Projection-based particle methods - latest achievements and future perspectives

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Abstract

The paper presents a concise review on the latest achievements made in the context of projection-based particle methods, including MPS and Incompressible SPH (ISPH) methods. The latest achievements corresponding to stability, accuracy, boundary conditions and energy conservation enhancements as well as advancements related to simulations of multiphase flows, fluid-structure interactions and surface tension are reviewed. The future perspectives for enhancement of applicability and reliability of projection-based particle methods are also highlighted.

Keywords: particle methods, projection method, Moving Particle Semi-implicit (MPS), Incompressible Smoothed Particle Hydrodynamics (ISPH), stability, accuracy, conservation

Introduction

Projection-based particle methods, including MPS [1] and Incompressible SPH (ISPH) [2] methods, are founded on Helmholtz decomposition of an intermediate velocity vector field into a solenoidal (divergence-free) one and an irrotational (curl-free) one. These methods potentially result in accurate solutions to the continuity and Navier-Stokes equations, especially in terms of pressure calculation and volume conservation. In particular, the prediction-correction feature of projection-based particle methods provides the opportunity for numerical error minimization through the application of, for instance, error mitigating functions in the source term of the Poisson Pressure Equation (PPE) [3,4]. This paper aims at illustrating a concise summary of the latest achievements made in the field of projection-based particle methods, as well as some future perspectives.

The latest achievements made in the field of projection-based particle methods correspond to enhancements of stability, accuracy, boundary conditions, energy conservation and enhanced simulations of multiphase flows, fluid-structure interactions, surface tension, etc. In this paper, these achievements will be concisely reviewed.

Latest Achievements

Stability enhancement: A distinct category of methods developed for enhancement of both stability and accuracy for both explicit and semi-implicit projection-based particle methods correspond to particle regularization schemes. For instance, Lind et al. [5] proposed a generalized **P**article **S**hifting (**PS**) technique on the basis of Fick's law of diffusion. Despite its simplicity and effectiveness, the particle shifting scheme may violate the overall conservation properties [5] including conservations of momentum and energy.

To ensure the stability of projection-based particle methods, Tsuruta et al. [6] presented a **D**ynamic **S**tabilization (**DS**) scheme which is aimed at producing exactly adequate repulsive forces in a momentum-conservative manner. The applicability and effectiveness of this scheme has to be further examined for a wider range of free-surface, internal and multi-phase flows. Recently, the authors have conducted a study on accuracy and conservation properties of particle regularization schemes including PS and DS schemes. Despite providing exact local and thus global momentum conservation, the DS scheme may result in small-scale particle perturbations. This issue can be seen from a simple and well-known numerical benchmark test, namely, the Taylor-Green vortex.

Fig. 1 shows a qualitative comparison in between DS and PS schemes through illustrating calculated normalized pressure and velocity fields at normalized time of tU/L = 1.0 for Re = 10^6 in a Taylor-Green vortex test [5]. In the performed simulations of Taylor-Green vortex, particles are considered to be 5 mm in diameter (d_0 = 0.005 m) resulting in a total number of 40,000 particles. The calculation time step is set based on Courant stability condition and a maximum allowable time step of Δt_{max} = 5.0E-4 s. Without a proper particle regularization scheme, a purely Lagrangian simulation of Taylor-Green vortices will be most likely characterized by unfavourable anisotropic particle distributions along the flow streamlines. Here both DS and PS schemes have been successful in providing stable calculations. Nevertheless, distribution of particles by PS appears to be more regular in comparison to that by DS. As previously stated, at least for this test, the DS scheme has apparently resulted in small-scale particle perturbations. This would indicate the need to revisit the derivation of this scheme and possibly present an enhanced version.

As for the PS scheme, a distinct issue arises for free-surface or multiphase flows. In other words, special care must be taken with application of this scheme to interface particles due to large concentration gradients. Lind et al. [5] proposed a special treatment (Eq. 27 of [5]) for free-surface and its nearby particles to eliminate shifting normal to the free-surface. Theoretically, this treatment is justified for proper implementation of PS to free-surface flows. However, several numerical challenges arise, especially in long term simulations, resulting in unphysical perturbations and/or accumulation of particles at free-surface (e.g. Fig. 17 [5]). In addition, in order to minimize the unphysical perturbations at free-surface, the PS scheme of Lind et al. [5] for free-surface contains two tuning parameters to allow slight diffusion normal to the interface. Recently, the authors proposed a new **OPS** (**O**ptimized **P**article **S**hifting) scheme to enhance the accuracy of PS at the phase interfaces (e.g. free-surface). Unlike PS, the OPS does not contain any tuning parameters. **Fig. 2** illustrates the improved performance of OPS with respect to PS in simulation of a square patch of fluid [7]. **Fig 2**(**c**) and (**d**) present the time histories of mechanical energy dissipation and calculated pressure at the center of the patch. In our performed simulations, the square's length, L, and angular velocity, ω, are considered as 1.0 m and 1.0 m/s, respectively. Particles are considered to be 0.01 m in diameter (d_0 = 0.01 m).

Accuracy enhancement: For both ISPH and MPS methods refined differential operator models have been proposed to enhance the accuracy of pressure calculation [3,8,9,10,11] and particle motion [3,11]. Refined differential operator models have been proposed for discretization of either source term [8,10] or Laplacian of pressure [9,12,13] in the PPE.

Inspired by the excellent work of Kondo and Koshizuka [10], Khayyer and Gotoh [3] proposed a so-called **ECS** (**E**rror **C**ompensating **S**ource) scheme to minimize the projection-related errors. The PPE incorporating the ECS is formulated as [3]:

