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IMPROVING THE INCOMPRESSIBILITY CONDITION OF THE EXPLICIT SPH METHOD USING THE CONTROL THEORY

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ABSTRACT

The conventional smoothed particle hydrodynamics (SPH) method is inherently an explicit scheme; the modeling of weakly compressible flows must imply an equation of state to link the mass density with the pressure. Unfortunately, the SPH scheme has an outstandingly high computational performance requirement, especially in the case of small time step sizes applied due to the large stiffness. Therefore in practice, the speed of sound is usually reduced artificially to meet the requirements of the given fluid flow problem in terms of the compressibility rate. Unfortunately, this approach still demands very low time step sizes in most cases. In this paper, we introduce an excessively simple improvement of the weakly compressible variant of the SPH scheme to achieve a considerably stiffer fluid without the demand for a smaller time step size and additional computational requirement. The present work's motivation was to eliminate the remnant density variance under constant pressure by introducing an integral and differential term in the equation of state analogously with ProportionalâĂŞIntegralâĂŞDerivative (PID) controls. The model was tested through simple two-dimensional hydrostatic and dam break cases.

Keywords: control theory, incompressibility, particle methods, smoothed particle hydrodynamics, SPH

NOMENCLATURE

K_d	$[m^2/s]$	Differential gain
K_i	$[m^2/s^3]$	Integral gain
K_p	$[m^2/s^2]$	Proportional gain
V	$[m^3]$	Particle volume
W	$[1/m^2]$	Smoothing kernel function
Δt	[s]	Time step size
c	[m/s]	Speed of sound
h	[m]	Smoothing distance
m	[kg]	Particle mass
n_b	[−]	Number of neighbours
p	[Pa]	Pressure
q	[−]	Dimensionless distance
$\underline{a}$	$[m/s^2]$	Particle acceleration
$\underline{g}$	$[m/s^2]$	Gravitational acceleration
$\underline{r}$	[m]	Particle position
$\underline{v}$	[m/s]	Particle velocity
γ	[−]	Specific heat ratio
ν	$[m^2/s]$	Kinematic viscosity
ρ	$[kg/m^3]$	Mass density
ρ_0	$[kg/m^3]$	Reference density

Subscripts and Superscripts

i	Index of the particle in interest
j	Index of neighbouring particles
n	Time level

1. INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) is a Lagrangian particle-based meshless collocation scheme introduced by Gingold and Monaghan in 1977 [1] and independently by Lucy [2]. The motivation was the accurate modeling of self-gravitating interstellar gases without boundary conditions. Later, in 1994 Monaghan presented the simulation of coastal free surface flows using the SPH method [3], providing a novel approach of fluid flow modeling in the field of coastal engineering. Since then, SPH has been used successfully in many engineering and scientific areas of solid and fluid mechanics [4, 5, 6, 7, 8]. During the past decades, the conventional SPH method has been significantly improved in terms of the artificial diffusion [9, 10], adaptive spatial resolution [11, 12], and the treatment of undesired compressibility [13, 14].

Due to the lack of kinematic relation between the pressure and the velocity fields, the conventional explicit SPH scheme requires a suitable equation of state [13], that allows small density variations of fluids fulfilling the requirements of the given engineering problem. In most cases, the speed of sound is artificially reduced so that the density variance becomes larger than in real fluids but kept below a de-

sired threshold [15]. However, higher speed of sound results in stiffer systems with the need for smaller time step sizes, which is known to be a significant bottleneck of the weakly compressible variant of SPH.

Using the pressure projection method for incompressible fluids introduced in [16] is widely used in conventional computational fluid dynamics (CFD). Some of the earliest models of truly incompressible SPH (ISPH) schemes implying Chorin's decomposition were introduced and improved in the late 1990s and 2000s [17, 18, 19, 20, 21]. Although the ISPH scheme facilitates the modeling of incompressible fluid flows by avoiding the small time step size of weakly compressible models, the computational requirement per time step is significantly larger, not to mention the implementation issues that came with the semi-implicit solution of the elliptic pressure Poisson equation (PPE) over the continuously changing particle configuration [22].

