{1}{2} \xi e^{-\xi} \cos \xi + \frac{1}{2} \xi e^{-\xi} \sin \xi + \frac{3}{4} \right]. \quad \text{(A.31)}$$

This reduces to the solution:

$$\langle u \rangle = \frac{k\omega A^2}{\sinh^2 kh} \left[ -e^{-\xi} \cos \xi + \frac{1}{2} e^{-\xi} \sin \xi + \frac{1}{4} e^{-2\xi} \right.$$

$$\left. - \frac{1}{2} \xi e^{-\xi} \cos \xi - \frac{1}{2} \xi e^{-\xi} \sin \xi + \frac{3}{4} \right]. \quad \text{(A.32)}$$

Note that this has to be modified to get the traditional Lagrangian steady-streaming formula of Longuet-Higgins, since we did not correct for Stokes’ drift here.

We can also compute the steady-streaming component of the wall stress:

$$\frac{\langle \tau_w \rangle}{\rho} = \nu \frac{\partial u}{\partial z}$$

$$= \frac{\nu k\omega A^2}{2\delta_S \sinh^2 kh} \quad \text{(A.33)}$$

$$= \frac{\nu k\omega A^2}{2\sqrt{2\nu/\omega} \sinh^2 kh} \quad \text{(A.34)}$$

$$= \frac{(k\delta_S)(A\omega)^2}{2\sinh^2 kh} \quad \text{(A.35)}$$

$$\frac{\langle \tau_w \rangle}{\rho U_0^2} = k\delta_S \quad \text{(A.36)}$$

$$\frac{\langle \tau_w \rangle}{\rho U_0^2} = \frac{k\delta_S}{2}. \quad \text{(A.37)}$$
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APPENDIX B

Hydrodynamics of wave-induced boundary layers

Much of this work has concerned simulations of turbulent flow. It is worthwhile to briefly review some of the properties of turbulence, and how it concerns both experimental and computational fluid dynamics.

B.1 Experimental fluid dynamics

The physical processes involved in turbulence have been studied since Reynolds [1] pioneering work on finding the criterion for flow through a pipe to be turbulent. Many texts have been written describing theories of these random flows (see e.g., Pope [2]). It is most important here to consider both how boundary layer flow can be analytically described and how turbulence varies at different length scales.

B.1.1 Boundary layer mean flow

Given a point within a boundary layer, the most important variable is typically the mean velocity. The mean velocity is determined by the combination of viscous and turbulent Reynolds stresses. For points very close to the wall in a steady boundary layer with no pressure gradient, this mean shear is essentially constant, and equal to the wall shear stress. From this observation, we can consider the two special cases where either the turbulent or viscous stresses are negligible – these are referred to the viscous and logarithmic layers, respectively.

For steady boundary layers with no pressure gradient, the variables to consider are the wall shear stress, \( \tau_w \), the kinematic viscosity, \( \nu \), the fluid density, \( \rho \), the height above the wall, \( y \), and the local velocity, \( U \). Traditionally, velocities are normalized with respect to the friction velocity, \( u^+ = U/u_r = U/\sqrt{\tau_w/\rho} \), and
lengths are normalized with respect to a wall unit, \( y^+ = u_+ y/\nu \).

Very close to the wall, turbulent Reynolds stresses are insignificant in comparison to the viscous shear stresses, and mean velocity is proportional to the distance from the wall:

\[
U = \frac{u_+^2}{\nu} y. \tag{B.1}
\]

This viscous sublayer is about 5 wall units thick (i.e., \( y^+ < 5 \)). Flow within the viscous sublayer is not necessarily laminar. In the upper parts of the viscous sublayer there are turbulent fluctuations, and the fluctuating component of the wall shear stress is transmitted through fluctuations in the friction velocity.

Far from a smooth wall, typically starting at somewhere around 70 wall units from the boundary, the turbulent Reynolds stresses dominate, and the mean velocity varies logarithmically with distance from the wall:

\[
\bar{U} = \frac{u_+}{\kappa} \log y^+ + u_f B \tag{B.2}
\]

where \( \kappa \) and \( B \) are known constants, about 0.41 and 5.5. In fact, each component of the Reynolds stresses tend toward constant values, which Monin and Yaglom [3] showed experimentally. The upper bound of the logarithmic layer, which is the upper bound of the constant stress layer, depends on the boundary layer thickness.

For distances between the viscous sublayer and the logarithmic layer, there is a buffer layer, where both viscous and Reynolds stresses are important. Unlike the mean velocity profiles for the viscous sublayer and the logarithmic layer, there is no theoretical basis for a mean velocity profile. When there is a need to have an equation to predict the mean velocity profile in the buffer layer, typically the van Driest [4] velocity profile is used:

\[
\bar{U} = 2u_+ \int_0^{y^+} \frac{dy^+}{1 + [1 + 4\kappa^2 y^+ 2[1 - \exp(-y^+/A)]^2]^{1/2}} \tag{B.3}
\]
While complicated, the advantage of the van Driest profile is that it is a smooth function which tends towards a linear profile for small $y^+$ and a logarithmic profile for large $y^+$. Unlike earlier explanations, which relied entirely on dimensional analysis and experimental observations, the van Driest profile depends on mixing length theory, whereby a turbulent eddy viscosity profile is assumed which obeys:

$$\nu_T = \left(\kappa y [1 - \exp(-y^+ / A)]\right)^2 \frac{d\bar{U}}{dy}$$ (B.4)

where $A$ is a constant coefficient equal to 25.

For rough walls, the steady, turbulent boundary layer dynamics additionally depend on the height of the roughness elements. While typically random in size and location (e.g., grains of sand on the seabed), their effect on the flow can be described by a parameter known as the Nikuradse roughness height, $k_s$. The dynamics of the boundary layer then depends on the additional parameter, the Reynolds roughness number, $k_s^+ = k_s u_* / \nu$. For $k_s^+ < 5$, the wall is hydraulically smooth. For $k_s^+ > 70$, the wall is completely rough, and there is no viscous sublayer. There is still a logarithmic layer, but of the form:

$$\bar{U} = \frac{u_*}{\kappa} \log \frac{y}{y_0}$$ (B.5)

where $y_0 = k_s / 30$.

For transitionally rough cases, there is less theoretical basis for a specific velocity profile, but empirical relationships have been proposed. Colebrook [5], for instance, used

$$\frac{\bar{U}}{u_*} = \frac{1}{\kappa} u_* \frac{\bar{U}}{u_*} + B - \Delta U^+$$ (B.6)

$$\Delta U^+ = \frac{1}{\kappa} \log(1 - 0.26k_s^+).$$ (B.7)

Other empirical relationships based on mixing length theory have been proposed in order to give a van Driest-like profile for rough and transitionally rough walls (e.g.,
Cebeci and Chang [6]). One should use caution when relying on mixing-length theory, because it is based on some faulty assumptions, as discussed later. Still, it provides closed-form solutions for mean velocity profiles which in some cases agree quite well with experiment. Other, newer variations of the log-layer have been used to understand turbulent flow in pressure gradients, including around the point of flow separation (e.g., Fourrière et al. [7]) as discussed in Manuscript 3.

For more complex flows, such as oscillating boundary layers, or flow over an obstacle, fluid particles can experience both laminar and turbulent and both smooth and rough flow over the course of a single oscillation. This means, as discussed in Manuscript 1, that the relationships between the flow regimes are more complicated, and there may be no simple mean velocity distribution. For fully turbulent oscillating boundary layers over a flat plate, though, the logarithmic layer has been shown to experimentally exist for most of the period of oscillation.

B.1.2 Turbulent fluctuations

Turbulence is not completely unpredictable. Rather, it acts on certain length-scales. We see this most notably in observations of the smallest coherent structures and the velocity spectra.

Coherent structures are structures which appear among vortices and retain their shape over time (see e.g., Davidson [8]). While there is no one accepted definition, they are generally taken to be a structure which in an instantaneous sense is distinct from the turbulence around itself. The most commonly known type of coherent structure is a hairpin vortex which can be on the order of the boundary layer thickness in length, but as thin as 5 wall units across. Alternatively, long pairs of vortex tubes are dominant very near the wall (within 70 wall units). These vortex tubes interact with the mean flow and induce low-speed streaks around 1000 wall units long. The low-speed streaks eventually experience a local adverse
pressure gradient, causing the flow to separate from the wall and be ejected. This bursting process extends from the upper regions of the viscous sublayer to the lower edge of the logarithmic layer. In general, there are vortices that exist on a variety of length scales from $O(10^0)$ to $O(10^3)$ wall units. Note that the physical process of bursting is a stochastic one. For hydraulically rough flows over large ripples, turbulence is in fact generated by the shedding of lee eddies.

Another technique for considering how turbulent fluctuations act on different length scales is to measure the spectrum of the velocity components, either in space or in time. The two types of spectral analysis are similar. At the largest scales, turbulent spectra are determined by the outer flow, and at the smallest scales, turbulent spectra are determined by dissipation. In between, energy is produced, dissipated, and changes scales by a number of different mechanisms. One of the best known results from spectrum analysis is Kolmogoroff’s -5/3 law.

Kolmogoroff’s -5/3 law refers to the energy spectrum of isotropic turbulence in the inertial subrange, which is of the form: $E \propto k^{-5/3}$. The formal derivation of the -5/3 law can be seen in many texts, but briefly, it is due to the combination of Kolmogoroff’s first and second hypotheses. Kolmogoroff’s first hypothesis is that turbulence in the universal equilibrium range is isotropic. If that is the case, then the energy spectrum function is a function of $\epsilon$, the dissipation of turbulent energy per unit mass and per unit time, $\nu$, the viscosity of the fluid, and $k$, the wavenumber. Kolmogoroff’s second hypothesis is that the maximum of the energy spectrum is at sufficiently large length scales, and that the maximum of the energy dissipation is at sufficiently small length scales, that there must be a range of wave numbers where there is no significant energy production or dissipation. In this inertial subrange, the inertial terms of the Navier-Stokes equations transfer energy from the larger length scales to the smaller ones. Because this is independent of
the viscosity of the fluid, dimensional analysis yields:

\[ E = A \epsilon^{2/3} k^{-5/3} \]  

(B.8)

where the constant \( A \approx 1.5 \) which has been found to hold for all turbulent flows (see e.g., Kundu and Cohen [9]). The presence of the -5/3 spectrum has been confirmed in many flows, both experimentally and in CFD results.

It is notable, as mentioned in Manuscript 1, that Hino et al. [10] found that in an oscillatory boundary layer the -5/3 spectrum is not always found. While Hino et al. does not discuss it, it seems possible that the reason for this is due to a violation of Kolmogoroff’s hypotheses – the flow is not isotropic, and in e.g., the decelerating phase of the oscillatory boundary layer, there is an adverse pressure gradient present.

Often one-dimensional velocity spectra are calculated instead of \( E(k) \), because it is relatively simple in comparison, yet Tennekes and Lumley [11] showed that one-dimensional spectra are misleading. For example, the velocity spectrum for an eddy of characteristic length \( L_{\text{eddy}} \) is peaked around \( k = \pi / L_{\text{eddy}} \), whereas the one-dimensional spectrum would be peaked around \( k = 0 \). As a result, one should use caution when analyzing velocity spectra.

### B.2 Computational fluid dynamics

Computational fluid dynamics (CFD) refers to the study of fluid flow using numerical methods. This includes models of potential flow, as is used by the numerical wavetank referenced in these works, and it could also include both the modeling and simulation of turbulent flow with some form of the Navier-Stokes equations. There is a distinction between a numerical methods referred to as “models” and “simulation”. A turbulence model is deterministic method, so that with the same initial data, a model will always provide the same results, whereas a simulation is a stochastic method, and like an experiment, a simulation is not
guaranteed to have the same results from one run to another, except in a statistical sense. When applying the Navier-Stokes equations to a turbulent flow, one can only refer to the statistical properties of the velocity field. Corresponding to different numerical approaches, there are presently three common numerical methods for CFD: direct numerical simulation (DNS); Reynolds-averaged Navier-Stokes (RANS) models; and large-eddy simulations (LES).

DNS considers the velocity field for one realization of the flow. RANS equations consider mean velocity field (i.e., ensemble averaged). LES equations solve for the resolved velocity field (i.e., spatially averaged), which itself is a random variable. Direct numerical simulation is a technique where the Navier-Stokes equations are discretized on spatial scales small enough to dissipate (i.e., the Kolmogorov scales). DNS is extremely computationally expensive, because for most engineering applications the Kolmogorov scale is vastly smaller than the characteristic scales of the flow. The numerical techniques used also are extremely demanding, because numerical dissipation needs to be significantly less than the viscous dissipation. More commonly, RANS or LES are applied. Because RANS models are better known, below we differentiate the two, and elaborate on the turbulence closures typically used by a large-eddy simulation.