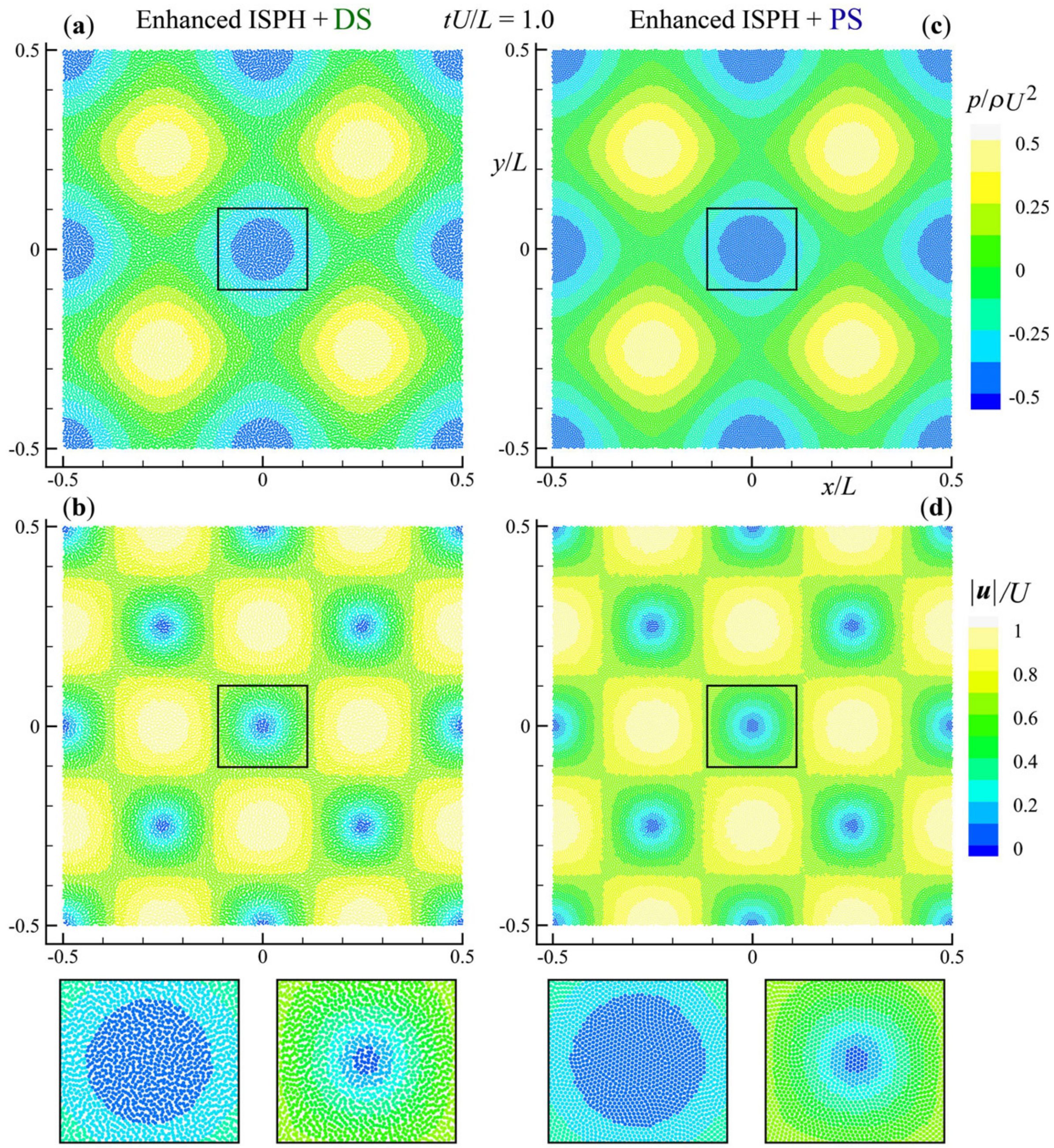

Fig. 1. Calculated normalized pressure (a,c) and velocity (b,d) by Enhanced ISPH + DS [6] (a,b) and Enhanced ISPH + PS [5] (c,d) - Taylor-Green flow (Re $=10^6$)

$$\left\langle \nabla^2 p_{k+1} \right\rangle_i = \frac{\rho}{n_0 \Delta t}\left(\frac{Dn}{Dt}\right)_i^* + \Lambda_{ECS}$$

$$\Lambda_{ECS} = \frac{\rho}{\Delta t}\left\{\frac{\alpha}{n_0}\left(\frac{Dn}{Dt}\right)_i^k + \frac{\beta}{\Delta t}\frac{n_i^k - n_0}{n_0}\right\} \quad ; \quad \alpha = \left|\frac{n_i^k - n_0}{n_0}\right| \quad ; \quad \beta = \left|\frac{\Delta t}{n_0}\left(\frac{Dn}{Dt}\right)_i^k\right| \tag{1}$$

where p, ρ, n, n_0, t, Δt, i and k represent pressure, density, particle number density, reference particle number density, time, calculation time step, target particle i and calculation step number, respectively. Hence, the source term of PPE is comprised of a main term and two error mitigating terms multiplied by dynamic coefficients (α, β) as functions of instantaneous