Due to the large neighbourhood of each particle and changing interparticle distances, one of the drawbacks of the SPH method in general or other particle-based schemes is the high computational performance requirement, which made them too expensive for practical applications for decades. However, recently, the more and more frequent presence of massively parallel architectures made these methods more capable for the computations of some specific problems compared to the finite volume method (FVM) [23]. Although there are numerous techniques for the SPH scheme that imply the solution of the PPE, this approach is less straightforward than in the case of the mesh-based FVM. On the one hand, the assembly of the linear system of the PPE is computationally expensive due to the changing particle configurations, while on the other hand, the efficient solution of the sparse linear system is a challenging task on massively parallel devices. Due to the loss of efficient massive parallelization, the latter appears to be an essential difficulty of the ISPH method.

As an alternative approach, the recent advances made in ISPH computations are frequently subjects of techniques maintaining the explicit solution to utilise the massively parallel devices but reducing the compressibility rate or allowing larger time step size beside the same or smaller density variance. These methods are often referred to as explicit ISPH (EISPH) [22, 24, 25, 26]. Similarly to the truly incompressible SPH schemes, EISPH methods are based on Chorin's decomposition but avoid the solution of the PPE with a computationally intensive implicit algorithm such as the biconjugate gradient stabilized method (BiCGSTAB). Instead, they deal with iterative algorithms, which provide lower accuracy but cheaper solution at the same time.

In the present paper, we introduce a simple and efficient improvement of the weakly compressible SPH scheme allowing the simulation of incompressible fluids with a significantly reduced density error but without the direct or iterative solution of the PPE.

2. THE CONVENTIONAL SPH METHOD

As a fully meshless Lagrangian scheme, the convective and local terms of the changing of any quantity can be expressed by a single term as

$$\frac{d\varphi}{dt} = \frac{\partial\varphi}{\partial t} + \underline{v}\nabla\varphi, \tag{1}$$

where φ is any function and $\underline{v}$ is the velocity field. Using (1), an inviscid fluid is governed by

$$\begin{aligned} \frac{d\underline{v}}{dt} &= -\frac{1}{\rho}\nabla p + \underline{g} \\ \frac{d\rho}{dt} &= -\rho\nabla\underline{v}, \end{aligned} \tag{2}$$

where p and ρ are the pressure and density fields of the fluid and $\underline{g}$ is the gravitational acceleration. As a relation between the the density and the pressure fields, we apply a barotropic equation of state

$$p = p(\rho). \tag{3}$$

2.1. The numerical scheme

Similar to the Finite Difference Methods (FDM), the SPH scheme converts a set of partial differential equations (PDEs) to a larger set of coupled ordinary differential equations (ODEs). The coupling between the equations is determined by the interparticle interactions, where the particles are considered as the smallest and atomic volumes of the discretized matter.

A fundamental step in the discretization process is the choice of the discrete differential operators, to fulfill specific requirements such as conservativity or a given order of consistency. Using the discrete convolution

$$< f >_i = \sum_i^{n_b} V_j f_j W_{ij}, \tag{4}$$

where f is an arbitrary function over a set of particles, V_j is the volume of the jth particle and $W_{ij} = W(|\underline{r}_j - \underline{r}_i|, h)$ is the radially symmetric smoothing kernel function. Throughout the present paper we use the fifth order polynomial Wendland kernel function [27] defined in two dimensions as

$$\begin{aligned} W(|\underline{r}_j - \underline{r}_i|, h) &= \frac{7}{4\pi h^2}\left(1 - \frac{q}{2}\right)(2q+1), \\ q &= \frac{|\underline{r}_j - \underline{r}_i|}{h}, \end{aligned} \tag{5}$$

with h being the smoothing radius. After a few simple steps presented in [28], one can see that the derivatives of an arbitrary function can be approximated by replacing the derivative on the smoothing kernel function, hence we obtain

$$< \nabla f >_i = \sum_j^{n_b} V_j f_j \nabla W_{ij}. \tag{6}$$

However, the operator (6) turns out to be a bad choice

for most problems, due to the low order of consistency, the sensitivity to particle layout and the lack of conservativity. To address these issues, the fluid equations are usually discretized using the operators