**B.2.1 Differences between RANS and LES**

The RANS equations are the Navier-Stokes that have had an ensemble average (denoted here by $\langle \cdot \rangle$) applied:

$$\frac{\partial \langle u_i \rangle}{\partial x_i} = 0 \quad \text{(B.9)}$$

$$\frac{\partial \langle u_i \rangle}{\partial t} + \frac{\partial \langle u_i \rangle \langle u_j \rangle}{\partial x_j} + \frac{\langle p \rangle}{\rho} \delta_{ij} - \nu \frac{\partial \langle u_i \rangle}{\partial x_j} + \tau_{ij} = 0. \quad \text{(B.10)}$$
The Reynolds stress tensor is given by the turbulence closure. One of many developed is the Wilcox $k-\omega$ model [12], governed by the two by the two equations:

\begin{equation}
-\tau_{ij} = 2\nu_T - \frac{2}{3}k\delta_{ij} \quad \text{(B.11)}
\end{equation}

\begin{equation}
\frac{\partial k}{\partial t} + \langle u_i \rangle \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ (\nu + \sigma^* \nu_T) \frac{\partial k}{\partial x_j} \right] - \langle u_i u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} - \beta^* k\omega \quad \text{(B.12)}
\end{equation}

\begin{equation}
\frac{\partial \omega}{\partial t} + \langle u_i \rangle \frac{\partial \omega}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ (\nu + \sigma \nu_T) \frac{\partial \omega}{\partial x_j} \right] - \frac{\gamma}{k} \left( \langle u_i u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} \right) - \beta k\omega^2 \quad \text{(B.13)}
\end{equation}

where $\gamma$, $\beta$, $\beta^*$, $\sigma$, and $\sigma^*$ are all model closure coefficients. The governing equations solved in a LES, however, are the Navier-Stokes equations that have had a spatial filter (denoted by an overbar) applied:

\begin{equation}
\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad \text{(B.14)}
\end{equation}

\begin{equation}
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{u}_j + \bar{p} \delta_{ij} - \nu \frac{\partial \bar{u}_i}{\partial x_j} + \tau_{ij} \right) = 0. \quad \text{(B.15)}
\end{equation}

where a typical subgrid-scale (SGS) model for turbulence closure is the Smagorinsky model [13]:

\begin{equation}
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_T \bar{S}_{ij} \quad \text{(B.16)}
\end{equation}

\begin{equation}
\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad \text{(B.17)}
\end{equation}

\begin{equation}
\nu_T = C_s \Delta^2 |\bar{S}| \quad \text{(B.18)}
\end{equation}

where $C_s$ is a model coefficient. Note that the RANS equations and the LES equations are essentially identical except how the Reynolds or subgrid-scale stresses are computed.

At first glance, the two types of CFD are nearly identical. While many RANS closures are two-equation models, and many SGS models for LES are based on the Smagorinsky approach, that does not define either approach. Transport equation-based SGS models, analogous to the two-equation closures used in RANS have been proposed (e.g., Gallerano et al. [14]), but experience has shown that the
additional computational cost of including transport equations to an LES is rarely advantageous [2]. The exceptions are for modeling reactive or buoyancy-driven flows, where significant energy is at the subgrid scales.

While the filtering of the Navier-Stokes equations for LES may seem very similar to a Reynolds decomposition, there are important differences. For a Reynolds decomposition, the mean velocity, \( \langle u_i \rangle \), is not a random variable, and a fundamental property of Reynolds averaging is that the mean of the fluctuating component of the velocity is everywhere zero. With an LES, the filtered velocity field, \( \bar{u}_i \), is a random variable. In general, the filtered residual is nonzero: i.e., if one decomposes the velocity vector into the mean and turbulent fluctuation

\[
    u_i = \langle u_i \rangle + u_i' \tag{B.19}
\]

Reynolds averaging gives the result:

\[
    \langle u_i u_j \rangle = \langle \langle u_i \rangle + u_i' \rangle \langle \langle u_j \rangle + u_j' \rangle \tag{B.20}
\]

\[
    = \langle \langle u_i \rangle \langle u_j \rangle \rangle + \langle u_i' \rangle \langle u_j' \rangle + u_i' \langle u_j \rangle + u_j' \langle u_i \rangle 
    \tag{B.21}
\]

\[
    = \langle \langle u_i \rangle \langle u_j \rangle \rangle + \langle u_i' u_j' \rangle \tag{B.22}
\]

but the equivalent expression is not true for a LES, for even \( \bar{u}_i \neq \bar{u}_i \).

Deciding whether an LES or RANS model is more useful is not necessarily possible a priori. However, note that RANS models can only model deterministic, and not stochastic, coherent structures in turbulence. The advantage of RANS models is that the eddies which need to be resolved in order to properly execute an LES are so small that simulations of boundary layers, unless wall models are used, require very fine grids. Large-eddy simulations utility is based on the size of the filter width compared to the scale of the turbulence. When the filter width is very small, LES will tend towards a DNS representation, which is often computationally cumbersome. At the other extreme when the filter width is very large, LES will
seem more similar to a RANS model, since the filtered velocity will tend toward the mean velocity. LES is most useful when the filter width (i.e., grid size) is in between, typically within the inertial subrange. When adding wall models to an LES are not useful, hybrid RANS-LES methods are often considered, such as a detached eddy simulation (DES) first studied by Spalart et al. [15], but current investigations do not show important advantages over LES for flow over a hill [16], which is geometrically very similar to flow over a buried cylinder. In general, a DES is a model where the turbulence closures of an LES and RANS model are written in similar ways such that each model is used in the region of flow best suited for it.

It is impossible to know in advance how important stochastic coherent structures are on oscillatory boundary layers. One could argue that for a horizontally homogenous oscillatory boundary layer that RANS models have provided adequate results in rough turbulent flows. The presence of the intermittently turbulent regime shows that small-scale perturbations that would not be captured by RANS models are important, although on the seafloor one would expect fully turbulent conditions to be most important when considering sediment transport. For more complicated flows, coherent structures could be very important. Hay and Bowen [17] showed from nearshore acoustic backscatter measurements that coherent structures are present in the suspended sediment concentration field. And it is well known that particles will settle more slowly in turbulent water than in still water, for instance [18]. And LES has been shown to be considerably more accurate than RANS models for flow around cylinders – a prototype for piles on a seabed, which are of great engineering interest.

One important difference between RANS and LES is also the way one compares with experiment. A large-eddy simulation results in a single instance of the
grid-filtered velocity, \( \bar{u}_i \). Turbulent statistics computed with the grid-filtered velocity neglect the subgrid scale contribution. While not done in this dissertation, it is possible to reintroduce the SGS term into the LES results before comparing with experiment. For example, consider the Reynolds stress. Zang [19] showed that the SGS contribution to the Reynolds stress can be approximately given by:

\[
\langle \tau_{ij} \rangle = \langle \bar{u}_i \bar{u}_j \rangle + \langle u'_i \bar{u}_j \rangle + \langle \bar{u}_i u'_j \rangle + \langle u'_i u'_j \rangle, \tag{B.23}
\]

where the Leonard term \( L_{ij} \) is

\[
L_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j. \tag{B.24}
\]

Zang was able to show that

\[
\bar{e}_{ij} = \bar{\epsilon}_{ij} + \langle \tau_{ij} \rangle - \langle L_{ij} \rangle \tag{B.25}
\]

where \( \bar{e}_{ij} \) is the measured Reynolds stress and \( \bar{\epsilon}_{ij} \) is the computed Reynolds stress.

### B.2.2 SGS turbulence closure

The most widely used models of the subgrid-scale (SGS) stresses in large-eddy simulations are based on variations of the Smagorinsky model [13], starting with Deardorff’s pioneering work [20] which is considered to be the first LES. Recently some non-Smagorinsky approaches have been developed, however (see e.g., Fureby and Grinstein’s monotonically integrated LES [21]). In the Smagorinsky approach, the local eddy viscosity is proportional to the resolved shear strain rate and a model coefficient. Early work by Lilly [22] showed that the Smagorinsky model agrees with the Kolmogorov turbulence spectrum for isotropic turbulence if the model coefficient \( C \) is approximately 0.16. The model applies too much dissipation near walls, however; predicts SGS stresses in laminar flow; and it assumes zero SGS energy backscatter (i.e., energy transfer from small scales to larger ones). One improvement to the Smagorinsky model being too dissipative in LES
of wall-bounded transitional flows \cite{23} is to apply the van Driest damping function \cite{4} or to otherwise adjust flow around the wall \cite{24}, but this does not fix the other problems, and creates additional parameters which must be tuned to each problem.

The simplest way to generalize Smagorinsky’s model is to vary the model coefficient with space and time. This can be done without empirical calibration by applying the Germano identity \cite{25}. The assumption behind the identity is that if the Smagorinsky approach is applied on the same velocity field, but at two different filter widths (i.e., the grid filter width and a “test” filter width), then the Smagorinsky model coefficient is equal (i.e., scale invariance). Based on this approach, Germano et al. \cite{26} developed the dynamic Smagorinsky model. The model coefficient is determined by finding the least squares error of the model assuming that the Germano identity holds \cite{27}. While this approach solves the problems mentioned earlier with the constant coefficient Smagorinsky model, the dynamic approach has several drawbacks. The dynamic Smagorinsky model and its variations have the unfortunate problem of being unstable unless the often noisy estimates of the model coefficient were heavily filtered (e.g., planar averaging). As well, negative values of the model coefficient can provide excessive SGS backscatter. One final problem that exists for Smagorinsky-like models is that the SGS stress tensor is aligned with the resolved strain rate tensor. The last point has been shown to be an important problem based on DNS results \cite{28}, and is a focus of many modern SGS closure schemes (e.g., Wand and Bergstrom \cite{29}).

Another approach to improving SGS models was proposed by Bardina et al. \cite{28}, where the SGS stress is separated into its resolved and unresolved components, with the goal of having the turbulence closure have to model less of the SGS stress. One of the requirements of a physically realistic SGS model is
that it should obey Galilean invariance. Speziale [30] found that Bardina et al.’s approach did not satisfy this requirement. Recent developments in Lagrangian-averaged Navier-Stokes equations (a relatively new approach to modeling turbulence introduced by Chen et al. [31]), however, show that to be accurate either the SGS turbulence should be directly modeled (e.g., as in the SGS estimation model of Domaradzki and Saiki [32] or the fractal interpolation method of Basu et al. [33]) or a decomposition like the Bardina model is necessary. The Bardina model has also been shown to be important in modeling SGS energy backscatter [34], and it also does not force the SGS stress tensor to be aligned with the resolved strain rate tensor.

The approaches of Germano and Bardina et al. have been combined by Zang [19] in a dynamic mixed model. Zang used a formulation of the turbulent stresses proposed by Germano [35], and since the dynamic mixed model has been successfully applied to a variety of geophysical flows [36, 37, 38] and more recently been applied to flows involving sediment transport [39]. The constant coefficient Smagorinsky model, dynamic Smagorinsky model, and dynamic mixed model were the three SGS models tested in Manuscript 1.

More recently proposed SGS closures include Salvetti and Banarjee’s dynamic two parameter model [40] and a Lagrangian averaged SGS model [41]. Lagrangian averaged SGS models are variants of the dynamic Smagorinsky approach which average the model coefficient over fluid pathlines. Early large-eddy simulations were often applied to two-dimensional problems, where the model coefficient could be averaged over homogeneous directions in order to stabilize the results. In fully three-dimensional problems, however, homogeneous directions no longer exist, so the averaging either has to be done over a local area (as in this work), or the averaging could be applied over fluid pathlines. This is essentially the application
of Taylor’s hypothesis that turbulent fluctuations are on a small enough scale that they are advected with the resolved fluid motions. More recently, Bou-Zeid et al. [42] has applied this approach to a Lagrangian averaged scale dependent dynamic model that takes into consideration the variation of the Smagorinsky model coefficient with scale. This involves a third filter of the Navier-Stokes equations and assumes a power-law behavior of the model coefficient rather than assuming scale-invariance as in the traditional dynamic Smagorinsky approach.

Note that SGS models are often not self-consistent. For example, in Lilly’s [27] least-squares approach to solving for the Smagorinsky model coefficient, at one point the coefficient is assumed to be a constant with regards to the spatial filtering operation (e.g., assuming that \( C_s = \bar{C}_s \)) – even though the purpose of using the dynamic approach is to allow the model coefficient to vary in space. Although other SGS models have been proposed which do not have this problem (see e.g., Ghosal et al. [43]), many SGS models are found to mathematically inconsistent. To some extend these faults are tolerated for the sake of computational efficiency, but also note that the Smagorinsky model was developed in 1963 [13], while laser Doppler velocimetry, important for making turbulence measurements and a predecessor to particle image velocimetry, was not developed until 1964 [44]. The models and measurements in fluid dynamics, like most of science, develop together – and the future of turbulence modeling depends on knowing what experiments need to be made to make those discoveries.

