Application of Localized Implicit Iterative Particle Shifting on Free Surface Flows

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I. INTRODUCTION

This study focuses on Weakly-Compressible SPH (WCSPH) [1], which conserves mass, linear, and angular momentum but suffers from irregular particle distributions which limits the accuracy of the spatial discretization. Particle Shifting Techniques (PSTs), like the Explicit shifting technique [2], improve the stability and accuracy by applying Fick's diffusion law [3], but do not guarantee uniform particle distribution throughout the simulation.

Recently, implicit shifting methods have been developed to address the limitations of explicit approaches. Among these, the Implicit Iterative Shifting (IIPS) technique introduced by Rastelli et al. [4] ensures a homogeneous particle distribution across the domain. However, this method is associated with high computational costs, large memory requirements, and large shifting magnitudes. To overcome these issues, A Novel Implicit Iterative Shifting (NIIPS) formulation that incorporates neighboring particles in the self-interaction term of the second kernel derivative (neglected in [4]) is proposed in the present work with the aim of producing a more stable particle distribution. Furthermore, to significantly reduce computational cost and memory usage, the NIIPS method is selectively activated in specific regions with irregular particle distribution, thereby localizing its application. This approach introduces the concept of Localized NIIPS (L-NIIPS). Additionally, in the L-NIIPS, shifting magnitudes are restricted to 5% of the particle spacing enhancing the overall accuracy and ensuring better coherency of the computed physical quantities.

In this work the Standard WCSPH formulation [1] is adopted to discretize the Navier-Stokes equation. Furthermore, the system is solved using a second-order Runge-Kutta (RK2) time integration scheme, with no diffusion terms [5] in the continuity equation as they might mask the effects of non-uniform particle distribution on the physical quantities. Finally, a linear approximation of first-order Taylor expansion is implemented to update the physical quantities at the new particle position. The proposed L-NIIPS algorithm is assessed using the oscillating droplet test case. To the best of the author's knowledge this work demonstrates, for the first time, the applicability of an implicit iterative shifting formulation to a scenario involving a time-varying free surface.

II. NOVEL IMPLICIT ITERATIVE SHIFTING (NIIPS)

The gradient of particle concentration is represented as a 2D function $\nabla C(\mathbf{X}, \mathbf{Y})$. Let $\mathbf{X} = (x_1, x_2, \ldots, x_i, \ldots, x_n)$ and $\mathbf{Y} = (y_1, y_2, \ldots, y_i, \ldots, y_n)$ be the arrays of particle positions. The objective of the IIPS procedure is to find new particle positions $\bar{\mathbf{X}} = (\bar{x}_1, \ldots, \bar{x}_i, \ldots, \bar{x}_n)$ and $\bar{\mathbf{Y}} = (\bar{y}_1, \ldots, \bar{y}_i, \ldots, \bar{y}_n)$ that satisfies the following equation [4]:

$$\nabla C_i(\bar{\mathbf{X}}, \bar{\mathbf{Y}}) = 0, \quad \forall \quad i = 1, \ldots, n. \tag{1}$$

Using the Eq. (1) as the inspiration point from IIPS formulation introduced by Rastelli et al. [4], led us to obtain the system of linear equations below (called NIIPS), with all the details and mathematical derivations to be presented in the conference.