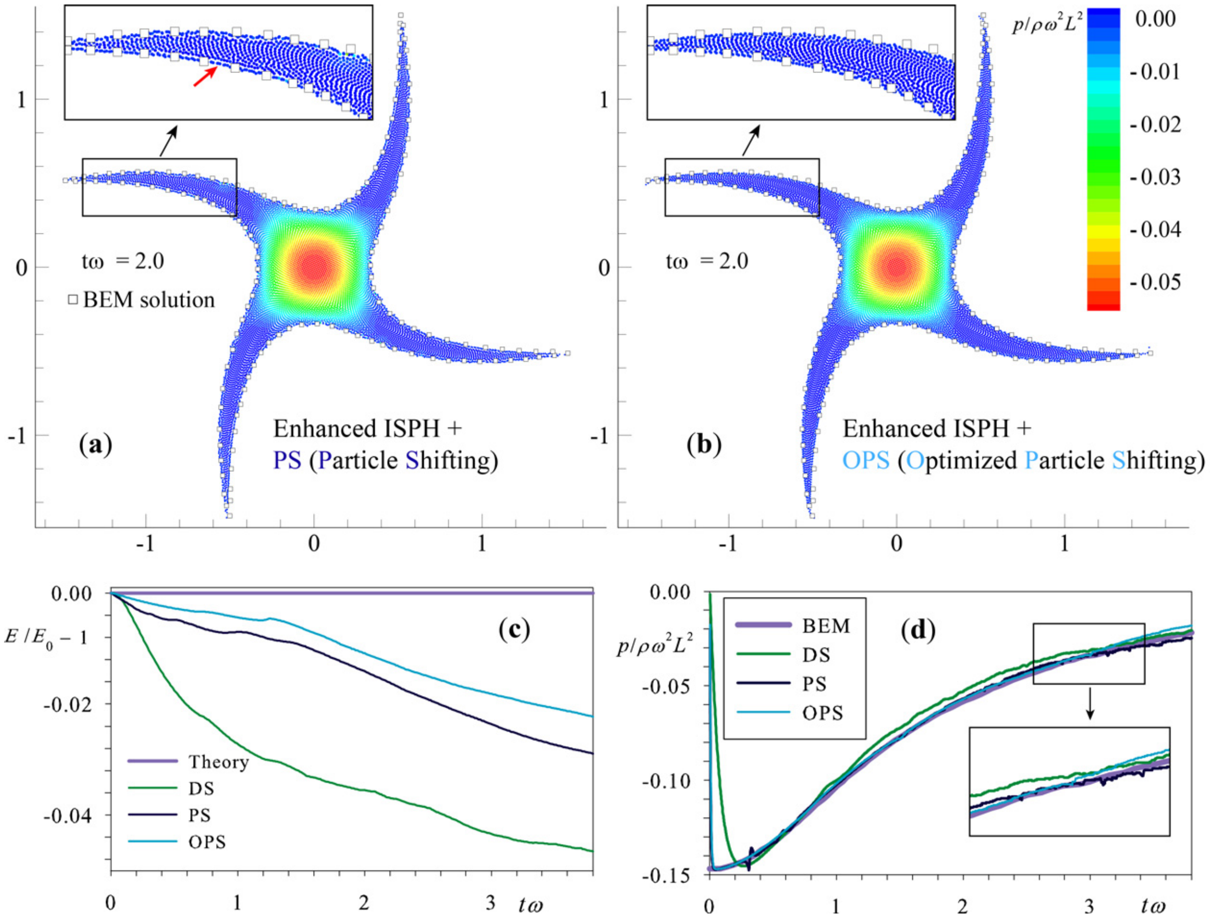

Fig. 2. Qualitative comparison in between PS [5] (a) and newly proposed OPS (b) schemes, elimination of unphysical discontinuity at free-surface (a) by OPS (b) - time histories of energy and normalized pressure at the center of the patch - evolution of a square patch of fluid [7]

flow field. The dynamic coefficients adjust the intensities of error mitigating terms depending on the instantaneous state of flow field. Similar ECS scheme has been formulated and validated for the ISPH [11].

Once an accurate pressure field is obtained, particles should be moved in space according to accurately computed accelerations corresponding to pressure gradient. In this regard, enhanced pressure gradient models with consistency-related corrections (e.g. [3,4,11,14,15,16]) have been proposed.

Improvement of boundary conditions: These improvements correspond to wall, free-surface and inflow/outflow boundary conditions.

Adami et al. [17] proposed a generalized wall boundary condition for SPH which correctly imposes no-slip conditions even for complex geometries. Despite being relatively simple for implementation, application of mirror particles may lead to inaccuracies in the convergence of differential operator models [18]. A more favored and recent approach is related to development of so-called semi-analytical wall boundary conditions. Di Monaco et al. [19] developed a semi-analytic approach for treatment of wall boundaries that can be considered as an integral version of the mirror particles of Adami et al. [17] for fixed boundaries. Similar approaches have been proposed by Ferrand et al. [20] and Mayrhofer et al. [21] that provide accurate and direct modeling of boundary integrals at the frontiers of the fluid domain resulting in precise pressure forces, wall friction and turbulent conditions. Recently, Leroy et al. [22] extended the unified semi-analytical wall boundary condition of Ferrand et al. [20] for the projection-based particle methods, and more precisely, the ISPH method.

In projection-based particle methods, a challenging issue is to detect free-surface particles accurately to impose the dynamic free-surface boundary condition, i.e. p equal to zero, to them. Khayyer et al. [23] proposed an auxiliary condition based on the non-symmetric distribution of free-surface particles to be used together with the original simple criterion. Ma and Zhou [24] proposed a Mixed Particle Number Density and Auxiliary Function Method (MPAM) for identifying the free surface particles in their Meshless Local Petrov-Galerin method based on Rankine source solution (MLPG-R) method. Park et al. [25] used a so-called Arc Method for an accurate assessment of free-surface particles. Nair and Tomar [26] presented a semi-analytical approach to impose Dirichlet boundary conditions on the free surface and thus eliminating the need for free-surface particle detection. This necessity was also eliminated by proposal of a new free-surface boundary condition referred to as Space Potential Particles (SPP [27]), through introduction of a potential in void space.

There have been a number of researches specifically targeting inlet/outlet boundary conditions in both weakly compressible (e.g. [28]) and incompressible (e.g. [29]) frameworks. In order to enhance the ISPH solution for both pressure and velocity near the boundaries including inlet/outlet ones, Hosseini and Feng [30] presented an approach which utilizes a rotational pressure-correction scheme with a consistent pressure boundary condition.

Energy conservation: Violeau [31] highlighted the compatibility, and more precisely, the skew-adjointness of gradient and divergence operators for energy conservation in calculations by particle methods. In the context of projection-based particle methods, this important property is required for an exact projection [32] which is a necessity for an exact energy conservation. A clear link exists also in between energy conservation and consistency of differential operator models and specifically, pressure gradient model.

Khayyer et al. [33] performed a study on energy conservation properties of projection-based particle methods. Their study highlighted the significance of Taylor-series consistent pressure gradient models and enhancing effect of a consistency-related gradient correction in providing enhanced energy conservation. Both ISPH and MPS were found to provide accurate predictions of physical dissipations in fluid impact problems. **Fig. 3** depicts improved MPS results corresponding to a normal impact of two rectangular fluid patches [34]. The rectangular patches have a length L, width $2H$ and the impact occurs at t = 0. The fluid is considered to be inviscid and incompressible, and thus the impact will be associated with a theoretically sudden loss of a fraction of the initial energy [35]. For the performed simulations L = 1.0 m, H = 0.33 m and U = 3.4 m/s. The maximum allowable time step is set as Δt_{max} = 5.0E-5 s and the particles are set to be of 0.01 m in diameter, i.e. d_0 = 0.01 m. A set of typical snapshots illustrating this phenomenon are presented in **Fig**. **3**(**a-c**). From **Fig**. **3**(**d**), the improved MPS method has provided an accurate estimation of energy loss corresponding to this impact.