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APPENDIX C

Large-eddy simulation setup

C.1 Installation

As described in Appendix D, the source code used for this dissertation was based on PCUI (used by Cui and Street [1]).

For file input and output, the CFD General Notation System (CGNS) file format is used. The CGNS standard is a machine-independent file format designed for storing CFD data. The current I/O routines for the LES are based on version 2.5 of the CGNS library. The use of the CGNS file format is an American Institute of Aeronautics and Astronautics (AIAA) Recommended Practice [2]. A variety of scientific visualization software exists to render the data stored in a CGNS file.

To install CGNS, after decompressing the library tarball, in the CGNS directory, type:

```
chmod +x configure
./configure --enable-64bit --prefix=$HOME
make
make install
```

This will compile the CGNS source for the local system in the current directory, and place files in the `~/include/` and `~/lib/` directories. This is typically necessary, since on most systems the CGNS library is not already installed, and root access is rare.

After CGNS is installed, go to the LES directory, and after adjusting the FC, FCFLAGS, and BINDIR variables in the Makefile in order to be appropriate for the local system, type:

```
make
make install
```

In order to run a simulation, it is simply a matter of calling the code, e.g.,

```
mpirun -np 8 cav
```
and is commonly called from a queue. The input file is prespecified as `cav.in`, within the current directory. Output files will be written as output*.cgns. Note that there is no command-line interface. This has several reasons. When submitting jobs to queues, command-line options may get confused with the call to mpirun, and as well, a standard for command-line interface was only established for Fortran recently.

### C.2 Hardcoded parameters

Because of the large number of options, it is not necessarily most efficient to have all simulation parameters set by input files. Two files may need to be altered depending on the test run: `size.inc` and `tank.f`.

`size.inc` is used to set the both the size of the grid and the way the domain is decomposed into the work accomplished by each processor. The grid size is $n_i$ by $n_j$ by $n_k$, where $i$ is the streamwise direction, $j$ is the wall-normal direction, and $k$ is the spanwise direction. This does not have to be the case, but the wall boundary conditions would have to be modified if this was changed. It is possible to alter this to have the LES code use allocatable arrays instead, but in some cases this can result in slower code, and computational efficiency is most important for this work. The parameters $p_x$, $p_y$, and $p_z$ are used in the domain decomposition: i.e., the product of the three is the number of processors required during the test run, and e.g., the domain is split into $p_x$ sub-domains in the $i$ direction.

`tank.f` is used to set the grid and the inviscid forcing. The variable `idomain` is used to set the type of domain. Three are considered in the manuscripts here: 1 for a computational box with a uniform grid spacing; 2 for a computational box with vertical grid stretching; and 3 for a rippled domain. `ratio` is the vertical stretching ratio. For rippled domains, `$eta$` and `$lambda$` are the ripple height and wavelength, respectively. The term `iforcing` is used to set the type of forcing:
1 for a purely oscillatory flow; 2 for a wave-induced flow; and 3 for oscillatory flow over ripples. For oscillatory flow, \( u_0 \) is the maximum free-stream velocity and \( \text{period} \) is the period of oscillation. For wave-induced flow, \( \text{amp} \) sets the wave amplitude, \( \text{period} \) sets the wave period, \( \text{depth} \) sets the wave depth, and \( k_1 \) sets the wave number (i.e., for simplicity, the wavenumber is computed and hardcoded for each test case). For flow over ripples, \( u_1 \) and \( u_2 \) are the magnitudes of the first and second harmonics of the oscillatory free-stream velocity, and \( \text{period} \) is the period of oscillation. It is possible to store this information in an input file, but experience has shown that it is usually easier to re-compile the LES source instead. One would require e.g., an additional program for preprocessing to create the grid and store it in another CGNS file, which would mean that there would be two programs which could have bugs to fix.

Finally, in \texttt{scal.f} the relative density, \( s \), of the sediment, and the critical Shields number, \( \text{shieldscr} \). Future revisions of the code may include this in the input file discussed below.

### C.3 Input file format

In addition to the hardcoded parameters, an input file, \texttt{cav.in} is used to set the remaining simulation parameters (Fig. C.1). Here \texttt{verbose} is used to describe how much information is displayed during a simulation run (i.e., higher numbers display more debugging information). At this point, \texttt{newrun} is always set to 1 for any tests in this work. \texttt{nstart}, \texttt{nfinal}, and \texttt{nsave} refer to how often output files are saved – starting after timestep \texttt{nstart}, data is saved every \texttt{nsave} timesteps, with the simulation ending at timestep \texttt{nfinal}. Each timestep is \texttt{dt} seconds long. The function of the remaining terms in the input file can roughly be divided into the grid definition, the SGS model, the pressure Poisson solver, the boundary conditions, and the reference state.
1 iverbose
1 newrun
1 periodic
0 iscalar
0 ieddy
0.021 smag
0 iaug
0 ibc
1 nstart
6400 nfinal
64 nsave
38.08973812790537d0 bx
0.025786364998628467d0 by
0.1d0bz
0.00044 d50
3.6667 z0
0.09375 dtime
1.36e-6 vis
1.0e-6 ak = vis
9.81 g
1 mg_level
10 maxstep
20 20 20 20 20 iterchk(1-5)
10 10 10 10 10 maxiter(1-5)
0.5e-2 factor
1.e-7 1.e-7 1.e-7 1.e-7 1.e-7 tol(1-5)
1.e-7 1.e-7 1.e-7 1.e-7 1.e-7 ter(1-5)
0.7 0.6 0.6 0.6 0.6 slowiter(1-5)

Figure C.1. Example input file.
C.3.1 Grid definition

The grid size is specified by \( b_x \), \( b_y \), and \( b_z \), specifying the length, height, and width of the domain in meters.

C.3.2 SGS model parameters

The SGS model used for the simulation is set by \( i_{eddy} \): for 0, no SGS model is used; for 1, the constant coefficient Smagorinsky model is used; for 2, the dynamic Smagorinsky model is used; and for 3, the dynamic mixed model is used. For the constant coefficient model, \( s_{mag} \) is the Smagorinsky model coefficient. In addition, several of the test runs involved a near-wall augmentation of the SGS stress – this is activated when \( i_{aug} \) is 1, and deactivated when it is 0.

C.3.3 Pressure Poisson solver

The pressure Poisson solver is based on a multigrid method which depends on a large variety of parameters, including \( mg\_level \), \( maxstep \), \( iterchk \), \( maxiter \), \( factor \), \( tol \), \( ter \), and \( slowiter \).

\( mg\_level \) sets the multigrid level between 0 and 5. Typically this value is \( \log_2 nx/px \). The method depends on a V-cycle which loops as many as \( maxstep \) times, unless the 2-norm of the residual is less than \( tol \), the infinity-norm of the residual is less than \( ter \), and the ratio of the residual to the magnitude of the right-hand side is less than \( factor \).

At each level of the V-cycle, the residual is smoothed \( iterchk \) times before checking the residual for convergence. And this process is repeated as many as \( maxiter \) times at each level. As well, at each level, if the residual does not decrease by at least a factor of \( slowiter \), the iteration is judged to be too slow, and the smoothing operation for that level is terminated early.
C.3.4 Boundary conditions

The boundary conditions are set by periodic and ibc. When periodic is 0, the domain is considered to be periodic in the spanwise direction, but not the streamwise direction; for periodic equal to 1, the domain is periodic in both the streamwise and spanwise direction.

C.3.5 Fluid reference state

The fluid viscosity and the acceleration of gravity is set by vis and g. The sediment diffusivity and settling velocity is set by ak and ws. In addition, the sediment diameter, d50, z0 of the surface, z0, also need to be set.

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APPENDIX D
Changes to existing code

The hybrid simulation code was not an original programming development. The vast majority of the resulting code is from either PCUI, a large-eddy simulation from Cui and Street [1], and the numerical wavetank, from Grilli and Subramanya [2]. Below an outline of the changes that were required is given.

D.1 Initialization

PCUI, in its original form, is designed to simulate a lid-driven cavity. For these manuscripts, the lid velocities are no longer needed, and so this was eliminated for the current model. It, like the other initialization procedures, are located in init.f. At the initial timestep, a number of other changes to variables are needed. The pressure term is set to zero. The scalar $\phi$, which is used to store the suspended sediment concentration, is set to zero. The total velocity, stored in $\text{ules}$ (separate from the perturbation velocity, stored as $u$, which previously was the velocity in PCUI), is also set to zero.

The gridding routine in cavity.f was changed in a substantial way – the grid-points are no longer stored at the cell centers, but at the cell vertices. The positions of the remaining metric parameters are unchanged, so the routines for computing these are changed somewhat. The grid itself is setup by tank.f, described below in D.9.

D.2 Eddy viscosity

From a theoretical point of view, nothing new was developed for the eddy viscosity model (with routines in eddy.f), but some substantial changes were made to the source code. Originally PCUI was designed to implement the dynamic mixed
model [3] for a grid with no-slip boundaries. It was modified to also handle the
dynamic Smagorinsky model [4], the constant coefficient Smagorinsky model [5],
as well as to consider enhanced eddy viscosity near a wall. The explicit filter
definition changed somewhat for points next to the wall (i.e., to follow the filter
definitions of Vasilyev et al. [6]), and near-wall enhanced eddy viscosity is now an
option.

Others with more experience with approximate boundary conditions (e.g.,
logarithmic) have shown good results without this near-wall enhancement (e.g.,
Radhakrishnan and Piomelli [7]), so the theoretical consistency here could be im-
proved. Another notable change is that the code does not change usage from \( u \)
to \( \mathbf{u} \) (i.e., the eddy viscosity is computed with only the perturbation velocity
field).

D.3 Predictor step

In the predictor step, most of the modifications relate to changes between using
the perturbation velocity and the total velocity, as discussed in Appendix E. In
addition, the Coriolis and bouyancy terms are removed. The inviscid contribution
to the convective and viscous terms are added. Ideally the inviscid velocity is
filtered at this point. This is generally not necessary, because the inviscid velocity
varies on length scales larger than the LES grid.

D.4 Pressure Poisson equation

The pressure Poisson equation has remained essentially unchanged since the
original LES code, other than relying on the perturbation velocity instead of the
total velocity field. The wall boundary condition does not change either, since the
pressure Poisson equation only depends on the flux at the boundaries.
D.5 Corrector step

In the corrector step, as a part of corr.f, the primary change is to add approximate boundary conditions, such as the log-layer assumption. This is done through modifying $u_{bc}$ and adding the subroutine: getufric and the function mybc. getufric obtains the friction velocity given the velocity at a point above the seabed for a given type of boundary condition. mybc is a function which is used to solve for the friction velocity for the modified log-layer approach considered in Manuscript 3.

As well, the inviscid fluxes (e.g., $u_{ixi}$) are computed from the inviscid forcing of the previous timestep in the corrector step.

D.6 Scalar transport

In scal.f, two primary changes were made to the governing equations for a passive scalar (which now represents suspended sediment). First, a settling velocity of $w_s$ is added to the convective terms. Also, at the lower boundary, the SSC boundary condition is applied based on the sediment pickup function, as described in Manuscript 3.

D.7 Message passing

The large-eddy simulation code runs calculations in parallel by using the Message Passing Interface (MPI). Only a few changes were needed for the MPI calls within mp.f.

For initialization, there is the issue of boundary conditions. A domain decomposition is used for parallelizing the algorithms, and because the large-eddy code uses a structured grid, a Cartesian topology is used as an efficient way to connect the processors. MPI_CART_CREATE is used to setup the relationships between the processor domains (i.e., west, east, north, south, front, back). Periodic bound-
ary conditions can easily be implemented through this function as well. The new code uses periodic boundary conditions for all test cases in this dissertation for the span-wise direction. The switch between the periodic and aperiodic boundary conditions affects only the streamwise direction.

As far as exchanging information between the processors, no changes are required for the vast majority of the variables. For the third manuscript, however, the pressure gradient above the wall is needed, which is a two-dimensional variable. A new routine, dp_exchange was written to exchange the information for this calculation.

D.8 Input and output files

The I/O routines in io.f have been rewritten substantially. The subroutine parameter has been rewritten to work with the altered cav.in format, as described in Appendix C. The output file format is now re-written to save the velocity, eddy viscosity, and suspended sediment concentration for a given timestep in a CGNS file.

D.9 Inviscid forcing

In terms of inviscid forcing, a new file, tank.f is created which contains routines mygrid and myNWT which control the inviscid forcing. mygrid creates the LES grid, and myNWT is used to specify what the inviscid velocity is at the next timestep – either an analytic expression, or reading an input from the NWT.