$$\underbrace{\begin{bmatrix} \nabla^2_x W_{11}\omega_1 - \phi_{1xx} & \nabla^2_{xy} W_{11}\omega_1 - \phi_{1xy} & \cdots & \nabla^2_x W_{1i}\omega_i & \nabla^2_{xy} W_{1i}\omega_i & \cdots & \nabla^2_x W_{1n}\omega_n & \nabla^2_{xy} W_{1n}\omega_n \\ \nabla^2_{yx} W_{11}\omega_1 - \phi_{1yx} & \nabla^2_y W_{11}\omega_1 - \phi_{1yy} & \cdots & \nabla^2_{yx} W_{1i}\omega_i & \nabla^2_y W_{1i}\omega_i & \cdots & \nabla^2_{yx} W_{1n}\omega_n & \nabla^2_y W_{1n}\omega_n \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \nabla^2_x W_{i1}\omega_1 & \nabla^2_{xy} W_{i1}\omega_1 & \cdots & \nabla^2_x W_{ii}\omega_i - \phi_{ixx} & \nabla^2_{xy} W_{ii}\omega_i - \phi_{ixy} & \cdots & \nabla^2_x W_{in}\omega_n & \nabla^2_{xy} W_{in}\omega_n \\ \nabla^2_{yx} W_{i1}\omega_1 & \nabla^2_y W_{i1}\omega_1 & \cdots & \nabla^2_{yx} W_{ii}\omega_i - \phi_{iyx} & \nabla^2_y W_{ii}\omega_i - \phi_{iyy} & \cdots & \nabla^2_{yx} W_{in}\omega_n & \nabla^2_y W_{in}\omega_n \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \nabla^2_x W_{n1}\omega_1 & \nabla^2_{xy} W_{n1}\omega_1 & \cdots & \nabla^2_x W_{ni}\omega_i & \nabla^2_{xy} W_{ni}\omega_i & \cdots & \nabla^2_x W_{nn}\omega_n - \phi_{nxx} & \nabla^2_{xy} W_{nn}\omega_n - \phi_{nxy} \\ \nabla^2_{yx} W_{n1}\omega_1 & \nabla^2_y W_{n1}\omega_1 & \cdots & \nabla^2_{yx} W_{ni}\omega_i & \nabla^2_y W_{ni}\omega_i & \cdots & \nabla^2_{yx} W_{nn}\omega_n - \phi_{nyx} & \nabla^2_y W_{nn}\omega_n - \phi_{nyy} \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} \delta x_1 \\ \delta y_1 \\ \vdots \\ \delta x_i \\ \delta y_i \\ \vdots \\ \delta x_n \\ \delta y_n \end{bmatrix}}_{\delta\mathbf{r}} \approx \underbrace{\begin{bmatrix} \nabla_x C_1 \\ \nabla_y C_1 \\ \vdots \\ \nabla_x C_i \\ \nabla_y C_i \\ \vdots \\ \nabla_x C_n \\ \nabla_y C_n \end{bmatrix}}_{\mathbf{B}} \tag{2}$$

This system represents a linear equation $\mathbf{A}\delta\mathbf{r} = \mathbf{B}$ to solve for the shifting vectors ($\delta\mathbf{r}$). The ϕ terms which are the novelty of this work, represent the contributions of neighbors in the self-interaction terms (main diagonal of the linear system) and are defined as follows:

$$\begin{cases} \phi_{1xx} = \sum_{k=2}^{K} \frac{\partial^2 W(x_{1k}, y_{1k})}{\partial x_1^2}\omega_k, \quad \phi_{1xy} = \sum_{k=2}^{K} \frac{\partial^2 W(x_{1k}, y_{1k})}{\partial x_1 \partial y_1}\omega_k, \quad \phi_{1yy} = \sum_{k=2}^{K} \frac{\partial^2 W(x_{1k}, y_{1k})}{\partial y_1^2}\omega_k \\ \phi_{ixx} = \sum_{k=1, k\neq i}^{K} \frac{\partial^2 W(x_{ik}, y_{ik})}{\partial x_i^2}\omega_k, \quad \phi_{ixy} = \sum_{k=1, k\neq i}^{K} \frac{\partial^2 W(x_{ik}, y_{ik})}{\partial x_i \partial y_i}\omega_k, \quad \phi_{iyy} = \sum_{k=1, k\neq i}^{K} \frac{\partial^2 W(x_{ik}, y_{ik})}{\partial y_i^2}\omega_k \\ \phi_{nxx} = \sum_{k=1, k\neq n}^{K} \frac{\partial^2 W(x_{nk}, y_{nk})}{\partial x_n^2}\omega_k, \quad \phi_{nxy} = \sum_{k=1, k\neq n}^{K} \frac{\partial^2 W(x_{nk}, y_{nk})}{\partial x_n \partial y_n}\omega_k, \quad \phi_{nyy} = \sum_{k=1, k\neq n}^{K} \frac{\partial^2 W(x_{nk}, y_{nk})}{\partial y_n^2}\omega_k \end{cases} \tag{3}$$