To further illustrate the performance of improved MPS in reproduction of physical dissipation the normal impact of two rectangular fluid patches with different masses is considered. An analytical expression for the energy loss during this specific impact is given by Rogers and Szymczak [36]. A set of snapshots corresponding to this interesting classical fluid mechanics problem are presented in **Fig 4**. The performed simulation is characterized by a Mach number

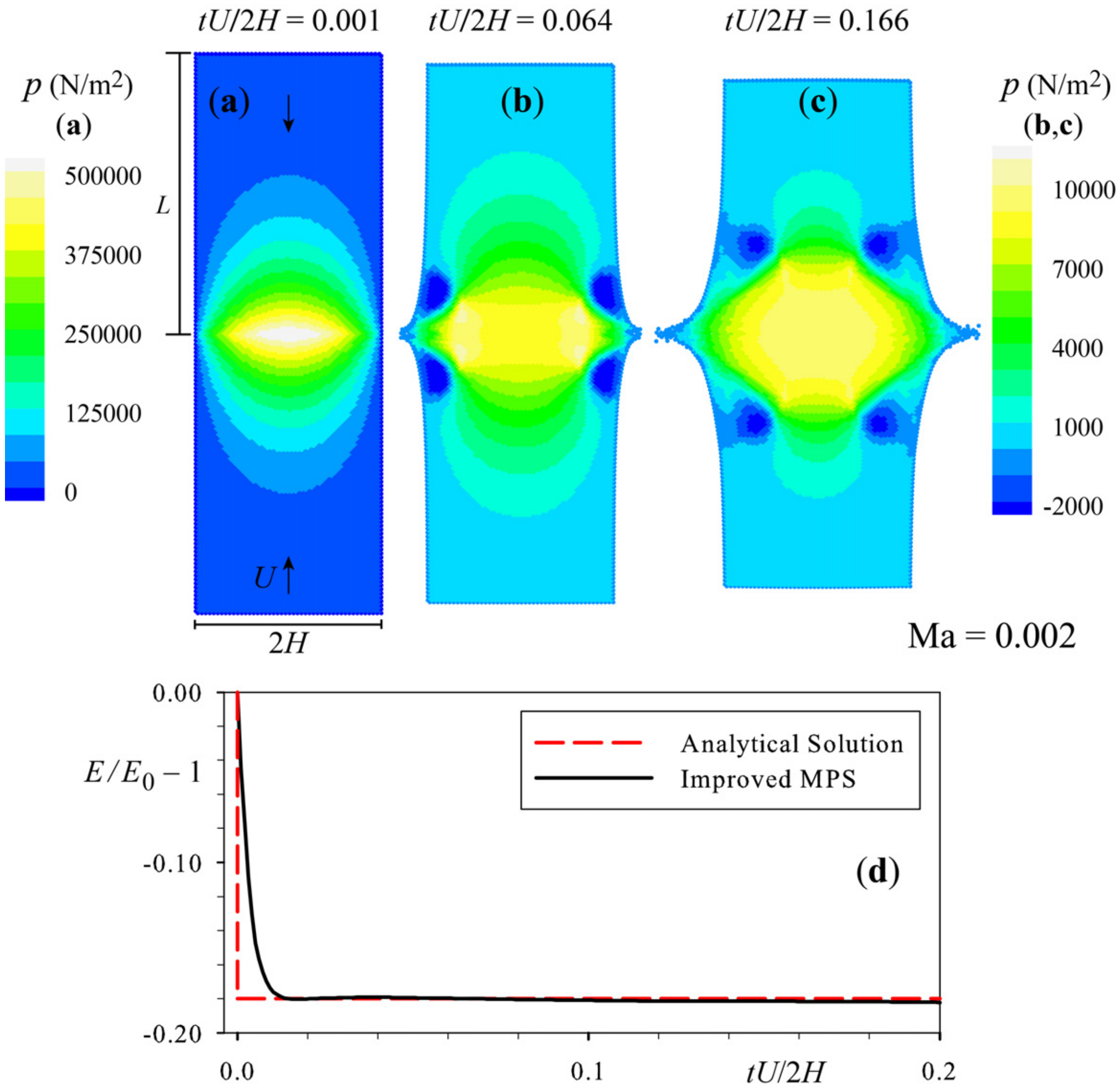

Fig. 3. Snapshots of particles together with pressure field (a-c), analytical [35] and calculated energy loss (d) - results by improved MPS - normal impact of two identical fluid patches [34,37]

of Ma = 0.2. For this simulation, the maximum allowable time step, Δt_{max}, is set as 5.0E-7 s, and particles are set to be of 0.01 m in diameter, i.e. d_0 = 0.01 m. **Fig. 4(e)** shows the excellent performance of improved MPS in providing almost accurate prediction of the energy loss for this impact.

The superior performance of improved MPS in predictions of energy loss in fluid impact problems as well as its excellent capability in shock capturing and propagation can be further pronounced by comparing the achieved results with those of advanced particle methods, including δ-SPH (e.g. Figs 14 and 15 in [37]) and Riemann SPH (e.g. Figs 9 and 10 in [34]). It should be noted in both of the mentioned references [34,37] weakly compressible SPH formulations are adopted.

Enhanced simulations of multiphase flows: Khayyer and Gotoh [4] presented an improved MPS method for multiphase flows characterized by large density ratios. The stability of their calculations was guaranteed through the application of a Taylor-series-based density smoothing scheme, and accuracy enhancement was achieved through the application of a PPE's error mitigating term, i.e. ECS scheme, and refined discretizations of source term and