D.10 Main loop

The changes to the main loop (in ns.f) for each timestep were relatively minor, primarily to call the new inviscid forcing routine.

In addition, the variable imass is used to describe whether or not the pressure Poisson equation is used. If imass is 1, then the perturbation pressure is
solved for normally. If \textit{imass} is 2, then as described in Manuscript 2, the vertical velocity is solved for by assuming that the streamwise velocities are orders of magnitude greater than the vertical velocities and by integrating the mass conservation equation directly.

\textbf{List of References}


APPENDIX E
Numerical implementation

E.1 Introduction

The numerical method of the hybrid model includes the numerical wavetank of Grilli and Subramanya [1] and the large-eddy simulation of Cui and Street [2], each large projects, so an attempt was made to minimize the amount of program restructuring.

The computational domain of the hybrid model (Fig. E.1) consists of the two- or three-dimensional NWT grid, and the three-dimensional LES grid. The hybrid model advances $\Delta t$ at a time until the end of the simulation or the CFL number exceeds 0.9. CFL numbers in excess of 0.9 typically cause in inaccurate results and in many cases instabilities in the velocity field. None of the results published in any of the four manuscripts were terminated early due to the CFL number.

Although independently all of the numerical methods presented below have been published by other authors, nowhere has all of the material below been produced in one location. So briefly, although this level of detail is not needed in the manuscripts, the numerical method for the hybrid method is given. This is divided into the various inviscid forcings and the many steps of the large-eddy simulation.

E.2 Inviscid forcings
E.2.1 Oscillating free-stream

The simplest oscillating inviscid forcing is that used for the Stokes boundary layer, e.g.:

$$u^I_1(t) = U_0 \sin \omega t.$$  \hspace{1cm} (E.1)

This velocity is applied uniformly at all points.
E.2.2 Analytic wave forcing

Both first- and second-order wave theories are considered. Using linear wave theory, the internal velocities of a progressive water wave over a flat bed are (see e.g., Dean and Dalrymple [3]):

\[ u_1(x, y, t) = \frac{a g k \cosh ky}{\omega \cosh kh} \cos(kx - \omega t) \]  \hspace{1cm} (E.2)

\[ u_2(x, y, t) = \frac{a g k \sinh ky}{\omega \cosh kh} \sin(kx - \omega t) \]  \hspace{1cm} (E.3)

for an amplitude \( a \), wavenumber \( k \), and angular frequency \( \omega \). While this can be applied for any amplitude, it is derived assuming small \( kH/2 \). It can often be useful to consider even when considering moderately steep waves. In contrast, second-order Stokes waves have the velocity forcing (see e.g., Dean and Dalrymple [3]):

\[ u'_1(x, y, t) = \frac{a g k \cosh ky}{\omega \cosh kh} \cos(kx - \omega t) + \frac{3 a^2 \omega k \cosh 2ky}{4} \sinh^4 kh \cos 2(kx - \omega t) \]  \hspace{1cm} (E.4)

\[ u'_2(x, y, t) = \frac{a g k \sinh ky}{\omega \cosh kh} \sin(kx - \omega t) + \frac{3 a^2 \omega k \sinh 2kh}{4} \sinh^4 kh \sin 2(kx - \omega t). \]  \hspace{1cm} (E.5)

In deriving these equations, there is a restriction on the Ursell number [4], such that \( L^2 H / h^3 << 64\pi^2 / 3 \). In shallow water, in order for the solution to remain single crested, this requirement is in fact \( L^2 H / h^3 < 8\pi^2 / 3 \). Higher-order Stokes
expansions are possible, but for many engineering applications first- and second-order theory is used.

### E.2.3 Analytic forcing over ripples

Another common situation is an oscillating flow over ripples. Instead of solving for the inviscid flow over ripples directly, we consider the flow obtained by the conformal mapping:

\[
x_1(\xi, \chi) = \xi - \frac{1}{2} \eta e^{-k\chi} \sin k\xi \\
x_2(\xi, \chi) = \chi + \frac{1}{2} \eta e^{-k\chi} \cos k\xi
\]

(E.6) (E.7)

or in complex notation (i.e., \(z = x_1 + ix_2\) and \(\zeta = \xi + i\chi\)):

\[
z = \zeta + \frac{1}{2} i \eta e^{ik\zeta} \\
\frac{dz}{d\zeta} = 1 - \frac{1}{2} k \eta e^{ik\zeta} \\
\frac{d\phi}{dz} = \frac{d\phi}{d\zeta} \frac{d\zeta}{dz}
\]

(E.8) (E.9) (E.11)

which results in the inviscid velocity:

\[
u_1^I(\xi, \chi, t) = u_\infty(t) \frac{1 - \frac{1}{2} k \eta \cos k \xi e^{-k\chi}}{1 - k \eta e^{-k\chi} \cos k \xi + \frac{1}{4} k^2 \eta^2 e^{-2k\chi}} \\
u_2^I(\xi, \chi, t) = u_\infty(t) \frac{-\frac{1}{2} k \eta \sin k \xi e^{-k\chi}}{1 - k \eta e^{-k\chi} \cos k \xi + \frac{1}{4} k^2 \eta^2 e^{-2k\chi}}
\]

(E.12) (E.13)

where

\[
u_\infty(t) = U_1 \cos(\omega t - \gamma) + U_2 \cos(2\omega t - 2\gamma)
\]

\[
\gamma = \arccos \left( \frac{\sqrt{U_1^2 + 8U_2^2} - U_1}{4U_2} \right)
\]

(E.14) (E.15)

where \(\gamma\) is the same phase shift as that used by van der Werf et al. [5] such that the initial velocity is zero.
E.2.4 Numerical wavetank

The exact numerical method used by the NWT is described by Grilli and Subramanya [1]. Here we outline the method.

For incompressible irrotational flows, we define \( u_i = \frac{\partial \Phi}{\partial x_i} \), with \( \Phi \) the velocity potential. With this definition, mass conservation becomes Laplace’s equation:

\[
\nabla^2 \Phi = 0 \quad (E.16)
\]

which is efficiently solved using a Boundary Element Method (BEM) based on Green’s second identity:

\[
\alpha \Phi(x_i) = \int_G \left\{ \frac{\partial \Phi}{\partial n} G - \Phi \frac{\partial G}{\partial n} \right\} \, d\Gamma \quad (E.17)
\]

where \( \Gamma \) denotes the NWT boundary, \( n \) is the outwards normal vector to the boundary, \( G \) is the free-space Green’s function. In two dimensions, \( G \) is given by:

\[
G(x, x_l) = -\frac{1}{2\pi} \log |x - x_l| \quad (E.18)
\]

where \( x_l \) is a collocation node.

Numerical wavetanks have no closed-form velocities, but instead the internal velocities are computed with a boundary integral equation:

\[
u(x_l) = \int_G \left\{ \frac{\partial \Phi}{\partial n}(\nabla_l G) - \Phi \left( \nabla_l \frac{\partial G}{\partial n} \right) \right\} \, d\Gamma. \quad (E.19)
\]

The resulting equations are discretized similar to Grilli and Subramanya [1], i.e., integrated in time using a second-order Taylor’s series expansion (i.e., using both \( \Phi \) and \( \frac{\partial \Phi}{\partial t} \)) and the fully nonlinear kinematic and dynamic boundary conditions can be applied for the free-surface:

\[
\frac{Dx}{Dt} = \frac{\partial \Phi}{\partial x_i} \quad (E.20)
\]

\[
\frac{D\Phi}{Dt} = -g x_3 + \frac{1}{2} \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_i} - \frac{p_o}{\rho} \quad (E.21)
\]
respectively, where \(x_3\) is the vertical coordinate, and a (Neumann) no-flow condition is specified on the other boundaries, including a wavemaker and the seabed. The boundary integral equation is discretized using a series of collocation nodes \(l = 1, ..., N_Γ\) on the boundary, and higher-order elements are used to interpolate between the nodes. The resulting linear system equations is solved at each timestep to provide boundary values of \(Φ\) and its normal and time derivatives. In the hybrid model, such internal points are selected at the grid cell centers of the submerged NS-LES domain, which is embedded within the NWT.

Wave generation in the NWT can be accomplished in several ways. Here a flap wavemaker is simulated at the leftward boundary of the NWT, \(Γ_w\), with a prescribed motion, \(x_w(t)\). This can easily be used to generate regular waves, similar to a physical wavetank (e.g., Grilli and Horrillo [6]; Grilli et al. [7]). In this work, however, besides regular waves, we also extended the NWT to generate a well controlled irregular wave climate, based on a specified incident energy spectrum.

In the far-field wave domain simulated in the NWT, incident waves propagate, transform, and shoal over the specified bottom topography. In the near-field, waves would eventually break and dissipate their energy. In the NWT, following Grilli and Horrillo [6], an absorbing beach (AB) is specified at the far shallow end of the NWT, in which energy dissipation is applied by a combination of free surface absorption and an actively absorbing piston (AP) boundary. The absorbing pressure is specified in the dynamic free surface boundary condition, proportional to the normal particle velocity as:

\[
p_a(x_1, t) = ν_a(x_1) \frac{∂Φ}{∂n}
\]

(E.22)

where \(ν_a\) denotes smoothly varying AB absorption function in the long NWT horizontal direction \(x_1\).
E.3 LES timestep

The large-eddy simulation is based around a predictor-corrector method, split into six essential steps (Algorithm 1).

Input: $[\bar{u}_i^P]^n$, $[\bar{u}_i^I]^{n+1}$
Output: $[\bar{u}_i^P]^{n+1}$

if LES then
    compute eddy viscosity, $\nu_T \equiv \nu_T(\bar{u}_i^P)$;
end

if scalar simulation then
    compute scalar RHS;
end

compute predictor step;
solve pressure Poisson equation;
compute corrector step;
if scalar simulation then
    solve scalar transport equation;
end

Algorithm 1: LES timestep algorithm.

E.3.1 Eddy viscosity

The eddy viscosity (and eddy diffusivity) is solved for with:

$$\nu_T = C_s \bar{\Delta}^2 |\bar{S}|$$  \hspace{1cm} (E.23)

$$\kappa_T = \frac{C_s \bar{\Delta}^2 |\bar{S}|}{Pr_T}$$  \hspace{1cm} (E.24)

where

$$C_s = \begin{cases} 
0.16 & \text{for Smagorinsky model} \\
\frac{-\ell_{ij} M_{ij}}{2 \bar{\Delta}^2 M_{ij} M_{ij}} & \text{for DSM} \\
\frac{-(\ell_{ij} - H_{ij}) M_{ij}}{2 \bar{\Delta}^2 M_{ij} M_{ij}} & \text{for DMM} 
\end{cases}$$  \hspace{1cm} (E.25)

$$\frac{1}{Pr_T} = \begin{cases} 
1.0 & \text{for Smagorinsky model} \\
\frac{-K_{ij} N_j}{C_s \bar{\Delta}^2 N_j N_j} & \text{for DSM} \\
\frac{-(K_{ij} - J_{ij}) N_j}{C_s \bar{\Delta}^2 N_j N_j} & \text{for DMM} 
\end{cases}$$  \hspace{1cm} (E.26)
and

\[ L_{ij} = \hat{u}_i \tilde{u}_j - \hat{u}_i \hat{u}_j \]  
(E.27)

\[ K_j = \hat{u}_j \hat{C} - \hat{u}_j \hat{C} \]  
(E.28)

\[ M_{ij} = \alpha^2 |\hat{S}| \hat{S}_{ij} - |\hat{S}| \hat{S}_{ij} \]  
(E.29)

\[ N_j = \alpha^2 |\hat{S}| \frac{\partial \hat{C}}{\partial x_j} - |\hat{S}| \frac{\partial \hat{C}}{\partial x_j} \]  
(E.30)

\[ H_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \]  
(E.31)

\[ J_j = \hat{C} \hat{u}_j - \hat{C} \hat{u}_j. \]  
(E.32)

For the DMM, two additional terms are also needed, which are used in the predictor step:

\[ L_{ij}^m = \overline{u_i u_j} - \overline{u_i \tilde{u}_j} \]  
(E.33)

\[ P_j = \overline{u_j \hat{C}} - \overline{u_j \hat{C}}. \]  
(E.34)

The algorithm for computing these expressions is relatively straightforward (Algorithm 2. Two discrete operations needed to evaluate these expressions: a
discrete differential which we will evaluate using center differencing; a
discrete filter (both grid- and filter-width) which we will evaluate using the trapezoidal rule.

Note that both the center differencing and filtering operations require boundary
conditions. In general, we apply linear extrapolation.