The matrix $\mathbf{A}$ is sparse with a size of $2n \times 2n$ in 2D, where n is the number of fluid particles in the domain. Following Rastelli et al. [4], we use the BiCGSTAB solver with the Jacobi preconditioner for faster convergence to solve the system of linear equations in Eq. (2).

III. LOCALIZATION PROCEDURE OF THE NOVEL IMPLICIT ITERATIVE SHIFTING (L-NIIPS)

In addition to the novel formulation described in the previous section, in the present work we reduced the high computational cost and memory usage (due to the size of the linear system) and the large shifting magnitude which is obtained for some particles if the standard IIPS formulation is adopted. We propose to shift only particles with ∇C above the pre-defined threshold, along with their neighbors, reducing the linear system size. These changes reduce memory usage and improve both efficiency and numerical accuracy by limiting shifting magnitudes to 5% of particle spacing. Algorithm 1 presents the L-NIIPS localization procedure and its application.

Algorithm 1

procedure LOCALIZATION OF THE NOVEL IMPLICIT ITERATIVE SHIFTING (L-NIIPS) TECHNIQUE
  Set a desired $L_\infty(\nabla C)_{\text{thr}}$
  Set a desired maximum shifting value
  Initialize an array named Shift_i to zero
  Initialize an array named Flag_i to zero
  Compute $h \cdot |\nabla C_i|$ for all particles and then $L_\infty(\nabla C)$
  For each fluid particle i:
  if $h \cdot |\nabla C_i| > L_\infty(\nabla C)_{\text{thr}}$ **then**
    $\text{Flag}_i = 1$
    $\text{Flag}_j = 1$, if particle j is a neighbor of particle i (except free surface and solid wall particles)
  end if
  while $(L_\infty(\nabla C) > L_\infty(\nabla C)_{\text{thr}}$ **and** $\max(\text{Shift}) >$ maximum shifting value) **do**
    Assemble the linear system with the particles where $\text{Flag}_i = 1$
    Solve the linear system to obtain shifting values $(\delta \mathbf{r}_i)$
    Shift_i += $(\delta \mathbf{r}_i)$
    Update particles' position
    Recompute $h \cdot |\nabla C_i|$, and then $L_\infty(\nabla C)$ (this time just for the particles where Flag $= 1$)
  end while
end procedure

IV. RESULTS (OSCILLATING DROPLET)

The formulation is tested against a single-phase oscillating droplet under the influence of a central conservative force field. This test case was chosen due to a time-evolving periodic free-surface condition that causes significant distortion in the particle distribution, other test cases cannot be included here due to the lack of space and they will be shown at the conference. In this study, the test case is simulated using the L-NIIPS proposed herein, along with the Explicit shifting approach [2]. The conservative force is defined as $\mathbf{f} = -\Omega^2 \mathbf{r}$ where Ω is a dimensional parameter. Initially, the droplet is circular and oscillates with period T, forming an ellipse. The oscillation period is $T \simeq 4.827R$. The analytical solution is used for validation under inviscid flow assumption [6], with initial simulation parameters detailed in Table I.

The time evolution of the droplet's axes, using the L-NIIPS formulation, is compared with the analytical solution in Fig. 1. As observed at the non-dimensional time $\frac{tU}{R} = 15.687$, the errors in the semi-major and semi-minor axes, with respect to the analytical solution, are 2.2% and 2.4%, respectively. Moreover the evolution of kinetic and potential energy is shown in Fig. 2. The numerical results align well with the analytical solution, with slight decreases in the axes and energy values over time due to numerical dissipation.