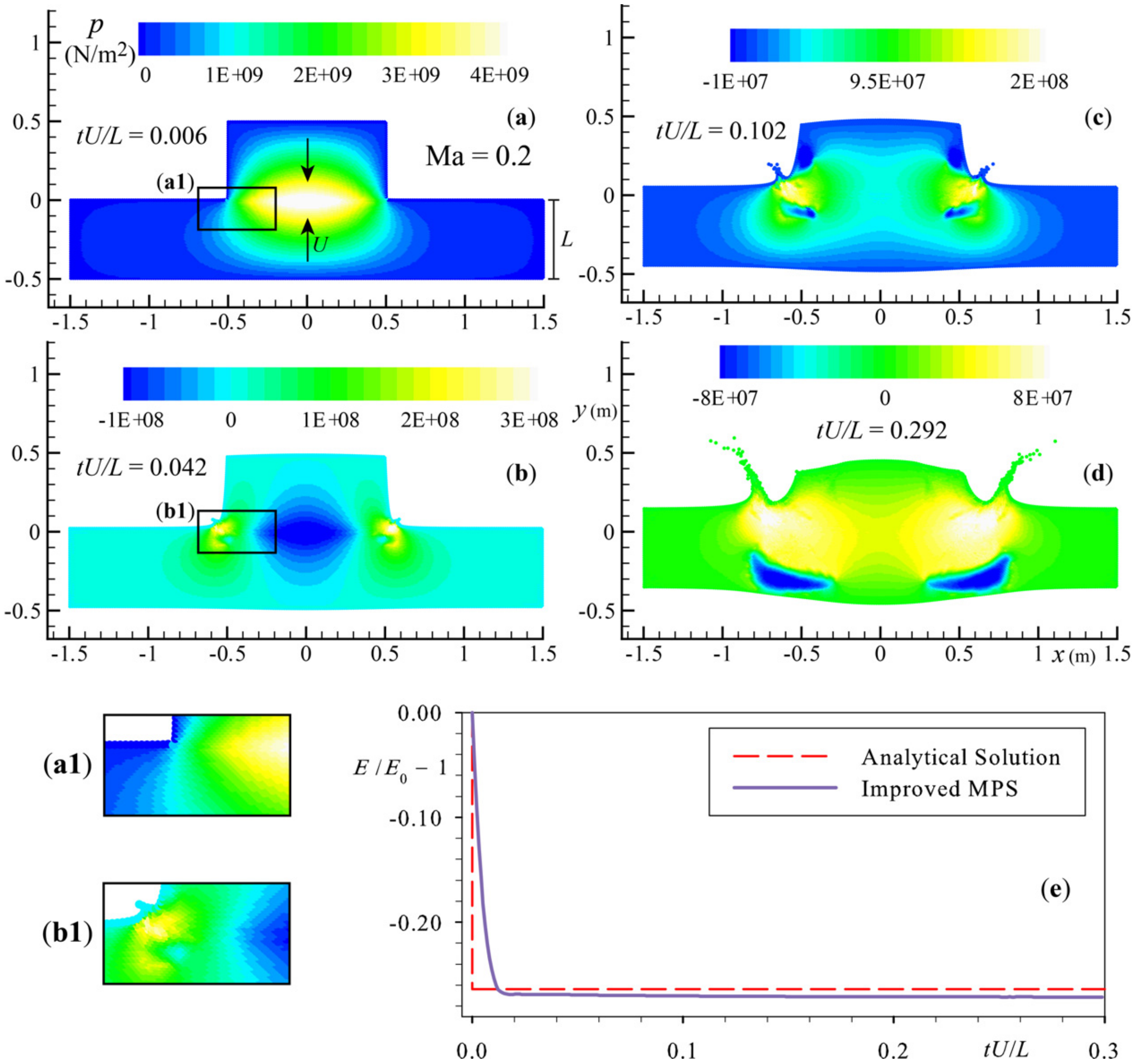

Fig. 4. Snapshots of particles together with pressure field (a-d), analytical [36] and calculated energy loss - results by improved MPS - normal impact of two fluid patches with different masses [34]

Laplacian of pressure. **Fig. 5** presents two typical snapshots corresponding to a multiphase violent sloshing flow characterized by air entrainment/entrapment with a realistic air/water density ratio of 1:1000. Conditions of the performed sloshing simulation corresponded to the experiment by Rognebakke et al. [38]. Sinusoidal excitations with maximum amplitude of 150 mm and frequency of 1.2 Hz were considered. The particles were 5.0 mm in diameter and the calculation time step was set according to the Courant stability condition and a maximum allowable time increment of 4.0E-5 s.

The ECS scheme was extended to minimize the projection-related errors in an incompressible-compressible multiphase calculation of wave slamming where actual speeds of sounds in air and water were implemented [39]. The newly proposed scheme was referred to as **CIECS** (**C**ompressible-**I**ncompressible **ECS**). The effectiveness of CIECS in minimization of projection-related errors in a typical Compressible-Incompressible multiphase flow, namely, slamming with entrapped air was shown through two sets of simulations corresponding to experiments by Lin and Shieh [40] and Verhagen [41].

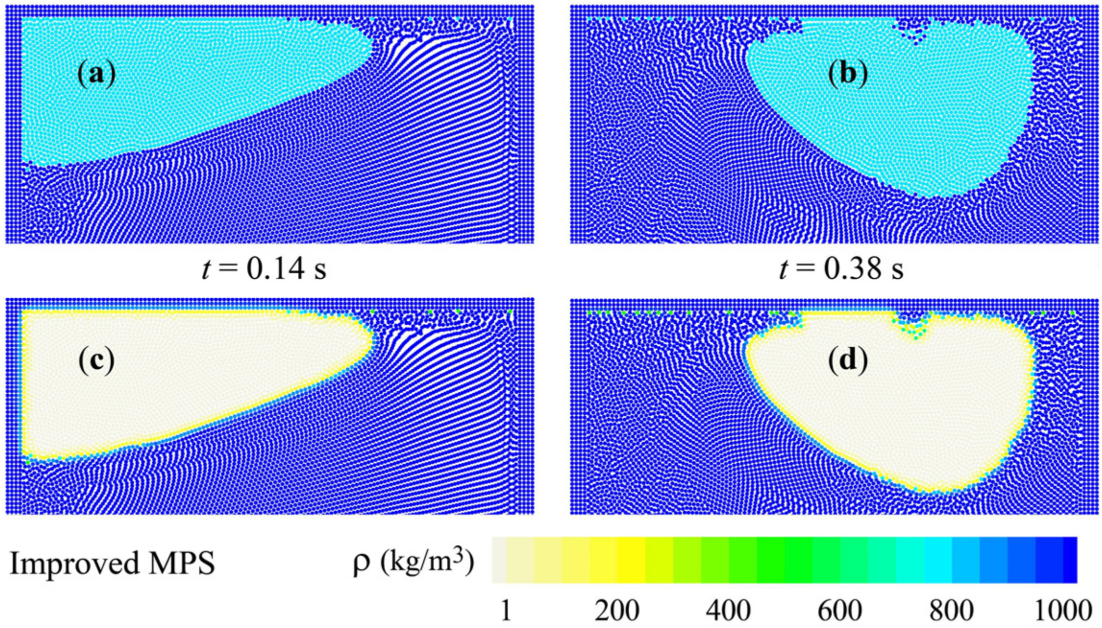

Fig. 5. Snapshots of gas and liquid particles (a,b) and calculated density fields (c,d) - muliphase simulation of a violent sloshing flow [38] by an improved MPS method [4]

