Extension of NHWAVE to Couple LAMMPS for Modeling Wave Interactions with Arctic Ice Floes

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LONG-TERM GOALS

1. Developing and testing a tightly-coupled wave-ice model system, including a nonhydrostatic wave model (NHWAVE, Ma et al., 2012) and a discrete element model (LAMMPS; Plimpton, 1995), for simulating wave interactions with arctic ice floes.
2. Using the coupled NHWAVE and LAMMPS models to investigate the relative importance of key physical processes governing the attenuation of wave energy in the marginal ice zone (MIZ).
3. Conducting comparative simulations to evaluate MIZ dissipation parameterizations used by larger-scale ice-ocean models.

OBJECTIVES

The study is a collaborative effort with Mark Orzech, Jay Veeramony and Joe Calantoni of the Naval Research Laboratory (separate internal NRL project, funded for FY14-16). The objectives of this study are to

1. extend NHWAVE to incorporate wave interactions with moving obstacles.
2. collaborate with the NRL LAMMPS group to develop matching boundary conditions for both NHWAVE and LAMMPS in a two-way coupling system.
3. collaborate with the NRL LAMPPS group to conduct a numerical study on determining the relative importance of key physical processes governing the attenuation of wave energy in the MIZ.

APPROACH

We have been developing additional capabilities in NHWAVE so that it can be tightly coupled to LAMMPS for use in modeling wave interactions with ice floes. This effort entails completion of the following approaches:

1. Implementation of 3D moving masks to represent ice floes in the computational image domain. A generalized vertical coordinate transformation is needed to make curvilinear coordinates fitting the ice floe boundaries.
2. Development of matching boundary conditions for coupling with LAMMPS. Both the kinematic and dynamic boundary conditions are developed. Specifically the kinematic boundary conditions are applied using the numerical fluxes defined at the fluid-ice interface. The dynamic boundary conditions include the pressure gradient boundary condition at the moving object boundaries, the wave-ice shear stress, and the form drag force proposed by Lu et al. (2011). The immersed boundary (IB, e.g., Udaykumar et al., 1999) method is applied at the fluid-ice interface for drag forces.
3. Enhancement of modularized NHWAVE to facilitate coupling interface development. The model architecture of NHWAVE is modified using object-oriented modularization techniques. To improve the model efficiency for modeling in an O(10km) scale domain, the Poisson pressure solver is enhanced using the Pressure Decimation and Interpolation Method.
4. Coordination with the LAMMPS model group in NRL to test coupled models. The work is a collaborative effort with the NRL group, who will focus on the mechanisms of wave-ice floe interaction using the coupled model and try to gain a better understanding of the relative importance of the major wave attenuation processes in the MIZ. We are focused on the development and testing of the coupled model and will assist the NRL group to carry out the process-based study.

WORK COMPLETED

1. NHWAVE has been extended to a generalized vertical coordinate system by using a generalized sigma-coordinate transformation. This extension allows the model to apply the natural kinematic boundary conditions at the bottom and top surfaces of the ice floe. The generalized vertical coordinate is not limited to analytical expressions of the traditional sigma-coordinate used in most ocean models. It is flexible and can fit complex top and bottom surfaces of ice floes. Figure 1 shows the generalized coordinate transformation, where k_t and k_b represent sigma levels at the top and bottom of an object, respectively. The wetting and drying algorithm is applied to represent the overtopping processes. The existing 2D mask in NHWAVE is extended to 3D, which can easily handle the movement and rotation of obstacles with the inclusion of mass conservation.

2. Formulations are implemented to compute kinematic and dynamic boundary conditions. Since the time-dependent boundary-fitted coordinate is applied at the top and bottom surfaces of an object, the kinematic boundary condition is naturally satisfied in the vertical direction at the fluid-object interfaces. In the horizontal directions, the numerical flux at the interface of fluid and object is calculated based on the conservative form of advection terms with limiters used in the TVD scheme. For the dynamic boundary conditions, pressure gradients are calculated using accelerations of the object at the fluid-object interface.

3. NHWAVE is modularized to make it easy to further develop an interface for a model coupling framework in a parallel computing environment without adopting additional coupling tool kits such as MCT or ESMF. Recent studies using Poisson solver-based non-hydrostatic models have shown that an accurate prediction of wave dispersion does not require a large number of

vertical layers if the dynamic pressure is properly discretized. We explored the possibility that the solution for the dynamic pressure field may, in general, be decimated to a resolution far coarser than used in representing velocities and other transported quantities, without sacrificing accuracy of solutions. We determine the dynamic pressure field by solving the Poisson equation on a coarser grid and then interpolate the pressure field onto the finer grid used for solving the remaining dynamic variables. With the Pressure Decimation and Interpolation (PDI, Shi et al., 2014) method, computational efficiency is greatly improved.