Figs. 3 and 4 show the particle distribution for the L-NIIPS formulation at the non-dimensional time $\frac{tU}{R} = 15.687$. As a brief recap of the method, free-surface particles (red) are not shifted, while free-surface neighbors (gray) are treated like inner fluid particles. After 3.25 oscillations, Fig. 4 demonstrate that the

TABLE I
OSCILLATING DROPLET, NUMERICAL SETUP

Symbol	Parameter	Value	Unit
Δ	Particle spacing	0.01	m
R	Radius	1.0	m
σ_0	Transient velocity	1.0	s^{-1}
Ω	Dimensional parameter	1.0	s^{-1}
t	Simulation time	20.0	s
C	Speed of sound	15.0	m/s
U	Reference velocity	1.0	m/s
ρ	Reference density	1000.0	kg/m^3
$\frac{h}{\Delta}$	-	1.5	-
α	Artificial viscosity	0.015	-
$L_\infty(\nabla C)_{\text{thr}}$	Threshold	0.01	-

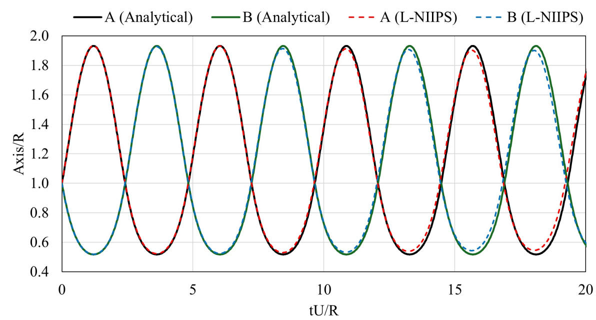

Fig. 1. Oscillating Droplet. L-NIIPS approach, validation of semi-major, semi-minor axes.

L-NIIPS achieves a uniform distribution, including the region near free surface, without any special treatment.

Fig. 5 shows the mechanical energy error (computed as the sum of kinetic and potential energy) for the Explicit shifting and L-NIIPS methods. As observed at the non-dimensional time $\frac{tU}{R} = 20.0$, the improved particle distribution achieved with the L-NIIPS method, enhances the dissipation of the numerical scheme by 43% compared to the Explicit shifting approach.

Finally, in Table II, a comparison for the computational cost of the Explicit shifting and L-NIIPS is shown, in comparison

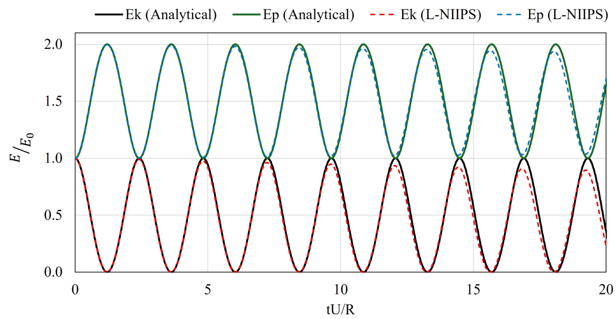

Fig. 2. Oscillating Droplet. L-NIIPS approach, validation of kinetic and potential energy

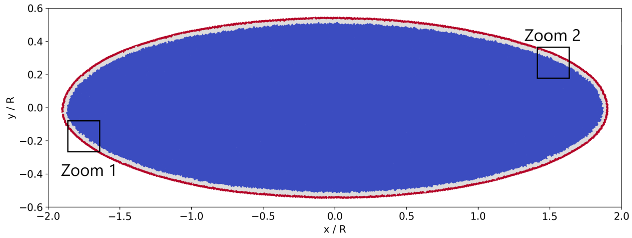

Fig. 3. Oscillating Droplet. L-NIIPS approach, particle distribution at the non-dimensional time $\frac{tU}{R}$ = 15.687 (T = 3.25).