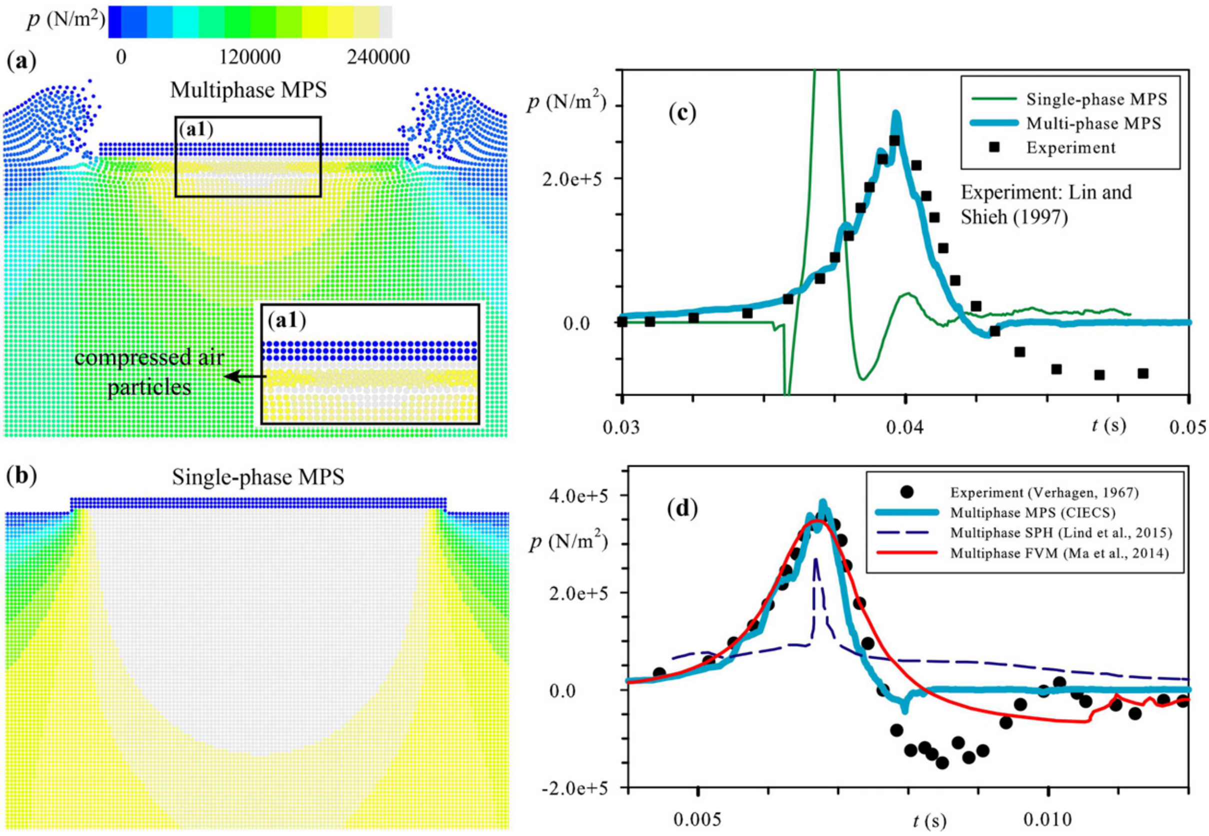

Fig. 6. Multiphase MPS with CIECS scheme applied to water slamming, experiments by Lin and Shieh [40] (a,c) and Verhagen [41] (d) - importance of air cushioning effect in prediction of slam induced pressure (c) and comparisons of multiphase MPS with multiphase SPH [42] and FVM [43] (d)

Fig. **6**(**a-c**) depicts the water slamming simulation results related to the experiment by Lin and Shieh [40] by multiphase and single-phase MPS methods. The figure portrays the importance of consideration of air and its cushioning effect for prediction of slamming-induced pressures.

Fig. **6**(**d**) presents a comparison in between the multiphase MPS with CIECS scheme with results by Lind et al. [42] and Ma et al. [43] with respect to the experiment by Verhagen [41]. A common experiment-simulation inconsistency seen in this figure corresponds to inaccurate prediction of post-impact negative pressure. The authors are investigating the probable reasons behind this apparent inconsistency. In the performed water slamming simulations, the diameter of particles was set as 3 mm. Considered viscosities for the water and air phases corresponded to their physical ones, i.e. ν_w = 1.0E-6 m^2/s and ν_a = 1.5E-5 m^2/s. The calculation time step was set based on the Courant stability condition and Δt_{max} = 1.0E-4 s.

Fluid-structure interactions: Particle methods including projection-based ones appear to be suitable computational tools for **FSI** (**F**luid-**S**tructure **I**nteraction) simulations, mainly due to their Lagrangian feature. These methods have been applied to simulate interactions in between fluid flows with either rigid (e.g. [44]) or flexible (e.g. [45]) structures. In the latter case, a proper structural model should be carefully coupled with the fluid solver.

In the context of projection-based particle methods, Lee et al. [46] developed a MPS-FEM coupled method to study incompressible fluid flow interactions with elastic structures. Rafiee and Thiagarajan [45] proposed a fully-Lagrangian SPH-based solver for simulation of incompressible fluid-hypoelastic structure interactions. In their study, the PPE was solved simply using an approximate explicit scheme. Hwang et al. [47] developed a fully-Lagrangian MPS-based FSI analysis method for incompressible fluid-linear elastic structure interactions. The key feature of this solver was absence of any artificial numerical stabilizers commonly applied in particle-based FSI solvers. This feature was achieved by implementation of an appropriate coupling algorithm.

