DEVELOPMENT OF 3D PARALLELIZED CMPS-HS WITH A DYNAMIC DOMAIN DECOMPOSITION APPROACH

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The paper presents a 3D parallelized improved particle method for simulation of violent free-surface fluid flows. The improved particle method is the Corrected Moving Particle Semi-implicit method with a Higher order Source term (CMPS-HS; Khayyer and Gotoh, 2009). The parallelization is carried out by a dynamic domain decomposition approach. Further, two different solvers are considered for the iterative solution process of the simultaneous linear equations corresponding to the Poisson pressure equation. The verification of the proposed method is carried out by simulating a 3D schematic dam break (Kleefsman et al., 2005) and by performing comparisons in terms of water surface profile and time history of pressure. The results by some other particle-based and grid-based methods are considered for more detailed comparisons.

Key Words **:** *particle method, parallelization, MPS, CMPS-HS, momentum conservation, pressure fluctuation*

1. INTRODUCTION

Particle methods have been increasingly used as powerful and versatile computational tools to simulate a wide variety of physical processes. Due to their Lagrangian and gridless features, these methods are well suited to simulate the convection-dominated problems involving large deformations as in case of violent free-surface fluid flows. For this class of problems, the MPS (Moving Particle Semi-implicit; Koshizuka and Oka, 1996) is a well-known particle method originally proposed on the basis of a projection-based approach for simulation of incompressible free-surface fluid flows.

Through the past years, the MPS method has been applied in a wide range of engineering applications including Coastal Engineering. For instance, Gotoh and his colleagues extended the MPS method to simulate wave breaking (Gotoh and Sakai, 1999, 2006), wave overtopping (Gotoh et al., 2005a) and sediment-water interactions (Gotoh et al., 2001, 2006). Gotoh et al. (2005b) also developed a 3D numerical wave flume based on the MPS method.

Despite its flexibility and wide-range of applicability, the MPS method has a few drawbacks including non-conservation of momentum (Khayyer and Gotoh, 2008) and existence of unphysical pressure fluctuations (Khayyer and Gotoh, 2009). By focusing on the momentum conservation properties of the MPS approximations for particle interacting forces and by deriving an anti-symmetric pressure gradient model, Khayyer and Gotoh (2008) proposed a revised version of the MPS method, namely, the CMPS (Corrected MPS) method. Improved conservation of both linear and angular momentum by the CMPS method resulted in refined reproductions of 2D plunging breaking waves and resultant splash-ups (Khayyer and Gotoh, 2008). Later, Khayyer and Gotoh (2009) revisited the derivation of the Poisson Pressure Equation (PPE) in the original MPS method and derived a higher order source term on the basis of a more accurate time differentiation of particle number density. Enhanced simulations of 2D wave impact pressure were obtained by the CMPS-HS (CMPS with a Higher order Source term) method.

An important issue in most hydrodynamic flows, however, is the three-dimensionality of the phenomenon. Hence, development of 3D CMPS-HS becomes indispensable. Moreover, since particle methods are computationally intensive and 3D simulations require considerably more particles, development of 3D parallelized CMPS-HS code becomes essential.

This paper presents a 3D parallelized CMPS-HS method. The 3D CMPS-HS is developed on the basis of 3D MPS (Gotoh et al., 2005b). The parallelization is carried out by a dynamic domain decomposition approach so that almost equal numbers of fluid particles are assigned to each processor throughout the calculation. Two different solvers, namely, PICCG-RP (Parallelized ICCG with Renumbering Process; Iwashita and Shimasaki, 2000) and SCG (Scaled Conjugate Gradient, Jennings and Malik, 1978) are applied for the iterative solution of the simultaneous linear equations corresponding to the Poisson Pressure Equation (PPE).

2. 3D CMPS-HS METHOD

The 3D CMPS-HS Method is explained in brief. Detailed descriptions on MPS and CMPS-HS have been provided by Koshizuka and Oka (1996) and Khayyer and Gotoh (2009). The governing equations are the continuity and the Navier-Stokes equations:

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} + \nabla\cdot\boldsymbol{u} = 0 \tag{1}$$

$$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = -\frac{1}{\rho}\nabla p + \boldsymbol{g} + \nu\nabla^2\boldsymbol{u} \tag{2}$$

where $\boldsymbol{u}$ is the particle velocity vector; t is the time; ρ is the fluid density; p is the pressure; $\boldsymbol{g}$ is the gravitational acceleration vector and ν represents laminar kinematic viscosity.