**Center differencing**

All non-convective terms of the time-stepping scheme are computed using
second-order center differences. For example for a quantity \( a \):

\[ \left[ \frac{\delta a}{\delta \xi_1} \right]_{i,j,k} \approx [a]_{i+1/2,j,k} - [a]_{i-1/2,j,k} \]  
(E.35)

which can be extended without loss of generality to the other two dimensions.
Input: \( \bar{u}_i, \bar{C} \)

Output: \( \nu_T, \kappa_T, \frac{\partial}{\partial \xi_m} \left( J \frac{\partial \xi_m}{\partial x_j} \right), L_{ij}^m \)

Compute \( \tilde{S}_{ij}, \frac{\partial \bar{C}}{\partial x_j}, |\tilde{S}|, |\tilde{S}| \tilde{S}_{ij} \);

if DSM or DMM then
   Test-filter to get \( \hat{|\tilde{S}|\tilde{S}_{ij}}, \hat{|\tilde{S}|}, \hat{\tilde{S}}_{ij} \);
   Compute \( M_{ij}, N_j \);
   Compute \( \bar{u}_i \bar{u}_j, \bar{C} \bar{u}_i \);
   Test-filter to get \( \hat{\bar{u}}_i \hat{\bar{u}}_j, \hat{\bar{C}} \hat{\bar{u}}_i, \hat{\bar{u}}, \hat{\bar{C}} \);
   Compute \( \mathcal{L}_{ij}, \mathcal{K}_{ij} \);
   Grid-filter to get \( \bar{u}_i, \bar{C} \);
   Apply BCs to \( \bar{u}_i, \bar{C} \);
   Compute \( \bar{u}_i \bar{u}_j, \bar{C} \bar{u}_i \);
   Test-filter to get \( \hat{\bar{u}}_i \hat{\bar{u}}_j, \hat{\bar{C}} \hat{\bar{u}}_i, \hat{\bar{u}}, \hat{\bar{C}} \);
   Compute \( \mathcal{H}_{ij}, \mathcal{J}_i \);
   Compute \( M_{ij} \bar{u}_i, M_{ij} \mathcal{L}_{ij}, M_{ij} \mathcal{H}_{ij}, N_i N_i, N_i \mathcal{K}_i, N_i \mathcal{J}_i \);
   Apply BCs;
   Filter \( C_s \);
end

Set \( \nu_T, \kappa_T \);
Apply BCs to \( \nu_T, \kappa_T \);
if DMM then
   Compute \( \bar{u}_i \bar{u}_j, \bar{C} \bar{u}_i \);
   Grid-filter to get \( \bar{u}_i \bar{u}_j, \bar{C} \bar{u}_i, \hat{\bar{u}}_i, \hat{\bar{C}} \);
   Compute \( L^m_{ij}, P_i \);
   Apply BCs to \( L^m_{ij}, P_i \);
   Compute \( \frac{\partial}{\partial \xi_m} \left( J \frac{\partial \xi_m}{\partial x_j} L^m_{ij} \right) \);
end

Algorithm 2: Process to compute SGS stress terms.
This can be used to evaluate the resolved strain rate tensor, i.e.,

\[
\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]

(E.36)

\[
= \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial \xi_k} \frac{\partial \xi_k}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial \xi_l} \frac{\partial \xi_l}{\partial x_i} \right)
\]

(E.37)

which using our discretized variables reads:

\[
[\bar{S}_{ij}]_{i,j,k} = \frac{[J^{-1}]_{i,j,k}}{8} \left( \left[ \bar{u}_i \right]_{i+1,j,k} - \left[ \bar{u}_i \right]_{i-1,j,k} \right) \left( \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i-1/2,j,k} + \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i+1/2,j,k} \right)
\]

\[
+ \left( \left[ \bar{u}_i \right]_{i+1,j,k} - \left[ \bar{u}_i \right]_{i-1,j,k} \right) \left( \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i-1/2,j,k} + \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i+1/2,j,k} \right)
\]

\[
+ \left( \left[ \bar{u}_i \right]_{i+1,j,k} - \left[ \bar{u}_i \right]_{i-1,j,k} \right) \left( \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i-1/2,j,k} + \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i+1/2,j,k} \right)
\]

\[
+ \left( \left[ \bar{u}_i \right]_{i+1,j,k} - \left[ \bar{u}_i \right]_{i-1,j,k} \right) \left( \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i-1/2,j,k} + \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i+1/2,j,k} \right)
\]

\[
+ \left( \left[ \bar{u}_i \right]_{i+1,j,k} - \left[ \bar{u}_i \right]_{i-1,j,k} \right) \left( \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i-1/2,j,k} + \left[ J \frac{\partial \xi_m}{\partial x_i} \right]_{i+1/2,j,k} \right)
\]

(E.38)

Filters

The grid-scale filter is implemented on a variable, e.g., \( \phi \), as:

\[
[\tilde{\phi}]_{i,j,k} = \frac{1}{8} \left( [\tilde{\phi}]_{i+1/4,j+1/4,k+1/4} + [\tilde{\phi}]_{i-1/4,j+1/4,k+1/4}
\]

\[
+ [\tilde{\phi}]_{i+1/4,j-1/4,k+1/4} + [\tilde{\phi}]_{i-1/4,j-1/4,k+1/4}
\]

\[
+ [\tilde{\phi}]_{i+1/4,j+1/4,k-1/4} + [\tilde{\phi}]_{i-1/4,j+1/4,k-1/4}
\]

\[
+ [\tilde{\phi}]_{i+1/4,j-1/4,k-1/4} + [\tilde{\phi}]_{i-1/4,j-1/4,k-1/4}
\]

(E.39)
but this can be rewritten so it uses fewer operations:

\[
[\bar{\phi}]_{i,j,k} = \left(\frac{1}{4} ([\bar{\phi}]_{i+1,j,k} + 2[\bar{\phi}]_{i,j,k} + [\bar{\phi}]_{i-1,j,k})
\right) \quad (E.40)
\]

\[
[\bar{\phi}]_{i,j,k}^* = \frac{1}{4} ([\bar{\phi}]_{i+1,j,1,k} + 2[\bar{\phi}]_{i,j,k}^* + [\bar{\phi}]_{i,j,k-1}^*) \quad (E.41)
\]

\[
\tilde{[\bar{\phi}]}_{i,j,k} = \frac{1}{4} ([\bar{\phi}]_{i,j,k+1}^* + 2[\bar{\phi}]_{i,j,k}^* + [\bar{\phi}]_{i,j,k-1}^*). \quad (E.42)
\]

The test-scale filter is implemented as:

\[
[\tilde{\bar{\phi}}]_{i,j,k} = \frac{1}{8} \left( ([\bar{\phi}]_{i+1/2,j+1/2,k+1/2} + [\bar{\phi}]_{i-1/2,j+1/2,k+1/2}
\right)
\]
\[
+ [\bar{\phi}]_{i+1/2,j-1/2,k+1/2} + [\bar{\phi}]_{i-1/2,j-1/2,k+1/2}
\]
\[
+ [\bar{\phi}]_{i+1/2,j+1/2,k-1/2} + [\bar{\phi}]_{i-1/2,j+1/2,k-1/2}
\]
\[
+ [\bar{\phi}]_{i+1/2,j-1/2,k-1/2} + [\bar{\phi}]_{i-1/2,j-1/2,k-1/2}
\right) \quad (E.43)
\]
which is similarly rewritten as:

\[
[\tilde{\bar{\phi}}]_{i,j,k} = \frac{1}{8} \left( ([\bar{\phi}]_{i+1,1,k} + 6[\bar{\phi}]_{i,j,k} + [\bar{\phi}]_{i-1,1,k})
\right) \quad (E.44)
\]

\[
[\tilde{\bar{\phi}}]_{i,j,k}^* = \frac{1}{8} \left( ([\bar{\phi}]_{i+1,1,k}^* + 6[\bar{\phi}]_{i,j,k}^* + [\bar{\phi}]_{i-1,1,k}^*)
\right) \quad (E.45)
\]

\[
\tilde{[\bar{\phi}]}_{i,j,k} = \frac{1}{8} \left( ([\bar{\phi}]_{i,j,k+1}^* + 6[\bar{\phi}]_{i,j,k}^* + [\bar{\phi}]_{i,j,k-1}^*)
\right). \quad (E.46)
\]

Along the wall, the filters should not be dependent on points outside of the domain, so they are rewritten using the expressions of Vasilyev et al. [8], i.e.,

\[
[\bar{\phi}]_{i,1,k}^* = \frac{1}{4} \left( (5[\bar{\phi}]_{i,1,k}^* - 2[\bar{\phi}]_{i,2,k}^* + [\bar{\phi}]_{i,3,k}^*)
\right) \quad (E.47)
\]

\[
[\bar{\phi}]_{i,1,k}^* = \frac{1}{8} \left( (9[\bar{\phi}]_{i,j+1,k}^* - 2[\bar{\phi}]_{i,j,k}^* + [\bar{\phi}]_{i,j-1,k}^*)
\right). \quad (E.48)
\]

**Boundary conditions**

For boundary conditions, we assume that the turbulent eddy viscosity and eddy diffusivity tends to zero at all boundaries (except periodic boundaries): e.g., to specify the eddy viscosity at the wall to be zero, the viscosity for the ghost cell
just outside the domain is the inverse of the eddy viscosity of the cell just inside the domain:

\[ [\nu_T]_{i,0,k} = -[\nu_T]_{i,1,k}. \]  

(E.49)

For the linear-extrapolation used on \( \bar{u}_i, \bar{C}, \) etc., linear extrapolation from two cells within the domain are used: e.g. along the wall, for a variable \( s, \)

\[ [s]_{i,0,k} = 2[s]_{i,1,k} - [s]_{i,2,k}. \]  

(E.50)

**E.3.2 SSC rhs**

The scalar transport equation:

\[
\left( I - \frac{\Delta t}{2J-1} F_I \right) \left( [\bar{C}]^{n+1} - [\bar{C}]^n \right) = \frac{\Delta t}{J-1} \left\{ \frac{3}{2}[E^n + F_E(\bar{u}_i) + \bar{S}_C^n] - \frac{1}{2}[E + F_E + \bar{S}_C]^{n-1} + [F_I]^n \right\} 
\]  

(E.51)

where

\[
E_C = -\frac{\delta}{\delta \xi_m} \left( \bar{U}_m \bar{C} - J \frac{\delta \xi_m}{\delta x_2} w_s \bar{C} \right) 
\]  

(E.52)

\[
F_I = \frac{\delta}{\delta \xi_m} \left( (\kappa + \kappa_T) G_{mn} \frac{\delta}{\delta \xi_n} \right), m = n 
\]  

(E.53)

\[
F_E = \frac{\delta}{\delta \xi_m} \left( (\kappa + \kappa_T) G_{mn} \frac{\delta}{\delta \xi_n} \right), m \neq n 
\]  

(E.54)

is solved for in two steps: the first is to compute the right-hand side. Second-order differencing is applied for all terms except for \( E_C, \) which requires the use of the interpolation method SHARP.

**SHARP**

A simple high accuracy resolution program (SHARP), which was first introduced by Leonard [9], is used to discretize the convective term, \( E. \) It is similar to the sharp monotonic algorithm for realistic transport (SMART) of Gaskell and Lau [10].
In order to describe it simply, we introduce locally normalized variables, whereby the concentration $\bar{C}$ can be normalized with respect to its upstream and downstream values:

$$\bar{C} = \frac{C - C_U}{C_D - C_U} \quad \text{(E.55)}$$

By interpolating based on a downstream ($C_D$), central ($C_C$), and upstream value ($C_U$), a normalized equation for interpolation can be made based only on the central value.