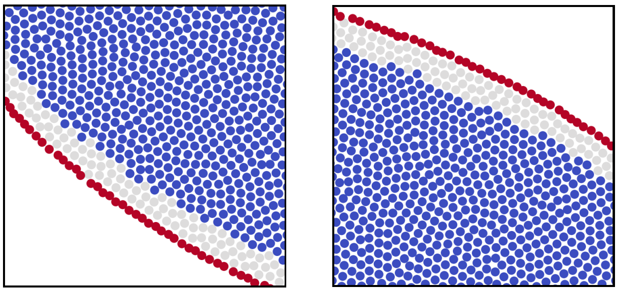

Fig. 4. Oscillating Droplet at the non-dimensional time $\frac{tU}{R} = 15.687$. L-NIIPS approach, two zoomed particle distribution (left) Zoom 1 and (right) Zoom 2.

with the computational cost relative to the simulation without any shifting (No-Shifting) procedure. As shown, the L-NIIPS is only 26% more expensive than the Explicit shifting. This is achieved mainly thanks to the localization procedure, which significantly reduces the size of the linear system of Eq. (2) iteratively solved every time that the L-NIIPS is activated. As shown in Fig. 6, less than 7% of the particles are included in the linear system of Eq. (2) in every timestep.

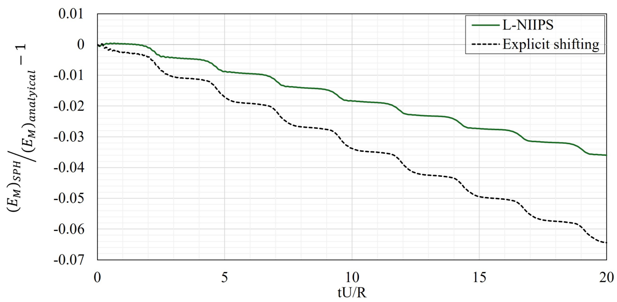

Fig. 5. Oscillating Droplet. Mechanical energy error.

TABLE II
OSCILLATING DROPLET. RELATIVE CPU TIME COMPARISON.

No-Shifting	L-NIIPS	Explicit Shifting
1.0	1.36	1.10

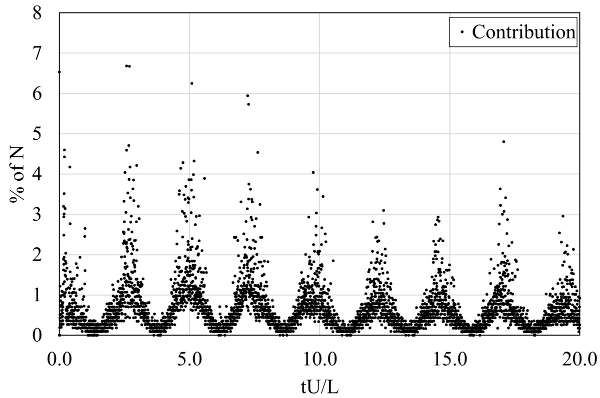

Fig. 6. Oscillating Droplet. L-NIIPS approach, contributed particles in the localization procedure.

V. Conclusion and Future Works

This paper introduces the Novel Implicit Iterative Particle Shifting (NIIPS) formulation as a more stable approach for achieving a guaranteed uniform particle distribution by accounting for the influence of neighboring particles. The Local NIIPS (L-NIIPS) procedure limits the shifting magnitude, and effectively reduces both computational cost and memory usage. The results demonstrate that L-NIIPS successfully simulates the oscillating droplet, a challenging SPH benchmark test case, due to its periodic free-surface condition. Finally, the proposed methods, along with their mathematical derivations, have been validated using test cases such as the Taylor-Green vortex, moving square box, impinging jet, and dam break, with detailed results to be presented during the oral presentation.

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