The pressure gradient is approximated by a radial and anti-symmetric gradient operator model as:

$$\langle\nabla p\rangle_i = \frac{D_s}{n_0}\sum_{j\neq i}\frac{(p_i+p_j)-(\hat{p}_i+\hat{p}_j)}{|\boldsymbol{r}_j-\boldsymbol{r}_i|^2}(\boldsymbol{r}_j-\boldsymbol{r}_i)\,w(|\boldsymbol{r}_j-\boldsymbol{r}_i|) \tag{3}$$

$$\hat{p}_i = \min_{j\in J}(p_i, p_j) \quad , \; J=\{j : w(|\boldsymbol{r}_j-\boldsymbol{r}_i|)\neq 0\} \tag{4}$$

where D_s = number of space dimensions = 3, $\boldsymbol{r}$ = coordinate vector of fluid particle, $w(r)$ = the kernel function and n_0 = the constant particle number density.

The kernel function applied in both MPS and CMPS-HS methods is the standard one proposed by Koshizuka and Oka (1996). The particle number density at a target particle i is defined as:

$$\langle n\rangle_i = \sum_{j\neq i} w(|\boldsymbol{r}_j-\boldsymbol{r}_i|) \tag{5}$$

The Laplacian operator is formulated as:

$$\langle\nabla^2\phi\rangle_i = \frac{2D_s}{n_0\lambda}\sum_{j\neq i}(\phi_j-\phi_i)w(|\boldsymbol{r}_j-\boldsymbol{r}_i|) \tag{6}$$

$$\lambda = \frac{\sum_{j\neq i} w(|\boldsymbol{r}_j-\boldsymbol{r}_i|)|\boldsymbol{r}_j-\boldsymbol{r}_i|^2}{\sum_{j\neq i} w(|\boldsymbol{r}_j-\boldsymbol{r}_i|)} \tag{7}$$

The Poisson Pressure Equation (PPE) is written as:

$$\langle\nabla^2 p_{k+1}\rangle_i = -\frac{\rho}{n_0\Delta t}\sum_{i\neq j}\frac{-r_e}{(r_{ij}^*)^3}\left(x_{ij}^* u_{ij}^* + y_{ij}^* v_{ij}^*\right) \tag{8}$$

where Δt = calculation time step.

3. PARALLELIZATION OF 3D CMPS-HS

In general, there are two approaches for parallelization of a particle method, particle decomposition and domain decomposition. Ikari and Gotoh (2008) showed that a domain decomposition approach outperforms a particle decomposition one in parallelization of 3D MPS method. In that study, a static domain decomposition strategy had been applied, i.e. the positions of sub-domains' interfaces were fixed in space throughout the simulation. This approach would surely lead to load imbalance especially in violent flow simulations. In the present study, we apply a Dynamic Domain Decomposition approach based on a simple one-dimensional Bisection Method. Inter-processor communications are performed using a MPI library on a distributed memory architecture.

Another important task in parallelization of a numerical method which consists of an iterative solution of simultaneous linear equations is to efficiently parallelize the iterative solver. In original MPS method the solution of the linear system of equations is obtained by the ICCG (Incomplete Cholesky Conjugate Gradient) method. Although the ICCG has been proven to be a robust method for solving a linear system of equations with a symmetric positive-definite matrix, the parallel processing of this method would be difficult due to inherent sequential nature of forward and backward substitutions performed for preconditioning. Iwashita and Shimasaki (2000) proposed a parallel processing technique for the ICCG on the basis of a renumbering process. The PICCG-RP (Parallelized ICCG with Renumbering Process) modifies the global matrix into a form similar to dissection ordering case. In this paper, the PICCG-RP is applied for parallel processing of the ICCG solver.