RESULTS

With the new components implemented in NHWAVE, the model is able to simulate the interaction between surface waves/currents and prescribed 3D moving objects. To validate the new model, we conducted a laboratory experiment of waves generated by a bouncing ball at NRL, Stennis Space Center, in July and August, 2014. A solid ball (bowling ball) with a diameter of 25.0 cm was forced to bounce at the water surface in a 2.0 m deep cylindrical tank with a 3.3 m diameter. The Reigl VZ1000 Lidar was used to capture the wave surface as well as the ball location. The labortary experiment setup is demonstrated in Figure 2.

NHWAVE was set up following the experiment configuration. Figure 3 shows the modeled surface elevations at different times (left panels) and model/data comparisons (right panels). The time series of the ball centroid is described in the top-right panel of the figure, which is obtained based on snapshots of the ball motion captured by the Lidar. Time series of water surface at r = 0.45, 0.65, 0.85 and 1.05 m, where r is the distance from the center of the domain, are shown in the rest of the right panels. The data points (crosses) are sparse due to the low scan frequency of the Lidar and are fitted by the dashed lines to better demonstrate the surface wave process at certain locations. The solid lines represent modeled surface elevations at the corresponding locations. The model/data comparison shows that the model is accurate in predicting waves generated by a prescribed moving object at the water surface, indicating its capability to model wave-surface object interactions when provided with realistic object motions by the coupled discrete element model.

As mentioned earlier, the coupling of NHWAVE and LAMMPS is a collaborative effort with the NRL group. The PI Fengyan Shi has been working closely with the NRL group since his 10-week summer visit to NRL at Stennis Space Center in June-August, 2014.

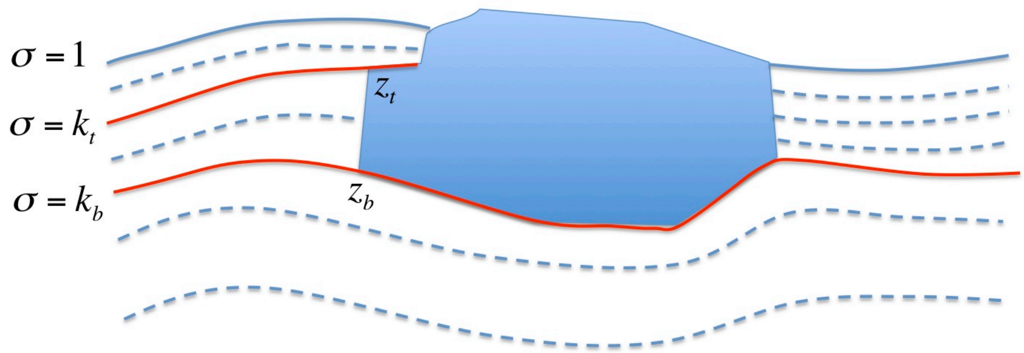

Figure 1. Flexible sigma-coordinate for modeling wave-ice floe interaction. k_t and k_b represent sigma levels and z_t and z_b represent z values of vertical coordinate at the top and bottom of an object, respectively.

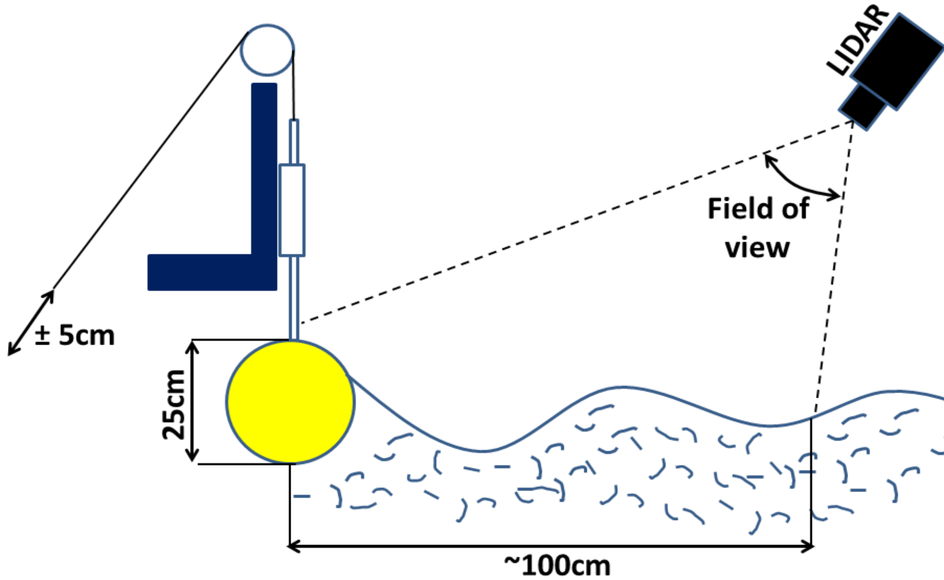

Figure 2. Lab experiment setup. A solid ball (bowling ball, yellow) with a diameter of 25.0 cm was forced to bounce at the water surface in a 2.0 m deep cylindrical tank with a 3.3 m diameter. The Reigl VZ1000 Lidar was used to capture the wave surface as well as the ball location.