In one-dimension, a computationally efficient approximation of the SHARP algorithm is written as:

$$\bar{C}_f = \begin{cases} 
\frac{1}{8} & \bar{C}_C < -1 \\
\frac{1}{2} + \frac{3}{8} \bar{C}_C & -1 < \bar{C}_C < 0 \\
\frac{1}{2} - \frac{5}{8} \sqrt{\bar{C}_C} & 0 < \bar{C}_C < \frac{1}{4} \\
\frac{1}{4} (1 - \bar{C}_C) & \frac{1}{4} < \bar{C}_C < 1 \\
-\frac{1}{4} (1 - \bar{C}_C) & 1 < \bar{C}_C < \frac{3}{2} \\
\frac{1}{8} & \frac{3}{2} < \bar{C}_C 
\end{cases} \quad \text{(E.56)}$$

### E.3.3 Predictor

The momentum equation is solved using a predictor-corrector method. The predictor step (Algorithm 3):

$$\frac{J}{\Delta t} \left( I - \frac{\Delta t}{2J} D_I \right) ([\bar{u}_i^P]^* - [\bar{u}_i^P]^n) = \frac{3}{2} [H]^n - \frac{1}{2} [H]^{n-1} + \frac{1}{2} D_I [\bar{u}_i^I]^{n+1} \quad \text{(E.57)}$$

can be evaluated much more efficiently than in its present form by applying an approximate factorization. The diagonal viscous terms are dimensionally split:

$$D_k = \frac{\delta}{\delta \xi_k} \left( \nu + \nu_T \right) G^{kk} \frac{\delta}{\delta \xi_k} \frac{\delta}{\delta \xi_k} \right]. \quad \text{(E.58)}$$
A second-order approximation can then be derived:

\[(I - \frac{\Delta t}{2J} D_1) \approx (I - \frac{\Delta t}{2J} D_1)(I - \frac{\Delta t}{2J} D_2)(I - \frac{\Delta t}{2J} D_3) + O(\Delta t^2) \quad (E.59)\]

compute convective terms;
add in LES self-similarity terms;
compute cross-viscous terms;
add source terms;
compute diagonal-viscous terms;
solve tridiagonal equation for \(i\)-direction;
solve tridiagonal equation for \(j\)-direction;
solve tridiagonal equation for \(k\)-direction;
update intermediate velocity;
apply intermediate velocity boundary conditions;
exchange intermediate velocity information between processors;

**Algorithm 3:** Predictor step.

The advantage of writing the predictor step this way is that with second-order center differencing being used to discretize \(D_k\), the resulting system of equations is tridiagonal. Then after the rhs of the predictor step is evaluated, these three tridiagonal problems are solved in turn.

**QUICK**

QUICK is used to interpolate the total velocities for the convective term, \(C_i\). It is a third-order method proposed by Leonard [11] that takes into account the upstream direction of flow. As described by Leonard, QUICK can be written as a linear interpolation corrected by a curvature term, but for implementation it is written in the more compact form:

\[
\phi_r = \begin{cases} 
-\frac{1}{8}\phi_L + \frac{3}{4}\phi_C + \frac{3}{8}\phi_R & u_r > 0 \\
-\frac{1}{8}\phi_{FR} + \frac{3}{4}\phi_R + \frac{3}{8}\phi_{CR} & u_r < 0. 
\end{cases} \quad (E.60)
\]

The QUICK routine is needed twice in the time-stepping algorithm: first to compute the convective term \(C_i\), and then later to compute the source terms for
the pressure Poisson equation. The convective term is found by applying center differencing to the QUICK interpolated velocities. If \( m = 1 \):

\[
C_i = \frac{\partial}{\partial \xi_1} \left( U_1 u_i - J \frac{\partial \xi_1}{\partial x_i} u_i^T u_j^T \right). \quad (E.61)
\]

We will solve the second term in the rhs using second-order center differences, e.g.:

\[
\left[ \frac{\partial}{\partial \xi_m} \left( J \frac{\partial \xi_1}{\partial x_i} u_i^T u_j^T \right) \right]_{i,j,k} = \frac{1}{2} \left[ J \frac{\partial \xi_1}{\partial x_i} \right]_{i+1/2,j,k} \left( \left[ u_i^T u_j^T \right]_{i,j,k} + \left[ u_i^T u_j^T \right]_{i+1,j,k} \right)
- \frac{1}{2} \left[ J \frac{\partial \xi_1}{\partial x_i} \right]_{i-1/2,j,k} \left( \left[ u_i^T u_j^T \right]_{i,j,k} + \left[ u_i^T u_j^T \right]_{i-1,j,k} \right)
\]

\( (E.62) \)

This does not contradict the upstream basis for the QUICK method because interpolating the inviscid velocities there should be no preference for the upstream value. The first term is found by:

\[
\left[ \frac{\partial}{\partial \xi_1} (U_1 u_i) \right]_{i,j,k} = [U_1 u_i]_{i+1/2,j,k} - [U_1 u_i]_{i-1/2,j,k}
\]

\( (E.63) \)

\[
= [U_1]_{i+1/2,j,k} [u_i]_{i+1/2,j,k} - [U_1]_{i-1/2,j,k} [u_i]_{i-1/2,j,k}
\]

\( (E.64) \)

where now QUICK can be used to interpolate \( u_i \). Notice that we can rewrite the first term in the rhs as:

\[
[U_1]_{i+1/2,j,k} [u_i]_{i+1/2,j,k} = [U_1]_{i+1/2,j,k} \left( -\frac{1}{8} [u_i]_{i-1,j,k} + \frac{3}{4} [u_i]_{i,j,k} + \frac{3}{8} [u_i]_{i+1,j,k} \right)
\]

\( (E.65) \)

when \([U_1]_{i+1/2,j,k} > 0\), or:

\[
[U_1]_{i+1/2,j,k} [u_i]_{i+1/2,j,k} = [U_1]_{i+1/2,j,k} \left( -\frac{1}{8} [u_i]_{i+2,j,k} + \frac{3}{4} [u_i]_{i+1,j,k} + \frac{3}{8} [u_i]_{i,j,k} \right)
\]

\( (E.66) \)

when \([U_1]_{i+1/2,j,k} < 0\).
Because the variable being interpolated is the velocity itself, then this formula can be written as one equation by first defining unidirectional fluxes:

\[
[f^+_m]_{i+1/2,j,k} = \frac{[\bar{U}_m]_{i+1/2,j,k} + |[\bar{U}_m]_{i+1/2,j,k}|}{2} \quad (E.67)
\]
\[
[f^-_m]_{i+1/2,j,k} = \frac{[\bar{U}_m]_{i+1/2,j,k} - |[\bar{U}_m]_{i+1/2,j,k}|}{2} \quad (E.68)
\]

and

\[
[a^+_m]_{i,j,k} = \frac{1}{2}[U_m]_{i+1/2,j,k} - \frac{1}{8}([f^+_m]_{i+1/2,j,k} - 2[f^-_m]_{i+1/2,j,k} - [f^-_m]_{i-1/2,j,k}) \quad (E.69)
\]
\[
[a^-_m]_{i,j,k} = -\frac{1}{2}[U_m]_{i-1/2,j,k} - \frac{1}{8}([f^-_m]_{i+1/2,j,k} + 2[f^+_m]_{i-1/2,j,k} - [f^-_m]_{i-1/2,j,k}) \quad (E.70)
\]

and then we see that the solution can be given as:

\[
\frac{\partial}{\partial \xi_1} (U_1 u_i)_{i,j,k} = \frac{1}{8}([f^-]_{i+1/2,j,k}[u_i]_{i+2,j,k} - [f^+]_{i+1/2,j,k}[u_i]_{i-2,j,k})
+ [a^+_m]_{i,j,k}[u_i]_{i+1,j,k} + [a^-_m]_{i,j,k}[u_i]_{i-1,j,k}
+ \left( [a^+_m]_{i,j,k} + [a^-_m]_{i,j,k} + \frac{1}{8}([f^-]_{i+1/2,j,k} - [f^+]_{i-1/2,j,k}) \right)
+ [U_m]_{i+1/2,j,k} - [U_m]_{i-1/2,j,k}) [u_i]_{i,j,k}
\quad (E.71)
\]

While complicated, this solution does not depend on any separate cases to be evaluated (which, considering the six sides to a control volume and two flow directions possible, would mean an unwieldy 64 possible cases). This formulation can easily be extended to three-dimensions.
Viscous terms

The diagonal viscous terms can be written as:

\[
D_I = \frac{\delta}{\delta \xi_m} \left[ (\nu + \nu_T) G^{mn} \frac{\delta}{\delta \xi_n} \right], \quad m = n \tag{E.72}
\]

\[
= \frac{\delta}{\delta \xi_n} \left[ (\nu + \nu_T) G^{mn} \frac{\delta}{\delta \xi_n} \right] \tag{E.73}
\]

\[
[D_I]_{i,j,k} \approx \frac{\delta}{\delta \xi_n} \left[ (\nu + \nu_T)(G^{11}[i+1/2,j,k] - G^{11}[i-1/2,j,k] + G^{22}[i,j+1/2,k} - G^{22}[i,j-1/2,k] + G^{33}[i,j,k+1/2] - G^{33}[i,j,k-1/2]) \right] + \frac{1}{2} \left[ (\nu_T)[i,j,k] + [\nu_T][i+1,j,k] \right] \right] G^{11}[i+1/2,j,k] (\|i+1,j,k - \|i,j,k)
\]

\[
+ (\nu + \frac{1}{2} \left[ (\nu_T)[i,j,k] + [\nu_T][i-1,j,k] \right] \right] G^{11}[i-1/2,j,k] (\|i-1,j,k - \|i,j,k)
\]

\[
+ (\nu + \frac{1}{2} \left[ (\nu_T)[i,j,k] + [\nu_T][i+1,j,k] \right] \right] G^{11}[i,j+1/2,k] (\|i+1,j,k - \|i,j,k)
\]

\[
+ (\nu + \frac{1}{2} \left[ (\nu_T)[i,j,k] + [\nu_T][i,j-1,k] \right] \right] G^{11}[i,j-1/2,k] (\|i,j-1,k - \|i,j,k)
\]

\[
+ (\nu + \frac{1}{2} \left[ (\nu_T)[i,j,k] + [\nu_T][i,j,k+1] \right] \right] G^{33}[i,j,k+1/2] (\|i,j,k+1 - \|i,j,k)
\]

\[
+ (\nu + \frac{1}{2} \left[ (\nu_T)[i,j,k] + [\nu_T][i,j,k-1] \right] \right] G^{33}[i,j,k-1/2] (\|i,j,k-1 - \|i,j,k)
\]

and the diagonal diffusive terms can be written analogously.

Likewise, the off-diagonal viscous terms can be written:

\[
D_E = \frac{\delta}{\delta \xi_m} \left[ (\nu + \nu_T) G^{mn} \frac{\delta}{\delta \xi_n} \right], \quad m \neq n \tag{E.76}
\]

\[
[D_E]_{i,j,k} \approx \frac{\delta}{\delta \xi_n} \left[ (\nu + \nu_T)(G^{31}[i+1/2,j,k] - G^{31}[i-1/2,j,k]
\]

\[
+ G^{31}[i+1/2,j,k] - G^{31}[i-1/2,j,k]
\]

\[
+ G^{12}[i,j+1/2,k] - G^{12}[i,j-1/2,k]
\]

\[
+ G^{21}[i,j+1/2,k] - G^{21}[i,j-1/2,k]
\]

\[
+ G^{13}[i,j,k+1/2] - G^{13}[i,j,k-1/2]
\]

\[
+ G^{23}[i,j,k+1/2] - G^{23}[i,j,k-1/2]
\]

\[
\tag{E.77}
\]

\[
\tag{E.78}
\]

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**Tridiagonal solver**

A version of the Thomas algorithm (the pipelined Thomas algorithm [12, 13]) is used to solve the many tridiagonal systems that are found in any timestep.

For a system of equations:

\[
[a]_i [x]_{i-1} + [b]_i [x]_i + [c]_i [x]_{i+1} = [f]_i
\]  
(E.79)

the Thomas algorithm gives a solution using modified variables:

\[
[f']_0 = \frac{[f]_0}{[b]_0}
\]  
(E.80)

\[
[c']_0 = \frac{[c]_0}{[b]_0}
\]  
(E.81)

using a forward substitution:

\[
[b']_k = \frac{1}{([b]_k - [a]_k [c]_{k-1})}
\]  
(E.82)

\[
[c']_k = [c]_k [b']_k
\]  
(E.83)

\[
[f']_k = ([f]_k - [a]_k [f]_{k-1})/([b]_k - [a]_k [c]_{k-1})
\]  
(E.84)

\[
[f']_{m+1} = ([f]_{m+1} - [a]_{m+1} [f]_m)/([b]_{m+1} - [a]_{m+1} [c]_m)
\]  
(E.85)

and back substitution:

\[
[x]_k = [f']_k - [c]_k [x]_{k+1}
\]  
(E.86)

\[
[x]_0 = [f']_0 - [c]_0 [f']_1.
\]  
(E.87)

The Thomas algorithm is on a serial system very efficient and is commonly used in engineering. For highly parallel computers, as considered here, there are more recent advances in tridiagonal solvers which may be faster.

For boundary conditions, notice that the lhs of the tridiagonal system can be
written in discrete form as, e.g., for $k = 1$:

$$
\left( I - \frac{\Delta t}{2J} D_1 \right) = \frac{\partial}{\partial \xi_1} \left( (\nu + \nu_T) G^{11} \frac{\partial}{\partial \xi_1} \right)
$$

$$
= \left( -\left( \nu + \frac{1}{2} \left( [\nu_T]_{j,k} + [\nu_T]_{i+1,j,k} \right) \right) \frac{\Delta t}{2J} [G^{11}]_{i+1/2,j,k} \right) \int_{i+1,j,k}
$$

$$
+ (a) \int_{i,j,k}
$$

$$
+ (a) \int_{i-1,j,k}.
$$

(E.88)

Instead of applying this to the boundary nodes as well, we apply

$$
([u_i^P]^* - [u_i^P]^n) = \frac{2\Delta t}{J} \frac{\partial [\phi]^n}{\partial \xi_m}
$$

(E.89)

(E.90)

notice that while this is a boundary condition, no assumption is needed for any boundary values.