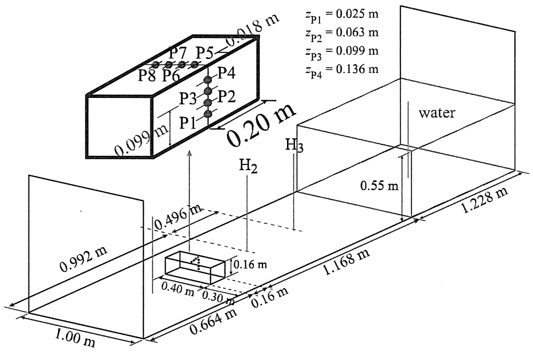

Fig. 1. A schematic sketch of calculation domain

Another alternative for solving the system of linear equations is to use the Scaled Conjugate Gradient (SCG) method which is 100% parallelizable (as there is no communication in the diagonal scaling) and at the same time benefits from a high convergence rate. In this study, the SCG method is considered as an alternative solver of linear equations.

4. VERIFICATION

The proposed method is verified by simulating a 3D schematic dam break and its impact against an obstacle (Kleefsman et al., 2005). This test has been considered as a benchmark test for verification of some particle-based (e.g. Moulinec et al., 2008) and grid-based (e.g. Park et al., 2009) methods. **Fig. 1** shows a schematic sketch of the calculation domain including the positions of the wave height probes and pressure sensors.

(1) Qualitative comparison

Fig. 2 shows snapshots of water particles at three instants by 3D parallelized CMPS-HS method. This figure portrays the concept of a dynamic domain decomposition approach and distributions of particles among the processors. At t = 0.0 s, an arbitrary distribution of sub-domains' interfaces is obvious. After this instant, however, almost equal numbers of particles are assigned to each of the four processors by applying a simple DDD approach. The slight differences in the numbers of particles are due to the one-dimensional decomposition as well as the employment of relatively course macro-cells for determination of instantaneous distribution of particles in the domain.

Fig. 3 depicts the experimental photo, snapshot of water particles and vertical velocity field (= w) at t = 0.56 s by 3D parallelized CMPS-HS and its corresponding high-order VOF snapshot presented

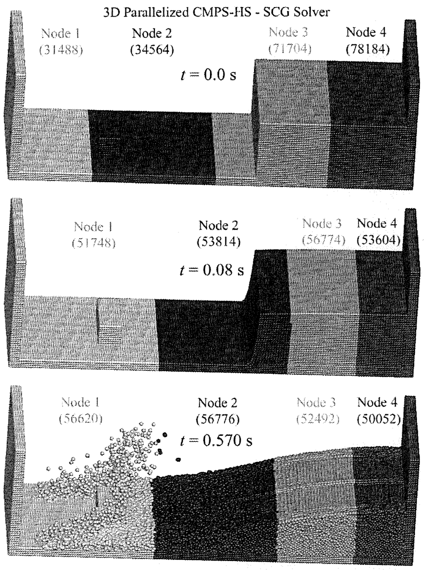

Fig. 2. Distribution of particles between four processors by a dynamic domain decomposition approach

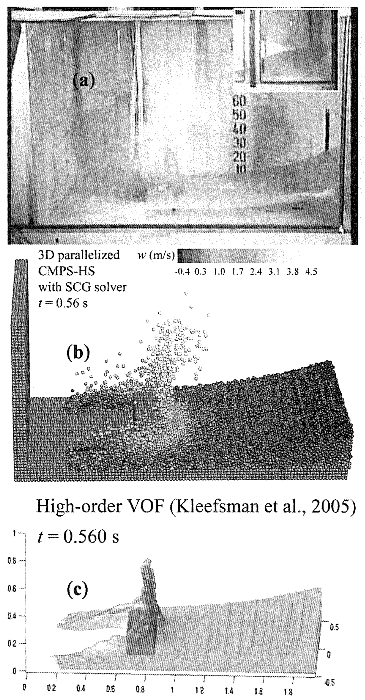

Fig. 3. Snapshots of water particles at t = 0.56 s – comparisons between (a) experiment (Kleefsman et al., 2005), (b) 3D parallelized CMPS-HS and (c) a high-order VOF

by Kleefsman et al. (2005). By focusing on Fig. 3(c), a straight, upward-directed and integrated jet is simulated by the high-order VOF method. However, the jet seen in the experimental photo (Fig. 3a) is