$$
\begin{aligned}
(\mathrm{grad}p)_i &= <\nabla p>_i = \rho_i \sum_j^{n_b} \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) m_j \nabla W_{ij}, \\
(\mathrm{div}\underline{v})_i &= <\nabla \cdot \underline{v}>_i = \sum_j^{n_b} V_j(\underline{v}_j - \underline{v}_i)\nabla W_{ij},
\end{aligned}
\tag{7}
$$

for the pressure gradient and the divergence of the velocity [28]. Thus the discretized form of (2) yields

$$
\begin{aligned}
\frac{d\underline{v}}{dt} &= -\sum_j^{n_b} \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) m_j \nabla W_{ij} + \underline{g}, \\
\frac{d\rho}{dt} &= -\rho_i \sum_j^{n_b} V_j(\underline{v}_j - \underline{v}_i)\nabla W_{ij}.
\end{aligned}
\tag{8}
$$

In the case of weakly compressible flows, the most frequently used equation of state is the Tait's equation written as

$$
p_i = \frac{c^2\rho_0}{\gamma}\left(\left(\frac{\rho_i}{\rho_0}\right)^\gamma - 1\right), \tag{9}
$$

where γ and ρ_0 are the specific heat ratio and the reference density respectively. For water, γ is often set to be 7, which results in a stiffer behaviour in terms of compressibility.

2.2. Integration in time

As a meshless particle based method, the discretisation (7) converts the governing PDE's into a set of ODE's, which can be solved by numerical integration. Here we use the velocity-Verlet scheme [29], which is expressed as

$$
\begin{aligned}
\underline{r}_i^{n+1} &= \underline{r}_i^n + \underline{v}_i^n \Delta t + \frac{1}{2}\underline{a}_i^n \Delta t^2, \\
\underline{v}_i^{n+1} &= \underline{v}_i^n + \frac{\underline{a}_i^n + \underline{a}_i^{n+1}}{2}\Delta t,
\end{aligned}
\tag{10}
$$

where the superscript n denotes the time level, $\underline{a}_i$ is the acceleration of the ith particle and Δt is the time step size. For the integration of the continuity equation we use the simple explicit Euler scheme:

$$
\rho_i^{n+1} = \rho_i^n + \left.\frac{d\rho}{dt}\right|_i^n \Delta t. \tag{11}
$$

The adaptive time stepping scheme applied in the present paper is written as

$$
\Delta t = CFL \cdot \min\left(\sqrt{\frac{h}{\max_i |\underline{a}|_i}}, \frac{h}{c}\right), \tag{12}
$$

where $CFL = 0.2$ is the Courant-Friedrichs-Lewy number.

3. MODIFIED EQUATION OF STATE

Apart from a few exceptions, the objective of liquid simulations in SPH reads as

$$
\mathrm{div}\underline{v} = 0. \tag{13}
$$

Unfortunately, the application of the equation of state (9) results in a remnant density deviation even in the case of hydrostatic problems. The reason is that the interparticle pressure forces can be considered as spring forces with complicated spring coefficients deduced from the equation of motion. Although the desired density field is

$$
\rho_i = \rho_0, \tag{14}
$$

it can never be reached using (9), because the corresponding pressure vanishes. This problem is in strong analogy with a simple mass-spring system, where the spring has to be deformed to compensate any constant forces acting on the mass, leading to a remnant offset of the position. It is obvious that the offset can be reduced by increasing the spring coefficient, but it cannot be eliminated without knowing the history of the motion.

One of the simplest techniques for the elimination of the remnant offset is the application of a controller with an integration term. Let us consider an error $\epsilon(t) = \phi(t) - \phi_0$, where ϕ_0 is the desired value for $\phi(t)$. The output of a PID-controller to minimise $\epsilon(t)$ can be written as

$$
u(t) = K_p\epsilon(t) + K_i \int_0^t \epsilon(\tau)d\tau + K_d\frac{d\epsilon(t)}{dt}, \tag{15}
$$

where the K coefficients are the proportional, integral and differential gains (cf. [30]). After rewriting (15) for the density and pressure, we obtain

$$
p_i = K_p(\rho_i - \rho_0) + K_i \int_0^t (\rho_i - \rho_0)d\tau + K_d\left.\frac{d\rho}{dt}\right|_i. \tag{16}
$$

