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A 3D parallel Particle-In-Cell solver for wave interaction with vertical cylinders

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ABSTRACT

In this paper, the Particle-In-Cell (PIC) based PICIN solver is extended to three spatial dimensions and parallelised using the Message Passing Interface (MPI) approach. The PICIN solver employs both Eulerian grid and Lagrangian particles to solve the incompressible Navier-Stokes equations for free-surface flows. The particles are employed to carry all the fluid properties, solve the non-linear advection term and track the free-surface, while the grid is used solely for computational efficiency in solving the non-advection terms. Validation of the new 3D model concentrates on test cases involving multiple wave types (including regular waves, focused waves and solitary waves) interacting with vertical cylinders in several spatial configurations. The results are compared with laboratory data and numerical results from state-of-the-art Volume of Fluid (VOF) based Eulerian solvers such as those from the OpenFOAM® suite. It is shown that the 3D parallel PICIN model is able to well simulate highly non-linear water waves, and the interaction of such waves with vertical cylinders, with a CPU efficiency similar to Eulerian solvers. Moreover, the innovative use of particles in PICIN, akin to meshless Lagrangian solvers, gives the model a particular flexibility in handling complex, full 3D, water-wave scenarios involving large free-surface deformations.

1. Introduction

The Particle-In-Cell (PIC) method was first invented at the Los Alamos National Laboratory in 1955 by Harlow (1955) and was further developed there until it became the practical methodology described in Harlow (1964). The PIC method was designed in an attempt to combine the advantages of Eulerian and Lagrangian methods, through a combined use of grid and particles. In particular, the particles are effectively used to solve the transport of fluid properties in a Lagrangian manner, while other non-advection terms are resolved on the underlying grid. In Harlow (1964), the fluid properties such as the mass and momentum are split between particles and grid; the velocity field needs to be transferred back and forth between particles and grid and thus it makes the solver highly dissipative. Following that, further developments of the PIC method can be found in, for example, Brackbill and Ruppel (1986) and Brackbill et al. (1988). In their PIC solver, the particles are assigned with all the fluid properties, and the grid is solely used for computational convenience in solving the governing equations for the velocity change (i.e. acceleration) on the grid, which is then used to increment particle velocity. This reduces the numerical dissipation significantly. The current 3D parallel PICIN solver follows the latter approach.

The PIC method was originally intended for compressible fluid flows and was extended to solve for incompressible flows by Harlow and Welch (1965) (via the Marker-and-Cell method which employs Eulerian advection) and Zhu and Bridson (2005). More recently, the PIC method has been developed by using innovative techniques, enabling the method to successfully model fluid-structure interaction processes in the coastal and offshore environment. Initially, Kelly (2012) developed a PIC-based solver to simulate the propagation and breaking of a solitary wave on an idealized beach. Kelly et al. (2015) then developed the PICIN solver for free-surface flows with fluid-solid interaction using a tailored Distributed Lagrange Multiplier (DLM) method. Chen et al. (2015) applied the PICIN solver to simulate the complex industrial problem of rock dumping through fall-pipes. Chen et al. (2016a) further validated the PICIN solver for 2D coastal flows. Later, Chen et al. (2016b) suggested that the DLM method used in PICIN may require further developments for simulating

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surface-piercing floating structures. They instead modified the PICIN model by incorporating a Cartesian cut cell based two-way strong coupling algorithm for fluid-structure interactions. In their study, the modified PICIN model was demonstrated to be capable of handling violent free-surface flows as well as the interaction of water waves with (surface-piercing) floating structures of arbitrary shapes and degree of freedoms.

In the studies mentioned above, the PICIN model was tested only in two spatial dimensions, showing nevertheless a great potential to be used as a numerical tool over a range of practical engineering applications. Extending PICIN to three spatial dimensions comes with additional requirements for computational resources due to the highly demanding memory storage, as a double grid system (i.e. particle and grid) is employed. To mitigate this problem, this paper chooses to parallelise the 3D PICIN model using the memory distribution based Message Passing Interface (MPI) approach, such that the model can make use of the High Performance Computing Service (HPCS). The major components of the parallelisation of the 3D PICIN model are detailed in this paper.

The validation tests are based on wave interaction with vertical cylindrical structures, which are widely employed in coastal and offshore engineering. Examples include the design of oil platforms, offshore wind turbine foundations and piled wharfs (Zhu and Moule, 1996). Numerous studies, both numerical and experimental, have been carried out on this topic. For example, Chen et al. (2014) employed the OpenFOAM® model to study the nonlinear effects of both regular wave and focused wave interaction with a single cylinder. This case was experimentally studied by Zang et al. (2010). Kamath et al. (2015) simulated regular wave interaction with multiple cylinders placed in groups in different configurations using the open-source CFD model REEF3D. Mo and Liu (2009) investigated non-breaking solitary wave interaction with a single cylinder or a group of three cylinders through a Volume of Fluid (VOF) based finite volume numerical solver and also physical experiments. Lara et al. (2013) and Leschka and Oumeraci (2014) also investigated solitary wave interaction with three vertical cylinders based on OpenFOAM®; in both works, different configurations of the cylinders are studied. In addition to the above-mentioned Eulerian methods, Lagrangian methods have also been widely employed for investigating these topics, such as the Smoothed Particle Hydrodynamics (SPH) method (Dalrymple and Rogers, 2006; Lind et al., 2016) and the meshless local Petrov-Galerkin method based on Rankine source solution (MLPG_R) (Zhou et al., 2009).