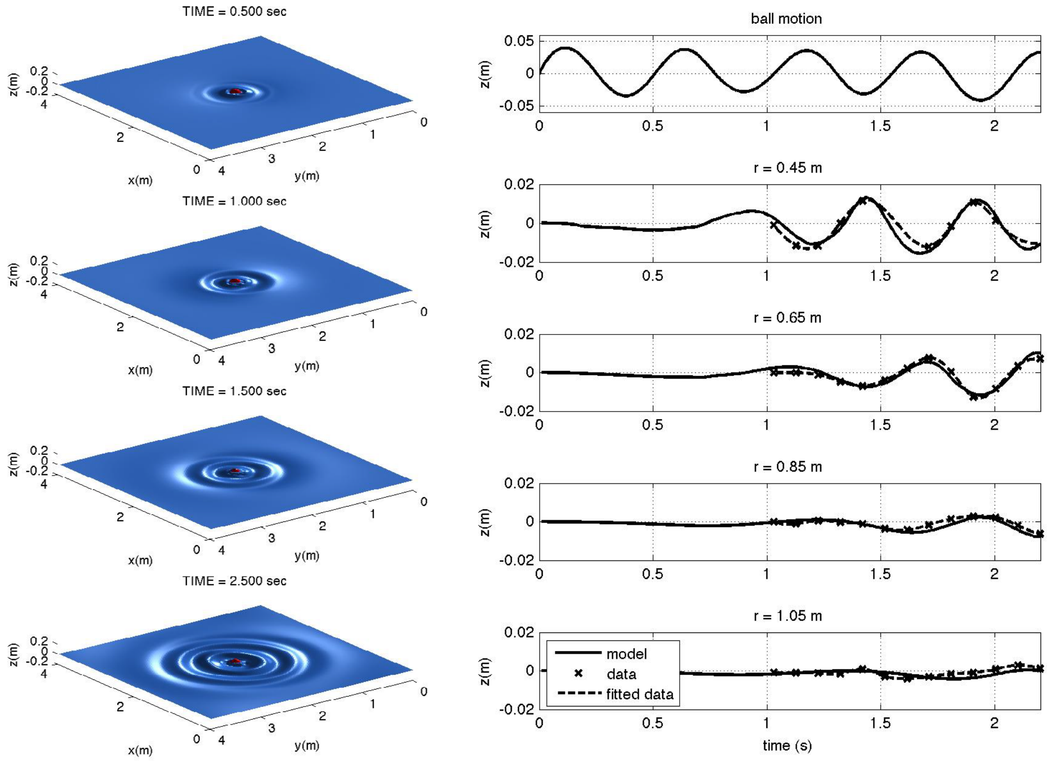

Figure 3. Model results of the bouncing-ball experiment conducted at NRL, Stennis Space Center. (Left) Snapshots of wave surface modeled by NHWAVE at time=0.5,1.0,1.5 and 2.5sec. (Right) comparison of surface elevation between model and data (crosses: data, dashed lines: data fitted lines, solid lines: model results).

IMPACT/APPLICATIONS

Further development of NHWAVE is also supported by the ONR Littoral Geosciences and Optics Program, RIVET II project (N00014-13-1-0188; PIs: Hsu, Shi and Kirby), a NSF project (OCE-1334325; PIs: Kirby, Hsu, Shi and Ma), and a NSF project (OCE-1435147, PIs: Kirby and Shi). The modularization of NHWAVE developed in the current project provides an important approach to enhancing the model efficiency for large-scale simulations.

RELATED PROJECTS

1. ONR RIVET II project. One of the main objectives is enhancement of NHWAVE with a high computational efficiency in order to carry out system-scale simulation with high resolution in the river plume nearfield. The Adaptive Mesh Refinement (AMR) scheme is developed and can be used in the current project.
2. NSF project (*OCE-1334325; Collaborative Research: The interaction of waves, tidal currents and river outflows and their effects on the delivery and resuspension of sediments in the near field; collaborate with Dr. Gangfang Ma of ODU*). The ongoing project is to study broader issues of wave-current interaction and sediment delivery in the nearfield of tidally-pulsed river plumes. NHWAVE is being extended to include more model components and boundary

conditions such as the wave-current aborbing-generating condition which can be used in modeling wave-ice floe interaction under strong current conditions.

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