It is worth remarking that the first term is identical with the right-hand side of the conventional SPH equation of state (9) when $\gamma = 1$ and $K_p = c^2$. The second term accumulates the density deviation in time and tunes the pressure value so that the density error becomes smaller. Finally, using (2) and the third term of (16) pressure gradient

$$
(\mathrm{grad}p)_i = \mathrm{grad}(\mathrm{div}\underline{v})_i \tag{17}
$$

becomes a bulk viscosity term. This term might also be used as an artificial viscosity in the momentum equation without the computation of any other particle interaction operator. Since the computation of the artificial viscosity proposed by Morris [31] can be eliminated, the computational cost per time step can be significantly reduced.

3.1. Setting the gain coefficients

For the sake of simplicity, we set the proportional term to be the same as in Tait's equation (9). However, to ensure numerical stability and efficiency in terms of density variance reduction, we propose

the gains for the integral and differential terms as

$$K_i = 0.001c^3/h, \qquad K_d = ch \tag{18}$$

which provide numerically stable simulation regardless of the particle size and artificial speed of sound. Thus the complete equation of state reads as

$$p_i = \frac{c^2\rho_0}{\gamma}\left(\left(\frac{\rho_i}{\rho_0}\right)^{\gamma} - 1\right) + \frac{c^3 h}{10^3}\int_0^t (\rho_i - \rho_0)d\tau + ch\left.\frac{d\rho}{dt}\right|_i, \tag{19}$$

where the numerical integration of the second term on the right hand side is computed using the explicit Euler scheme

$$R_i^{n+1} = R_i^n + \Delta t(\rho_i^n - \rho_0), \tag{20}$$

where

$$R_i^n \approx \int_0^{n\Delta t} (\rho_i - \rho_0)d\tau. \tag{21}$$

It can be seen that the pressure computed using the improved equation of state (19) does not require any significant additional operations. The temporal derivative of the density is computed in (8) regardless of the modification, while the integral term sums the error per particle without the computation of any particle interactions.

4. RESULTS

In this section, we present simple SPH benchmark cases using the conventional Tait's equation (9) and the modified equation of state (19), including the integral and differential terms.

4.1. 2D hydrostatic problem

The first test case has been chosen as the simplest verification of the improved model by monitoring the temporal density variation of the fluid and the steady-state density distributions compared to the conventional equation of state. The investigated hydrostatic problem is shown in Figure 1.

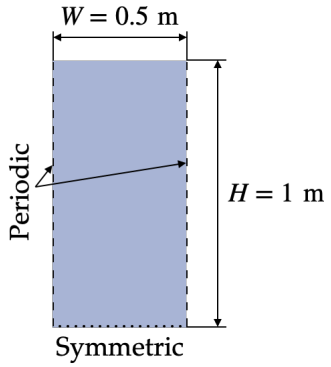

Figure 1. Geometry of the hydrostatic problem. The boundary conditions are periodic at the vertical and symmetric at the bottom boundaries.

The initial condition of the discretisation is chosen to be a relaxed particle layout but with a spatially constant density distribution $\rho = \rho_0$. As a weakly compressible fluid, the density distribution changes in time due to the gravitational forces until a steady-state is reached, when the weight of the liquid and the pressure forces counterbalance each other. The time series of the average density in the case of the original and improved models can be seen in Figure 2. The oscillations of the density are similar; however, the improved equation of state provides a more accurate steady-state density with virtually zero deviation from the reference density. The spatial distributions of the density and pressure are shown in Figure 3. As expected, the pressure distributions are similar, but the densities are different. This is because the density and pressure fields are no longer in total correspondence with the novel equation of state. Using the integral term in (19) the density becomes constant in case of a hydrostatic problem. However, the modified equation of state is accountable for the small fluctuations in the pressure distribution caused by the slightly less uniform particle layout of the hydrostatic case.