E.3.4 Pressure Poisson equation

The pressure Poisson equation

$$
\frac{\delta}{\delta \xi_m} \left( G^{mn} \frac{\delta [\phi]^{n+1}}{\delta \xi_n} \right) = \frac{1}{\Delta t} \frac{\delta [U_m^P]^*}{\delta \xi_m}.
$$

(E.91)

is solved with a multi-grid alternating direction implicit (MADI) method (Algorithm 4). Three sweeps of the domain are made, one for each dimension of the grid. Before calling the pressure Poisson solver, the grid geometry is known (i.e., $[\bar{u}_i^P]$, $J \frac{\partial \xi_i}{\partial x_j}$), the timestep is known ($\Delta t$), the pressure correction from the previous timestep is known ($[\phi]^n$), and $[\bar{u}_i^P]^*$ has been computed by the predictor step.

The rhs of Eq. E.91 is evaluated by using QUICK to find $[U_m^P]^*$ and then center differencing. The resulting discretized pressure Poisson equation has 19 nonzero
coefficients:
\[
\left[ \frac{\delta}{\delta \xi_m} \left( G_{mn}^{\delta \phi} \right) \right]_{i,j,k} \approx [G^{11}]_{i+1/2,j,k}(\phi)_{i+1,j,k} - [\phi]_{i,j,k} + [G^{11}]_{i-1/2,j,k}(\phi)_{i-1,j,k} - [\phi]_{i,j,k}
\]
\[
+ [G^{11}]_{i-1/2,j,k}(\phi)_{i-1,j,k} - [\phi]_{i,j,k} + [G^{22}]_{i,j+1/2,k}(\phi)_{i,j+1,k} - [\phi]_{i,j,k} + [G^{22}]_{i,j-1/2,k}(\phi)_{i,j-1,k} - [\phi]_{i,j,k} + [G^{33}]_{i,j,k+1/2}(\phi)_{i,j,k+1} - [\phi]_{i,j,k} + [G^{33}]_{i,j,k-1/2}(\phi)_{i,j,k-1} - [\phi]_{i,j,k}
\]
\[
+ [G^{12}]_{i+1/2,j,k}(\phi)_{i+1,j,k} - [\phi]_{i,j-1,k} + [\phi]_{i+1,j+1,k} - [\phi]_{i+1,j-1,k}
\]
\[
- [G^{12}]_{i-1/2,j,k}(\phi)_{i-1,j,k} - [\phi]_{i,j-1,k} + [\phi]_{i-1,j+1,k} - [\phi]_{i-1,j-1,k}
\]
\[
+ [G^{13}]_{i+1/2,j,k}(\phi)_{i,j,k+1} - [\phi]_{i,j,k-1} + [\phi]_{i+1,j,k+1} - [\phi]_{i+1,j,k-1}
\]
\[
- [G^{13}]_{i-1/2,j,k}(\phi)_{i,j,k-1} - [\phi]_{i,j,k-1} + [\phi]_{i-1,j,k+1} - [\phi]_{i-1,j,k-1}
\]
\[
+ [G^{23}]_{i,j+1/2,k}(\phi)_{i,j,k+1} - [\phi]_{i,j,k-1} + [\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}
\]
\[
- [G^{23}]_{i,j-1/2,k}(\phi)_{i,j,k-1} - [\phi]_{i,j,k-1} + [\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}
\]
\[
+ [G^{21}]_{i,j+1/2,k}(\phi)_{i,j,k} - [\phi]_{i,j,k} + [\phi]_{i+1,j,k} - [\phi]_{i-1,j,k}
\]
\[
- [G^{21}]_{i,j-1/2,k}(\phi)_{i,j,k} - [\phi]_{i,j,k} + [\phi]_{i+1,j,k} - [\phi]_{i-1,j,k}
\]
\[
+ [G^{31}]_{i,j,k+1/2}(\phi)_{i+1,j,k} - [\phi]_{i-1,j,k} + [\phi]_{i+1,j,k+1} - [\phi]_{i-1,j,k+1}
\]
\[
- [G^{31}]_{i,j,k-1/2}(\phi)_{i-1,j,k} + [\phi]_{i+1,j,k} - [\phi]_{i-1,j,k} - [\phi]_{i-1,j,k-1}
\]
\[
+ [G^{32}]_{i,j,k+1/2}(\phi)_{i,j,k+1} - [\phi]_{i,j,k} + [\phi]_{i,j,k+1} - [\phi]_{i,j,k+1}
\]
\[
- [G^{32}]_{i,j,k-1/2}(\phi)_{i,j,k-1} - [\phi]_{i,j,k} + [\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}
\]

(E.92)

The primary boundary condition applied here is one of no-flux. From the corrector step, we can see that:

\[
[U_m^P]^* = \Delta t \left( G_{mn}^{\delta \phi} \phi^n + O(\Delta t^2) \right)
\]

(E.93)

which was derived by Kim and Moin [14], following the method of LeVeque and Oliger [15].
Input: $[\phi]^n, G^{mn}, \Delta t, [\bar{u}_i]^*, J \frac{\partial \xi_i}{\partial x_j}$
Output: $[\phi]^{n+1}$
Compute source terms with QUICK
Apply BC for source terms
Call smooth
for $n=1$ to maxstep do
  if $mg\text{ level bigger than }1$ then
    Call thrd_f2c
    (restriction operator) Call smooth
    (smoothing) if $mg\text{ level bigger than }2$ then
      Call thrd_f2c
      Call smooth
    if $mg\text{ level bigger than }3$ then
      Call thrd_f2c
      Call smooth
    if $mg\text{ level bigger than }4$ then
      Call thrd_f2c
      Call smooth
      Call thrd_c2f
      (interpolation operator) Call smooth
    end
    Call thrd_c2f
    Call smooth
  end
  Call thrd_c2f
  Call smooth
end
end
Algorithm 4: Process to solver pressure Poisson equation.
First QUICK is used to find the intermediate perturbation fluxes, \([U_{m}^{P}]^{*}\), for all cell walls. The values of the fluxes on the exterior cells are imposed using the boundary conditions derived earlier. The source terms are found by applying second-order differencing to the resulting fluxes. For the source terms on the cells outside the domain, quadratic extrapolation based on the velocity field is used.

**Source terms**

The rhs of the pressure Poisson equation is found by using QUICK:

\[
\bar{U}_{m}^{P} = J \frac{\delta \xi_{m}}{\delta x_{i}} \bar{u}_{i}^{P}
\]  

(E.94)

so for e.g., \(m = 1\), and if \([\bar{U}_{1}]^{n} \geq 0\):

\[
[U_{m}^{P}]_{i+1/2,j,k}^{*} = \left[J \frac{\delta \xi_{1}}{\delta x_{1}}\right]_{i,j,k} \left(-\frac{1}{8}[\bar{u}_{1}]_{i-1,j,k} + \frac{3}{4}[\bar{u}_{1}]_{i,j,k} + \frac{3}{8}[\bar{u}_{1}]_{i+1,j,k}\right) \\
+ \left[J \frac{\delta \xi_{1}}{\delta x_{2}}\right]_{i,j,k} \left(-\frac{1}{8}[\bar{u}_{2}]_{i-1,j,k} + \frac{3}{4}[\bar{u}_{2}]_{i,j,k} + \frac{3}{8}[\bar{u}_{2}]_{i+1,j,k}\right) \\
+ \left[J \frac{\delta \xi_{1}}{\delta x_{3}}\right]_{i,j,k} \left(-\frac{1}{8}[\bar{u}_{3}]_{i-1,j,k} + \frac{3}{4}[\bar{u}_{3}]_{i,j,k} + \frac{3}{8}[\bar{u}_{3}]_{i+1,j,k}\right)
\]  

(E.95)

Note that this formula does not follow the true three-dimensional QUICK formula, but instead relies on one-dimensional QUICK in each direction. There are additional, transverse curvature terms as described by Leonard [16] that are left out for computational efficiency.

**Gauss-Siedel smoother**

The pressure Poisson equation is solved by a multigrid method. A V-cycle is used with three smoothing iterations at each level. Multigrid methods were developed by Brandt [17] and used previously in connection to this type of LES by Perng and Street [18].

For the downward pass of the V-cycle, a relaxation is performed, then for every coarser level, a restriction operator (through the subroutine `thrd_f2c`) is
**Input:** Intermediate velocities and solution to pressure equation

**Output:** Velocities for the next timestep

Compute residual

for \( n=1 \) to \( \text{maxiter} \) do

  for \( m=1 \) to \( \text{maxiter} \) do

    Smooth in \( j \) direction
    Smooth in \( k \) direction
    Smooth in \( i \) direction
  end

  Compute residual

  if converges too slowly then
    return
  end

end

**Algorithm 5:** Smooth routine.

applied:

\[
P_{ic,jc,ke} = [P_{if,jf,kf} + P_{if+1,jf+1,kf} + P_{if,jf+1,kf} + P_{if+1,jf+1,kf} + P_{if,jf,kf+1} + P_{if+1,jf+1,kf+1} + P_{if,jf+1,kf+1} + P_{if+1,jf+1,kf+1}].
\]  

(E.96)

After the relaxation is performed at the coarsest level, linear interpolation (through function \( \text{thrd\_c2f} \)) brings the solution back to finer grids:

\[
P_{if,jf,kf} = \frac{1}{16}[9P_{ic,jc} + 3P_{ic+1,jc} + 3P_{ic,jc+1,kf} + P_{ic+1,jc+1,kf}] \quad (E.97)
\]

\[
P_{if+1,jf,kf} = \frac{1}{16}[3P_{ic,jc} + 9P_{ic+1,jc} + P_{ic,jc+1,kf} + 3P_{ic+1,jc+1,kf}] \quad (E.98)
\]

\[
P_{if,jf+1,kf} = \frac{1}{16}[3P_{ic,jc} + P_{ic+1,jc} + 9P_{ic,jc+1,kf} + 3P_{ic+1,jc+1,kf}] \quad (E.99)
\]

\[
P_{if+1,jf+1,kf} = \frac{1}{16}[P_{ic,jc} + 3P_{ic+1,jc} + 3P_{ic,jc+1,kf} + 9P_{ic+1,jc+1,kf}] \quad (E.100)
\]

which requires no special boundary consideration.

The relaxation process is based on a dimensional splitting of the transformed Laplacian:

\[
L = \left[ \frac{\delta}{\delta \xi_m} \left( G^{mn} \frac{\delta}{\delta \xi_n} \right) \right]_{i,j,k}.
\]  