Khayyer et al. [48] presented an enhanced version of Hwang et al.'s method by incorporating several refined schemes for the fluid phase and presenting an improved calculation of fluid force to structure. The achieved enhancements as well as applicability of developed MPS-based FSI solver are portrayed in **Fig**. **7**, corresponding to simulations of an entry of a deformable aluminum beam into an undisturbed water [49] and a dam break flow impacting on an elastic plate [50]. **Fig**. **7**(**a**) presents a representative snapshot of the pressure and stress fields in fluid and beam. A schematic sketch of this beam entry test and time histories of deflection at point C is shown in **Fig. 7**(**b**), where improved results are obtained by the enhanced coupled MPS [48]. For this aluminum beam entry test, the analytical solutions were derived by Scolan [51], on the basis of the hydrodynamic Wagner's model and linear Wan's theory. The material properties of the aluminum beam, namely, its Young's modulus, Poisson ratio and density were considered as 67.5 GPa, 0.34 and 2700 kg/m^3, respectively. Both structural and fluid particles were 0.01 m in size. **Fig**. **7**(**c**) and (**d**) portray two typical snapshots by coupled MPS [47] and enhanced coupled MPS [48] solvers together with their corresponding experimental photo as well as the result by a FDM-FEM solver [50] for the second FSI test. The superior performance of enhanced MPS is clearly illustrated in this figure as this method provides more consistent deflections of the elastic plate.

Surface tension: Surface tension modeling in the context of particle methods have been performed using either potential approach or continuum one. In the so-called potential approach surface tension is modeled by assuming that microscopic cohesive intermolecular forces can be mimicked by macroscopic inter-particle forces. The main advantage of this approach is related to its computational simplicity in that surface tension is modeled via particle-particle interactions explicitly without the necessity of calculating surface normals and curvatures, as required in the continuum approach. The main disadvantage of potential

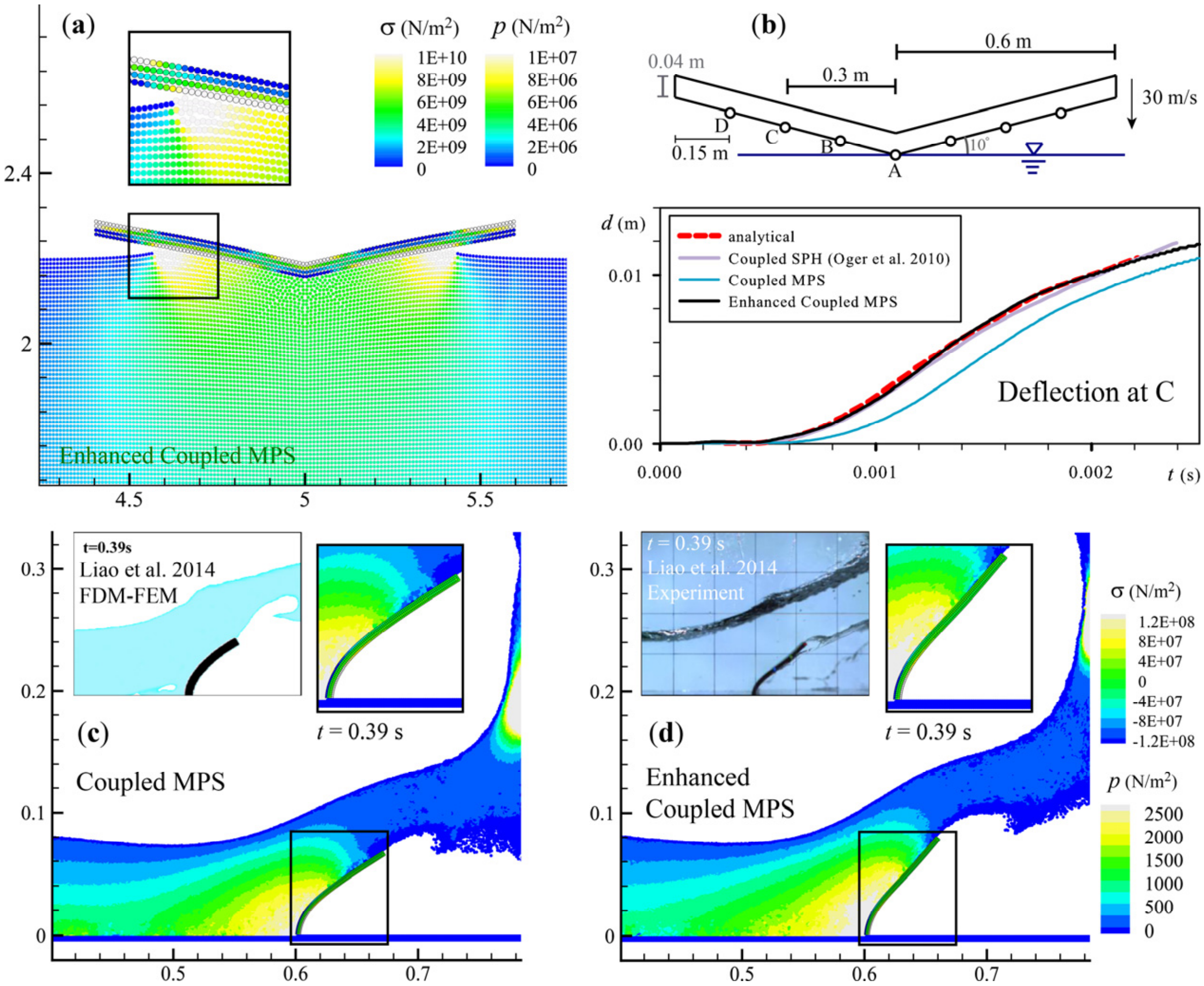

Fig. 7. Entry of an aluminum beam into undisturbed water [49] (a,b) and dam break with elastic plate [50] (c,d), results by an enhanced coupled MPS solver [48] (a,d) and a coupled MPS solver [47] (c)

approach corresponds to the fact that the surface tension forces depend on the intensity of particle-particle interactions. These interactions have to be adjusted numerically by varying the macroscopic input parameters depending on the simulation case to reproduce desired surface tension forces.