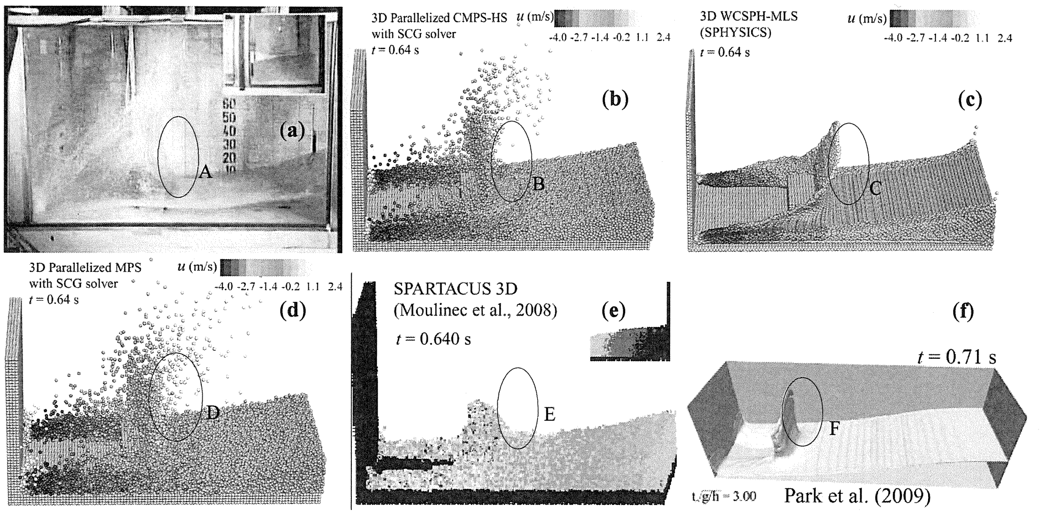

Fig. 4. Snapshots of water particles at t = 0.64 s – comparisons between (a) experiment (Kleefsman et al., 2005), (b) 3D parallelized CMPS-HS, (c) 3D WCSPH-MLS (SPHysics code, Gomez-Gesteira et al., 2008), (d) 3D parallelized MPS, (e) SPARTACUS 3D (Moulinec et al., 2008) and (f) a hybrid VOF-Level Set method (Park et al., 2009)

curled back towards the incoming flow. Further, the experimental jet is characterized by considerable fluid fragmentations which are not reproduced in the VOF snapshot. On the contrary, 3D parallelized CMPS-HS has been able to simulate the backward curl of the jet and the fluid fragmentations.

Fig. 4(a-f) shows the snapshots of water particles at t = 0.64 s by the 3D parallelized CMPS-HS, the 3D WCSPH-MLS (SPHysics, Gomez-Gesteira et al., 2008), the 3D parallelized MPS methods and the results by a WCSPH-based code (SPARTACUS 3D, Moulinec et al., 2008) and a hybrid two-phase VOF-Level Set method (Park et al., 2009). The WCSPH-MLS method provides an integrated jet without the reproduction of fluid fragmentations. The backward curl of the jet is simulated to some extend by this method. The snapshot by the 3D parallelized MPS consists of considerable unphysical dispersed particles (e.g. the particles seen in the region D in **Fig. 4(d)**). The snapshot by the 3D parallelized CMPS-HS is in a moderately good agreement with the experiment as the height of jet, its curling back and physical fluid fragmentations are fairly well simulated. From **Fig. 4(e)**, SPARTACUS 3D has not simulated the backward curl of the jet. Further, the velocity field by this code contains considerable numerical noise in the vicinity and left hand side of the reproduced jet. Comparable to the VOF result seen in **Fig. 3(c)**, the two-phase VOF-Level Set snapshot shows a straight upward and integrated jet. It appears that reproductions of fluid fragmentations and complicated behaviour of violent fluid flows (such as backward curling of a jet, backward breaking) are difficult to be simulated by the grid-based numerical methods even the high-order ones.

