A New Surface Tension Model for Particle Methods with Enhanced Splash Computation

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Surface tension plays a key role in splash generation. However, accurate modeling of surface tension is challenging due to the numerical difficulties in calculating the interface curvature. This paper presents a new surface tension model for macroscopic particle methods on the basis of Continuum Surface Force (CSF) concept. The new model is characterized by a novel formulation for curvature estimation using direct second order derivatives of color function via a meticulous and comprehensive discretization. The new model is referred to as Laplacian-based surface tension model which applies a high-order Laplacian scheme including the approximation of boundary integrals. A set of benchmark tests are considered for simple and comprehensible verifications and then the model is applied to a water drop impact test to investigate its appropriateness in calculation of splash generation. Comparisons are also made with two commonly applied surface tension models in the context of particle methods, namely, divergence-gradient based model and the arc fitting one.

Key Words: splash, surface tension, particle method, Laplacian, curvature

1. INTRODUCTION

Surface tension plays a key role in splash generation due to finger-jet break-up at the tip of the wave-breaking jet. The splash generation drastically increases the surface area of water drops which enhances gas exchange between atmosphere and seawater. Hence, surface tension modeling is of significant importance in Coastal Engineering.

In the context of particle methods (e.g. MPS, SPH), there are two surface tension modeling approaches, namely, the potential approach and the Continuum Surface Force (CSF) one. The potential approach assumes that the microscopic intermolecular forces can be mimicked by inter-particle forces. But, due to significant differences in scales of molecule and particle, the model is not free from tuning parameters. Hence, the preferable approach for particle-based modeling of surface tension would be the CSF model which is derived directly from the Young-Laplace equation.

The most challenging problem of CSF-based surface tension models is related to calculation of interface curvature. This difficulty mainly arises from the fact that interface curvature corresponds to the calculation of divergence of a normalized gradient of color function by local, incomplete particle-based interpolation schemes.

In most cases of CSF particle-based modeling, calculation of interface curvature has been performed via a double summation scheme, and thus double approximations, comprising of an approximation of a normalized gradient and then an approximation of divergence of this estimated gradient. An alternative approach for curvature estimation is to formulate it using direct second order derivatives (of color function) and then meticulously discretize it via an accurate single summation scheme.

This paper presents a novel and simple surface tension model on the basis of CSF concept and by considering the above mentioned alternative approach. The distinct feature of the proposed model corresponds to accurate estimation of interface cur-
ture via deriving a single summation, Laplacian-based scheme that applies a high-order Laplacian model\textsuperscript{2} and includes approximations of the boundary integrals\textsuperscript{3}. This scheme and all other considered surface tension models are applied together with an enhanced and broadly verified MPS method\textsuperscript{4}.

2. NEW SURFACE TENSION MODEL

In the CSF-based models the pressure jump corresponding to the Young-Laplace equation is applied via a volume force normal to the interface. This volume force, $F_i$, is formulated as\textsuperscript{5}:

$$ F = -\sigma \kappa n \delta $$

(1)

where $\sigma$ denotes the surface tension coefficient, $\kappa$ is the local surface curvature, $n$ represents the unit normal vector and $\delta$ signifies the surface delta function that localizes the force to the interface and is defined as $\delta = |n|$.

In order to approximate the characteristics of the interface, i.e. normal direction and curvature, a volume fraction function, usually referred to as color function $C$, is defined. Mathematically, the color function defines the presence or absence of a given fluid at a spatial point $x$. Following Morris\textsuperscript{5}, a smoothed color function in the MPS context is defined as:

$$ C_i = \frac{\sum w_i |I_{ij} - I_{ij}|}{n_b} = \frac{\sum w_i}{n_b} $$

(2)

representing the discrete volume fraction of considered fluid in the influential circle of target particle $i$. In Eq. (2), $w$ represents the kernel function, $r$ represents the position vector and $n_b$ symbolizes the constant particle number density.