The most common approach for incorporation of surface tension in macroscopic particle-based simulations is the continuum approach and specifically those based on the **C**ontinuum **S**urface **F**orce (**CSF**) model introduced by Brackbill et al. [52]. In this approach, the surface tension is treated as a continuous, three-dimensional effect across the interface, derived directly from the Young-Laplace equation. Morris [53] showed several possible implementations of CSF model in SPH and highlighted the challenges in accurate calculations of interface curvature. These challenges are not only limited to difficulties in accurate particle-based calculation of Laplacian of color function for approximation of interface curvature, but also to the fact that a smoothed color function is usually used. The use of a smoothed color function may become problematic for approximation of interface normals near the boundaries and sharp-angled areas.

In MPS-based simulations of surface tension, the CSF based simulations can be categorized into two distinct groups, depending on the computational procedure for calculation of the curvature and the normal vector. These two categories are: arc fitting at interface [54] and differential approach (e.g. [55]). As the name indicates the arc fitting approach is aimed at approximating the normal vector and curvature by constructing local arcs at the surface particles via specific computational procedures. The accuracy of arc fitting approach is highly dependent upon the instantaneous smoothness of the free-surface. In the differential approach, the continuum surface forces are calculated by applying differential operator models for both gradient and Laplacian so that potentially accurate approximations of the unit normal vector and the curvature can be obtained.

Khayyer et al. [56] proposed a new differential CSF-based model in the context of MPS. Their model benefits from a novel formulation for curvature estimation using direct second order derivatives of color function via a precise discretization. By applying a high-order Laplacian scheme [9] including the approximation of boundary integrals, relatively accurate approximation of interface curvature and thus surface tension could be achieved. Accordingly, the Laplacian of color function, C, at an interface target particle i was calculated as [56]:

$$\left(\nabla^2 C\right)_i = \frac{1}{n_0}\sum_{i \neq j}\left\{\frac{\partial C_{ij}}{\partial r_{ij}}\frac{\partial w_{ij}}{\partial r_{ij}} + C_{ij}\left(\frac{\partial^2 w_{ij}}{\partial r_{ij}^2} + \frac{D_s - 1}{r_{ij}}\frac{\partial w_{ij}}{\partial r_{ij}}\right)\right\} + BI \tag{2}$$

where $C_{ij} = C_j - C_i$, $r_{ij} = r_j - r_i$, w represents kernel function, D_s stands for number of space dimensions and BI denotes the boundary integrals [57] formulated as:

$$BI = \int_{\partial\Omega} \nabla C \cdot \boldsymbol{n} w_{ij}\, dS \approx \frac{1}{n_0}\sum_{j \in \partial\Omega} \frac{C_{ij}\, \boldsymbol{r}_{ij} \cdot \boldsymbol{n}_j}{\left|\boldsymbol{r}_{ij}\right|^2} w_{ij}\, S_j \tag{3}$$

where $\boldsymbol{n}$ denotes interface normal, $\boldsymbol{r}$ symbolizes position vector and for 2D simulations S_j signifies the length (diameter) of boundary particle j. Therefore, the surface tension force is evaluated via achieving a direct Laplacian-based approximation of curvature. The enhanced performance of the Laplacian-based surface tension model [56] with respect to the arc fitting one [54] is illustrated in **Fig. 8**, corresponding to simulations of a water drop impact [58] for Froude and Weber numbers of 639 and 395, respectively. The figure portrays the superior performance of Laplacian-based surface tension model in better reproduction of crown development and splash drops.

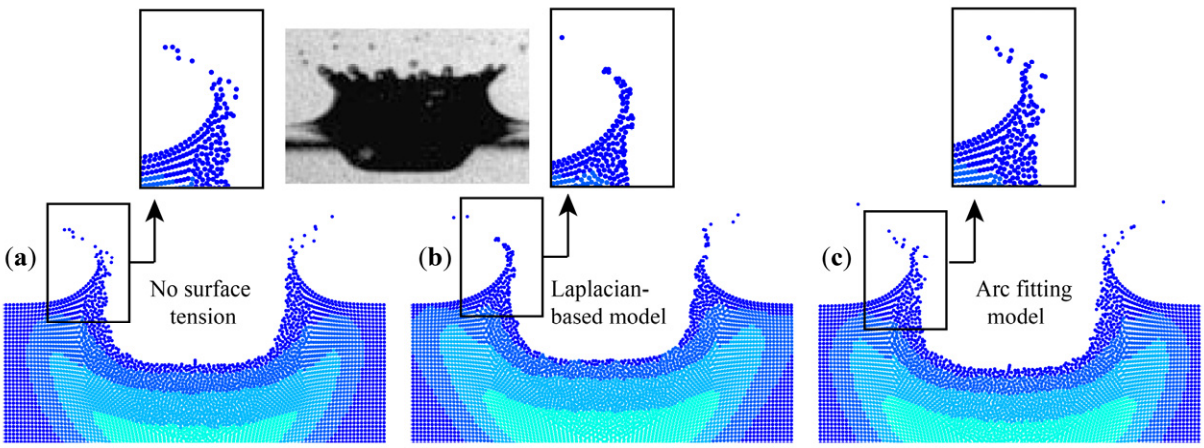

Fig. 8. Improved MPS results of a water drop impact [58], no surface tension model (a), Laplacian-based surface tension model [56] (b) and arc fitting surface tension model [54] (c)

Future Perspectives

In spite of the achieved advancements, rigorous researches should continue to be conducted to further enhance the reliability and accuracy of particle methods for practical engineering and scientific purposes. In particular, important issues of stability, conservation, convergence, boundary conditions, turbulence modeling [59,60], multi-scale and multi-physics simulations [61] will be among the future perspectives corresponding to projection-based particle methods.

For extended engineering and industrial applications, it is important to keep the developed computational methods free of any numerical term with constants that may require calibration. Several key insights on extended engineering and industrial applications of particles methods are highlighted in excellent review papers by Koshizuka [62] and by Violeau and Rogers [63]. Indeed, prior to any practical application, precise verification of particle-based codes must be conducted by consideration of appropriate benchmark tests with analytical solutions in terms of reproduced velocity and pressure together with comprehensive investigations on conservation and convergence properties.

Further advanced multi-scale and multi-physics applications of particle methods are expected to be achieved with forthcoming theoretical and computational enhancements. In particular, rigorous enhancements of stability, accuracy and conservation properties of particle methods along with advancements made in high performance computing as well as developments of accurate variable resolution schemes [64] will enable particle methods, including projection-based ones, to serve as advanced, reliable and efficient computational methods.

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