(E.101)
In order to apply the MADI scheme, the Laplace operator is split into five matrices:

\[ L = L_1 + L_2 + L_3 + L_\Sigma + L_R \]  \hspace{1cm} (E.102)

where

\[ L_1 = [G^{11}]_{i+1/2,j,k}([\phi]_{i+1,j,k}) + [G^{11}]_{i-1/2,j,k}([\phi]_{i-1,j,k}) \]

\[ [G^{21}]_{i,j+1/2,k}([\phi]_{i+1,j,k} - [\phi]_{i-1,j,k}) - [G^{21}]_{i,j-1/2,k}([\phi]_{i+1,j,k} - [\phi]_{i-1,j,k}) + [G^{31}]_{i,j,k+1/2}([\phi]_{i+1,j,k} - [\phi]_{i-1,j,k}) - [G^{31}]_{i,j,k-1/2}([\phi]_{i+1,j,k} - [\phi]_{i-1,j,k}) \]  \hspace{1cm} (E.103)

\[ L_2 = [G^{22}]_{i,j+1/2,k}([\phi]_{i,j+1,k}) + [G^{22}]_{i,j-1/2,k}([\phi]_{i,j-1,k}) + [G^{12}]_{i+1/2,j,k}([\phi]_{i,j+1,k} - [\phi]_{i,j-1,k}) - [G^{12}]_{i-1/2,j,k}([\phi]_{i,j+1,k} - [\phi]_{i,j-1,k}) + [G^{32}]_{i,j,k+1/2}([\phi]_{i,j+1,k} - [\phi]_{i,j-1,k}) - [G^{32}]_{i,j,k-1/2}([\phi]_{i,j+1,k} - [\phi]_{i,j-1,k}) \]  \hspace{1cm} (E.104)

\[ L_3 = [G^{33}]_{i,j,k+1/2}([\phi]_{i,j,k+1}) + [G^{33}]_{i,j,k-1/2}([\phi]_{i,j,k-1}) + [G^{13}]_{i+1/2,j,k}([\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}) - [G^{13}]_{i-1/2,j,k}([\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}) + [G^{23}]_{i,j,k+1/2}([\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}) - [G^{23}]_{i,j,k-1/2}([\phi]_{i,j,k+1} - [\phi]_{i,j,k-1}) \]  \hspace{1cm} (E.105)
The relaxation process is done by solving three tridiagonal systems:

\[
L_\Sigma = [G^{11}]_{i+1/2,j,k}(-[\phi]_{i,j,k}) + [G^{11}]_{i-1/2,j,k}(-[\phi]_{i,j,k}) + [G^{22}]_{i,j+1/2,k}(-[\phi]_{i,j,k}) + [G^{22}]_{i,j-1/2,k}(-[\phi]_{i,j,k}) + [G^{33}]_{i,j,k+1/2}(-[\phi]_{i,j,k}) + [G^{33}]_{i,j,k+1/2}(-[\phi]_{i,j,k}) \tag{E.106}
\]

\[
L_R = [G^{12}]_{i+1/2,j,k}([\phi]_{i+1,j+1,k} - [\phi]_{i+1,j-1,k}) - [G^{12}]_{i-1/2,j,k}([\phi]_{i-1,j+1,k} - [\phi]_{i-1,j-1,k}) + [G^{13}]_{i+1/2,j,k}([\phi]_{i+1,j,k+1} - [\phi]_{i+1,j,k-1}) - [G^{13}]_{i-1/2,j,k}([\phi]_{i-1,j,k+1} - [\phi]_{i-1,j,k-1}) + [G^{23}]_{i,j+1/2,k}([\phi]_{i,j+1,k+1} - [\phi]_{i,j+1,k-1}) - [G^{23}]_{i,j-1/2,k}([\phi]_{i,j-1,k+1} - [\phi]_{i,j-1,k-1}) + [G^{21}]_{i,j+1/2,k}([\phi]_{i+1,j+1,k} - [\phi]_{i-1,j+1,k}) - [G^{21}]_{i,j-1/2,k}([\phi]_{i+1,j-1,k} - [\phi]_{i-1,j-1,k}) + [G^{31}]_{i,j,k+1/2}([\phi]_{i+1,j,k+1} - [\phi]_{i-1,j,k+1}) - [G^{31}]_{i,j,k-1/2}([\phi]_{i+1,j,k-1} - [\phi]_{i-1,j,k-1}) + [G^{32}]_{i,j,k+1/2}([\phi]_{i,j+1,k+1} - [\phi]_{i,j-1,k+1}) - [G^{32}]_{i,j,k-1/2}([\phi]_{i,j+1,k-1} - [\phi]_{i,j-1,k-1}) \tag{E.112}
\]

The relaxation process is done by solving three tridiagonal systems:

\[
L_1p^r = (L - L_1)p^{r-1} + \frac{1}{\Delta t} \frac{\partial[U_{i,m}^{p*}]}{\partial \xi_m} \tag{E.113}
\]

\[
L_2p^r = (L - L_2)p^{r-1} + \frac{1}{\Delta t} \frac{\partial[U_{i,m}^{p*}]}{\partial \xi_m} \tag{E.114}
\]

\[
L_3p^r = (L - L_3)p^{r-1} + \frac{1}{\Delta t} \frac{\partial[U_{i,m}^{p*}]}{\partial \xi_m}. \tag{E.115}
\]
This relaxation procedure is iterated a number of times, $N_{\text{iter-chk}}$, after which the residual is computed. If the solution has converged then the procedure moves to the next level; if not, it repeats a maximum number of $N_{\text{iter-max}}$ times. After completing the V-cycle, if the solution has not converged, another V-cycle is completed.

This technique might be improved in the future with simultaneous over-relaxation (SOR), but experience has shown that the multigrid method converges in so few iterations most of the time that accelerating it is not necessary.

**Residual**

The coefficients of the stencil for the pressure Poisson equation are given by:

$$
\left[ \frac{\delta}{\delta \xi_m} \left( \frac{\delta}{\delta \xi_n} \right) \right]_{i,j,k} \approx \frac{\delta}{\delta \xi_m} \left( G^{m1} \right)_i^{i+1/2,j,k} - \left( G^{m1} \right)_i^{i-1/2,j,k} \\
+ G^{m2} \left( i,j+1/2,k \right) - G^{m2} \left( i,j-1/2,k \right) \\
+ G^{m3} \left( i,j,k+1/2 \right) - G^{m3} \left( i,j,k-1/2 \right) 
$$

(E.116)
which can be expanded:

\[
\left[ \frac{\delta}{\delta \xi_m} \left( G_{mn}^{\xi} \frac{\delta}{\delta \xi_n} \right) \right]_{i,j,k} \approx [G^{11}]_{i+1/2,j,k} \left( [i+1,j,k] - [i,j,k] \right)
- [G^{11}]_{i-1/2,j,k} \left( [i,j,k] - [i-1,j,k] \right)
+ [G^{21}]_{i,j+1/2,k} \left( [i+1/2,j+1/2,k] - [i-1/2,j+1/2,k] \right)
- [G^{21}]_{i,j-1/2,k} \left( [i+1/2,j-1/2,k] - [i-1/2,j-1/2,k] \right)
+ [G^{31}]_{i,j,k+1/2} \left( [i+1/2,j,k+1/2] - [i-1/2,j,k+1/2] \right)
- [G^{31}]_{i,j,k-1/2} \left( [i+1/2,j,k-1/2] - [i-1/2,j,k-1/2] \right)
+ [G^{12}]_{i+1/2,j,k} \left( [i+1/2,j,k] - [i+1/2,j,k] \right)
- [G^{12}]_{i-1/2,j,k} \left( [i-1/2,j,k] - [i-1/2,j,k] \right)
+ [G^{22}]_{i,j+1/2,k} \left( [i,j+1,k] - [i,j,k] \right)
- [G^{22}]_{i,j-1/2,k} \left( [i,j,k] - [i,j-1,k] \right)
+ [G^{32}]_{i,j,k+1/2} \left( [i,j+1/2,k+1/2] - [i,j-1/2,k+1/2] \right)
- [G^{32}]_{i,j,k-1/2} \left( [i,j+1/2,k-1/2] - [i,j-1/2,k-1/2] \right)
+ [G^{13}]_{i+1/2,j,k} \left( [i+1/2,j,k] - [i+1/2,j,k] \right)
- [G^{13}]_{i-1/2,j,k} \left( [i-1/2,j,k] - [i-1/2,j,k] \right)
+ [G^{23}]_{i,j+1/2,k} \left( [i,j+1/2,k] - [i,j,k+1/2] \right)
- [G^{23}]_{i,j-1/2,k} \left( [i,j,k] - [i,j,k] \right)
+ [G^{33}]_{i,j,k+1/2} \left( [i,j,k+1] - [i,j,k] \right)
- [G^{33}]_{i,j,k-1/2} \left( [i,j,k] - [i,j,k] \right)
\]

(E.117)

Convergence

E.3.5 Corrector

The corrector step for integrating the momentum equation is

\[
[u_i^{n+1}]_{i,j,k} = [u_i^n]_{i,j,k} - \frac{J \Delta t}{2} \left( J^{-1} \frac{\delta \xi_m}{\delta x_i} \frac{\delta \phi}{\delta \xi_m} \right). \tag{E.118}
\]
e.g., for $i = 1$:

$$
[\bar{u}_1^P]_{i,j,k}^{n+1} = [\bar{u}_1^P]_{i,j,k}^* - \frac{J \Delta t}{2} \left( J^{-1} \frac{\delta \xi_m}{\delta x_1} \frac{\delta [\phi]^n}{\delta \xi_m} \right) 
\quad \text{(E.119)}
$$

$$
= [\bar{u}_1^P]_{i,j,k}^* - \frac{[J]_{i,j,k}\Delta t}{2} \left( J^{-1} \frac{\delta \xi_m}{\delta x_1} \right)_{i+1/2,j,k} \left( [\phi]_{i,j,k} + [\phi]_{i+1,j,k} \right)
\quad \text{(E.120)}
$$

$$
- \left[ J^{-1} \frac{\delta \xi_m}{\delta x_1} \right]_{i-1/2,j,k} \left( [\phi]_{i-1,j,k} + [\phi]_{i,j,k} \right)
+ \left[ J^{-1} \frac{\delta \xi_m}{\delta x_1} \right]_{i,j+1/2,k} \left( [\phi]_{i,j,k} + [\phi]_{i,j,k+1} \right)
- \left[ J^{-1} \frac{\delta \xi_m}{\delta x_1} \right]_{i,j-1/2,k} \left( [\phi]_{i,j-1,k} + [\phi]_{i,j,k} \right)
+ \left[ J^{-1} \frac{\delta \xi_m}{\delta x_1} \right]_{i,j,k+1/2} \left( [\phi]_{i,j,k} + [\phi]_{i,j,k+1} \right)
- \left[ J^{-1} \frac{\delta \xi_m}{\delta x_1} \right]_{i,j,k-1/2} \left( [\phi]_{i,j,k-1} + [\phi]_{i,j,k} \right)
$$

In all cases considered here, the bottom boundary condition is a no-flux condition with a shear stress applied depending on the flow conditions, i.e.,

$$
\tau_w = \rho u^2/\nu \quad \text{(E.121)}
$$

where $\tau_w$ is the wall shear stress and $n$ is the normal direction to the wall. This is numerically implemented through ghost cells outside of the domain. Combining this with the condition that the eddy viscosity is zero along the bed, we can implement the boundary condition through the viscous stress terms:

$$
\left[ \frac{\partial u}{\partial n} \right]_{y=0} = \frac{1}{\nu} u_*^2. \quad \text{(E.122)}
$$

where $u_*$ is the friction velocity, which is related to the wall shear stress ($\tau_w = \rho u_*^2$).

Then the fluxes are corrected:

$$
[\bar{V}_m^P]^{n+1}_{i,j,k} = [\bar{V}_m^P]_{i,j,k}^* - (\Delta t) G_{mn} \delta [\phi]^{n+1}_{\xi_n} \quad \text{(E.123)}
$$
e.g., for \( m = 1 \):

\[
[\bar{U}^P]^n_{i+1/2,j,k} = [\bar{U}^P]_i^{n+1}_{i+1/2,j,k} - (\Delta t)G^1\delta[\phi]_{i,j,k}^{n+1}/\delta\xi
\]

\[
= [\bar{U}^P]_i^{n+1}_{i+1/2,j,k} - (\Delta t)\left([G^{11}]_{i+1/2,j,k}([\phi]_{i+1,j,k}^{n+1} - [\phi]_{i,j,k}^{n+1})
+ [G^{12}]_{i+1/2,j,k}([\phi]_{i,j,k+1}^{n+1} - [\phi]_{i,j,k}^{n+1} + [\phi]_{i,j,k+1}^{n+1} - [\phi]_{i,j,k+1}^{n+1})
+ [G^{13}]_{i+1/2,j,k}([\phi]_{i,j+1,k}^{n+1} - [\phi]_{i,j,k}^{n+1} + [\phi]_{i,j+1,k}^{n+1} - [\phi]_{i,j+1,k}^{n+1} - [\phi]_{i,j+1,k}^{n+1})\right)
\]

(E.124)

\[
= [\bar{C}]_{i,j,k}^{n+1} - [\bar{C}]_{i,j,k}^{n} = \Delta tJ^{-1}\{3/2[E^n + FE(\bar{u}_i) + SC^n] - 1/2[E + FE + SC^{n-1} + F_l^n]\}
\]

(E.125)

### E.3.6 SSC solver

Finally, the scalar transport equation is split similarly to the predictor:

\[
\left(I - \frac{\Delta t}{2J^{-1}}F_1\right)\left(I - \frac{\Delta t}{2J^{-1}}F_2\right)\left(I - \frac{\Delta t}{2J^{-1}}F_3\right)\left([\bar{C}]^{n+1} - [\bar{C}]^n\right) = \frac{\Delta t}{J^{-1}}\{3/2[E^n + FE(\bar{u}_i) + SC^n] - 1/2[E + FE + SC^{n-1} + F_l^n]\}
\]

where

\[
F_k = \frac{\delta}{\delta\xi_k} \left[(\kappa + \kappa_T)G^{kk}\delta\xi_k\right].
\]

(E.127)

The resulting equation is solved in each direction with the pipelined Thomas algorithm, as before.

After the SSC solver has finished, the CFL number is checked to make sure the simulation is not becoming unstable and the time is advanced by one timestep.

**List of References**


BIBLIOGRAPHY


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