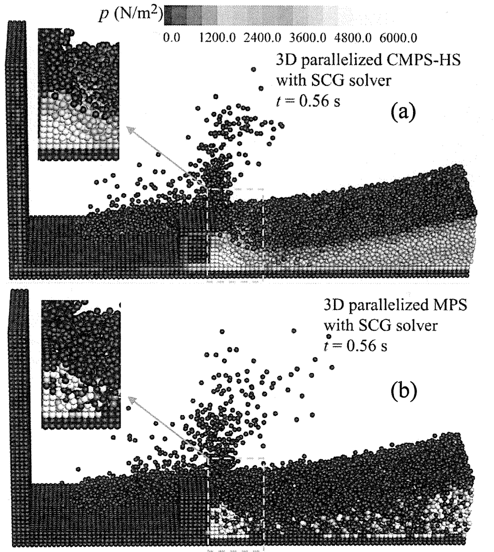

Fig. 5. Qualitative comparison in terms of the reproduced pressure field by the 3D parallelized CMPS-HS (a) and the 3D parallelized MPS (b) methods (t = 0.56 s)

Fig. 5 illustrates the enhancement in simulation of pressure field by 3D parallelized CMPS-HS in comparison to 3D parallelized MPS from a qualitative aspect. The 3D parallelized CMPS-HS has resulted in a remarkably improved pressure field in a wave impact type phenomenon.

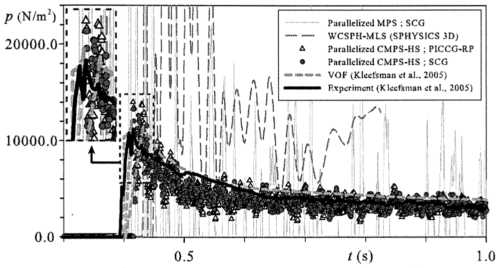

Fig. 6. Time histories of pressure at measuring points P1

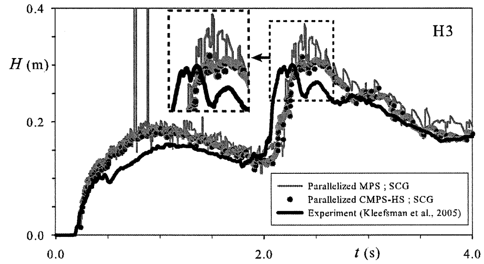

Fig. 7. Time histories of water height at measuring point H_3

(2) Quantitative comparison

Fig. 6 shows the pressure time histories at measuring point P1. From this figure, 3D parallelized CMPS-HS results in a significantly enhanced time variation of pressure (in comparison to 3D parallelized MPS) and an acceptable calculation of peak pressure together with its rise and declination. From Fig. 6, the pressure results by 3D parallelized CMPS-HS are comparable to those by the high-order VOF method but appear to be slightly more fluctuating. Yet, as seen in Fig. 3, the 3D parallelized CMPS-HS provides a more realistic reproduction of the jet.

Fig. 7 depicts time variation of water height at measuring probe H_3. From this figure, the 3D parallelized CMPS-HS method provides an enhanced estimation of water height variations at H_3. Despite slight overestimations of water height value and rise time, the overall trend of the water height variations has been fairly well predicted by the 3D parallelized CMPS-HS method.

5. CONCLUDING REMARKS

The paper presents a 3D parallelized version of an improved particle method and its application to simulation of violent free-surface fluid flows and wave impact pressure. The improved particle method is an enhanced version of the MPS method (Koshizuka and Oka, 1996), namely, the CMPS-HS method (Khayyer and Gotoh, 2009). The CMPS-HS method is extended to 3D and is parallelized for the enhancement of computational efficiency.

The parallelization is carried out by a dynamic domain decomposition approach. Two different solvers are tested for the iterative solution process of the simultaneous linear equations corresponding to the Poisson Pressure Equation (PPE).

Qualitative and quantitative comparisons are made in terms of the overall flow features and the time histories of pressure and water height. The results by some other particle-based and grid-based methods are considered for detailed comparisons.

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