The normal vector $n$ is determined as the normalized gradient of color function and curvature is obtained by taking the divergence of the normal vector, i.e.

$$ n = \nabla C / |\nabla C| \quad , \quad \kappa = -\nabla \cdot n $$

(3)

In order to calculate the surface curvature, we may firstly find the unit normal vector $n$ by utilizing the gradient model and then applying the divergence model to this approximated value (divergence-gradient surface tension model). However, as it has been frequently stated by several researchers\textsuperscript{5}, this double approximation procedure will bring about substantial errors in curvature evaluation. The incompleteness of differential operator models will also further add to the related numerical errors.

Another approach for curvature evaluation is to formulate it using direct second order derivatives and then carefully discretize it via an accurate and complete single summation scheme. From Eq. (3):

$$ \kappa = -\nabla \cdot n = -\nabla \left( \frac{\nabla C}{|\nabla C|} \right) = -\frac{\nabla C \cdot \nabla \nabla C + \nabla C \cdot \nabla |\nabla C|}{|\nabla C|^2} $$

(4)

The above equation will be discretized using enhanced MPS gradient\textsuperscript{4} and Laplacian models\textsuperscript{2}.

Discretization of the Laplacian of $C$ is founded on the HL scheme\textsuperscript{3} with incorporation of boundary integrals. Since the HL scheme applies a SPH gradient model (derived by application of Gauss theorem), inclusion of the boundary or surface integrals will be important, in particular, when we consider the nature of the gradient of color function which reaches its maximum at the interface. Hence, the Laplacian of $C$ at an interface target particle $i$ is calculated as:

$$ (\nabla^2 C)_i = \frac{1}{n_b} \sum_{j \neq i} \left( C_{ij} \frac{\partial^2 w_i}{\partial r_{ij}^2} - C_{ij} \frac{\partial w_i}{\partial r_{ij}} \right) + \text{BI} $$

(5)

where $C_{ij} = C_i - C_j$, $r = |r|$, $r_{ij} = r_i - r_j$ and BI denotes the boundary integrals formulated as\textsuperscript{3}:

$$ \text{BI} = \int_{\Omega} \nabla C \cdot \nabla |r_i - r_j| \cdot n \, dS $$

(6)

where 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.

3. VERIFICATION

The newly proposed Laplacian-based surface tension model is verified by considering a set of benchmark tests including a static circle, an equilibrium rod\textsuperscript{3} and a non-equilibrium rod\textsuperscript{6}.

3.1 A Static Circle

In order to demonstrate the accuracy of proposed model in evaluation of surface curvature, a static circle of radius $R$ is considered. Theoretically, the product of curvature $\kappa$ and radius $R$ should be 1.0.

Fig. 1 shows the spatial distribution of approximated surface curvatures by Laplacian-based model (a), divergence-gradient model (b) and arc fitting model\textsuperscript{9} (c).
Fig. 1. Approximated curvature of a static circle by different surface tension models.

Fig. 2. An equilibrium rod - initial arrangement (a) and results by different surface tension models (b-c).

From this figure, the distribution of approximated curvature by the Laplacian-based model tends to be by far closer to the theoretical value, where the other two models have resulted in unreliable and fluctuating curvature estimations.

(2) Equilibrium rod
A common and simple benchmark test applied for verification of surface tension models is a static liquid drop subjected solely to surface tension forces. Due to the absence of other external forces (gravity or viscosity), this considered static liquid drop has to become fully spherical.

A fluid drop with radius of $R = 0.1$ m, density of $\rho = 1000$ kg/m$^3$ and surface tension coefficient of $\sigma = 0.10$ N/m is considered. The fluid drop is formed by about 7800 particles arranged within a 0.002 m spacing.

Fig. 2(a) shows the initial distribution of particles. Since the initial arrangement of particles does not form an exact circular rod, the particles' positions should be adjusted due to surface tension forces until a fully circular drop is formed. Fig. 2(b) and (c) present the simulation results after a stable state at $t = 0.01$ s by divergence-gradient model (b) and the Laplacian-based model (c).