This paper aims to contribute to further understanding the processes of the interaction between different waves and single or multiple vertical cylinders, in terms of wave elevations around the cylinders, wave run-up and wave loading. More importantly, attention has been focused on the comparison of results between the PICIN model and VOF-based Eulerian models such as OpenFOAM®. We show that the innovative use of particles to track the free surfaces in PIC can handle large free-surface deformations such as wave breaking more advantageously. We also demonstrate that with the MPI parallelisation the PIC-based PICIN model is capable of modelling large scale 3D water wave problems, with an efficiency (in terms of CPU cost) that is of the same magnitude as the OpenFOAM® model.

The paper is organised as follows: section 2 gives an overview of the 3D parallel PICIN model including the governing equations, major numerical implementations and the parallelisation using the MPI approach. Next, section 3 compares the results of the present model with experimental measurements and numerical predictions from other state-of-the-art numerical solvers for two idealized test cases. Finally, in section 4 conclusions are drawn.

2. The 3D PICIN model

2.1. Governing equations

The PICIN model solves the incompressible Newtonian Navier-Stokes equations for single-phase flows:

$$\nabla\cdot\boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \boldsymbol{f} - \frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u}, \tag{2}$$

where, in 3D, $\boldsymbol{u} = [u, v, w]^T$ is the velocity field; t is time; p is pressure; $\boldsymbol{f} = [0.0, 0.0, -9.81\ \mathrm{m/s^2}]^T$ represents the body force due to gravity, and ρ and ν are the density and kinematic viscosity of the fluid, respectively. According to the PIC methodology, both grid and particles are employed to solve the governing equations. In particular, a staggered grid is employed following Harlow and Welch (1965), where pressures are stored at cell centres, whose positions along the x-, y- and z-directions are numbered by indexes i, j and k, respectively, and velocities are computed at relevant cell faces, whose positions are labelled with half-integer values of the indexes. Fig. 1 shows a schematic of the computational setup, where the staggered grid and fluid particles are also depicted. In the current 3D PICIN model, 8 particles are initially seeded in each cubic cell. Cells occupied by the particles are marked as fluid cells, while air cells correspondingly have no particles inside. The particles carry the fluid properties such as the mass and momentum, and are used to track the configuration of the fluid body (including the free-surface position) and solve the nonlinear advection term (the second term on the left hand side of the momentum equation), while the underlying grid is employed solely for computational convenience for solving the non-advection terms. The solution procedure is divided into two major steps: an Eulerian step and a Lagrangian step. During the Eulerian step the governing equations, ignoring the nonlinear advection term, are resolved on the grid. After that, in the Lagrangian step, the solution on the grid is used to update the particle velocity and the remaining advection term is then handled using the particles in a Lagrangian manner. More details of the solution procedure are given in the following sections. We note that no turbulence models are incorporated in the current numerical model, and thus the test cases presented in section 3 are carefully selected.

2.2. Eulerian step

2.2.1. The pressure projection algorithm

In the Eulerian step, the governing equations, ignoring the nonlinear advection term in the momentum equation, are solved on the grid. Prior to the solutions, the velocity field $\boldsymbol{u}^n$ at the nth time-step on the grid is mapped from the velocity field carried by the particles; this is discussed in section 2.4.

The solution in this step uses the pressure projection method proposed in Chorin (1968). A tentative velocity $\tilde{\boldsymbol{u}}$ is first computed by applying the body force and physical viscosity term as an Euler step in time:

$$\frac{\tilde{\boldsymbol{u}} - \boldsymbol{u}^n}{\Delta t} = \nu\nabla^2\boldsymbol{u}^n + \boldsymbol{f}, \tag{3}$$

where Δt is the time step. The body force and the viscosity term are both treated explicitly on the grid, and the viscosity term is resolved using the central differencing method. The next step is then to find a pressure field p^{n+1} to maintain the incompressibility condition (Eq. (1)). Recalling the remaining pressure gradient part of the momentum equation, we have:

$$\frac{(\boldsymbol{u}^{n+1} - \tilde{\boldsymbol{u}})}{\Delta t} = -\rho^{-1}\nabla p^{n+1}. \tag{4}$$

Taking the divergence of both sides of Eq. (4) and recalling that the velocity at the next time-step must satisfy the divergence-free condition lead to a pressure Poisson equation (PPE):

$$\Delta t\rho^{-1}\nabla^2 p^{n+1} = \nabla\cdot\tilde{\boldsymbol{u}}. \tag{5}$$

The PPE is discretised and solved in a finite volume sense by integrating