From Fig. 2(b), divergence-gradient model has resulted in a fully dispersed interface. This dispersive motion of fluid particles is mainly caused by an imprecise curvature approximation similar to that seen in Fig. 1(b). Similar results are obtained by other MPS-based surface tension models, for instance, Fig. 7 in Liu et al. From Fig. 2(c), the new Laplacian-based surface tension model has provided a neat and an almost perfect circular rod thanks to an accurate estimation of curvature and unit normal vectors by this model.

(3) Non-equilibrium rod
As another interesting theoretical benchmark test, we consider the oscillation of an initially square drop under the action of surface tension forces. This test has been theoretically solved and has been frequently considered for verification of surface tension models.

The initial square is an inviscid liquid with a diameter of $D = 4$ mm, density of $\rho = 1000$ kg/m$^3$ and surface tension coefficient of $\sigma = 0.10$ N/m. The particle size is considered to be 0.10 mm. Due to the initial square shape of drop with theoretically
infinite surface tension forces at the corners, the drop is set into oscillations towards an equilibrium circular shape.

Fig. 3 shows a comparison in between the snapshots of fluid particles at final states obtained by the Laplacian-based model (a) and arc fitting one (b). In contrast to the Laplacian-based model, the arc fitting model has not been able to result in a circular drop. Further, the snapshot by this model is characterized by a ragged and dispersed free surface.

4. WATER DROP IMPACT AND SPLASH

The impact of a circular water onto a water surface has been considered to investigate the appropriateness of developed surface tension model for splash computation. This test corresponds to the experiments by Liow. A set of three simulations corresponding to different Froude (Fr) and Weber (We) numbers are carried out. The water drop is considered to be 4.5 mm in diameter represented by a set of particles with a diameter of 0.2 mm.

Fig. 4 presents a set of snapshots corresponding to Fr and We numbers of 639 and 395, respectively. The snapshots (a c d) correspond to the experimental photos by Liow and Fig. 4b illustrates the pressure field at the impact instant. Fig. 4c depicts the initiation of splash and Fig. 4d shows a fully developed crown with splash drops, which is in agreement with the experiment in terms of the reproduced crown shape, splash drops and the angle of their ejection (45° to the horizontal).

Fig. 4a and (b) depict snapshots of particles corresponding to two other cases with with Fr = 301 and We = 186 (Fig. 5a), and Fr = 490 and We = 296 (Fig. 5b). These snapshots correspond to the experimental photos shown in Fig. 5a1 and (b1), respectively. Consistent with the experiment, Fig. 5a illustrate the formation of a mild annular spray. The reproduced free-surface profile including the curvature of annular spray are in agreement with the experiment. For the case depicted by Fig. 5b, the crown is not fully developed at the shown instant, consistent with the experiment.
Fig. 5 Water drop impact - results by improved MPS with the Laplacian-based surface tension model for $Fr = 301$ and $We = 186$ (a), and $Fr = 490$ and $We = 296$ (b) - experiment photos by Liow.

Fig. 6 Water drop impact - results by improved MPS without any surface tension models (a), with Laplacian-based surface tension model (b) and with arc fitting one (c) - $Fr = 639$ and $We = 395$ - experiment photo by Liow.

Fig. 6 shows a comparison in between the Laplacian-based surface tension model and arc fitting one. The snapshot shown in Fig. 6(a) corresponds to the improved MPS without any surface tension models, characterized by moderate unphysical fragmentations so that a clear formation of splash drops cannot be seen. Incorporation of Laplacian-based surface tension model has resulted in a better reproduction of the crown development as well as splash drops (Fig. 6b). The arc fitting model$^{9}$, in contrary, has somehow deteriorated the simulation results as it has apparently increased the unphysical particle dispersiveness at the free-surface (Fig. 6c).

5. CONCLUDING REMARKS

A novel surface tension model is proposed for macroscopic particle methods. The distinct feature of the newly proposed model corresponds to a novel scheme presented for a direct and precise evaluation of curvature by a meticulous approximation of Laplacian of color function.

The new surface tension model is applied together with an enhanced MPS method for splash computation corresponding to a water drop impact. The enhanced performance of the Laplacian-based model has been further verified via comparisons made with two other surface tension models.

REFERENCES