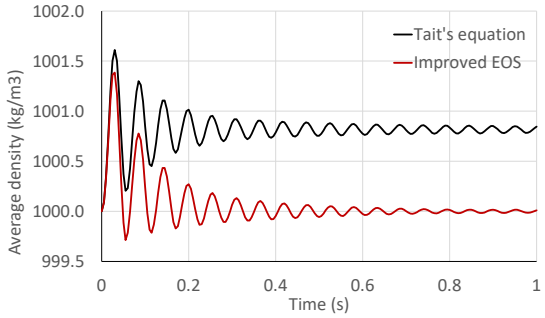

Figure 2. Time series of the average density in case of *a*. Tait's equation and *b*. the improved equation of state (EOS).

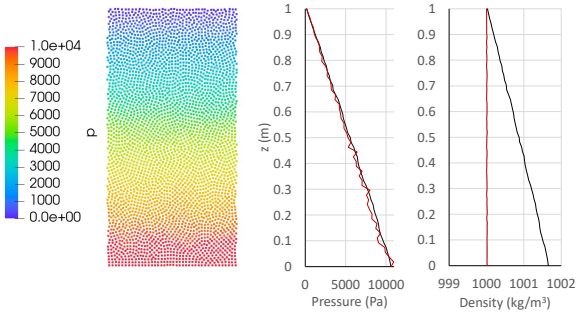

Figure 3. Density and pressure distributions along the vertical axis. Black and red lines show the distributions obtained from the original and modified equation of states respectively.

4.2. 2D dam break

The dam break problem is one of the most frequently referred benchmark cases of the SPH method. Here we present the results of a two-

dimensional case adopted from the DualSPHysics examples [32]. The geometry and the initial layout are presented in Figure 4. The fluid column is initially at rest at the bottom left corner and released at $t = 0$. Like the hydrostatic case, we performed the computations with both the conventional and the improved equation of states. The total number of particles was 21000, while the average time step size was $4.741 \cdot 10^{-5}$ s in both cases, resulting in the same computational time. In Figure 5, the time series

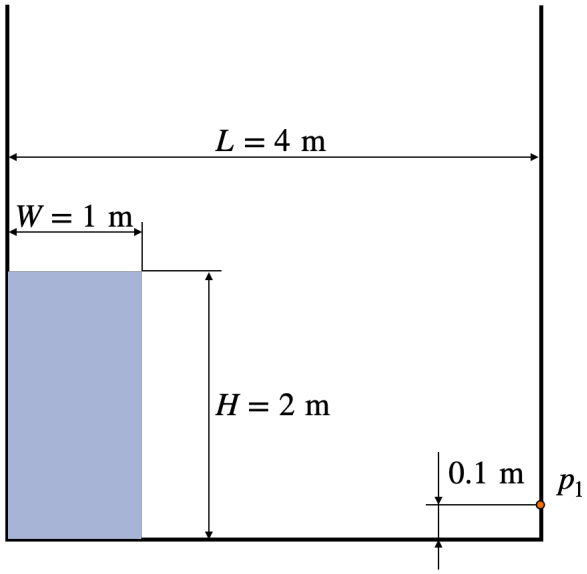

Figure 4. Initial layout of the dam break problem. The p_1 point marks the location of the pressure probe.

of the pressure at the p_1 probe shows that the original and the improved model are in good agreement. However, as expected, due to the additional integral term in (19), the proposed scheme provides consistently higher pressure values at the wall in order to force the density values closer to the reference density. The same behaviour can be observed in terms of the global average of the density in Figure 6. Although the qualitative behaviour is similar, the density approaches the reference value more accurately than the original simulation. The instantaneous

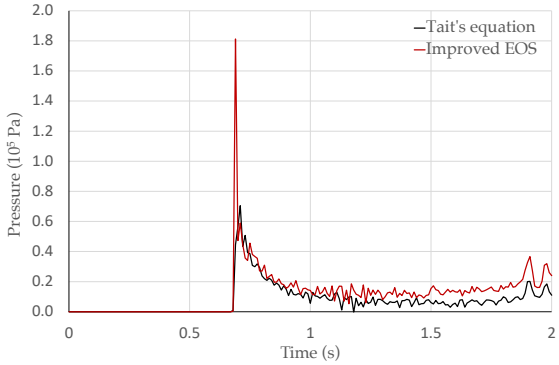

Figure 5. Pressure time series at point p_1.

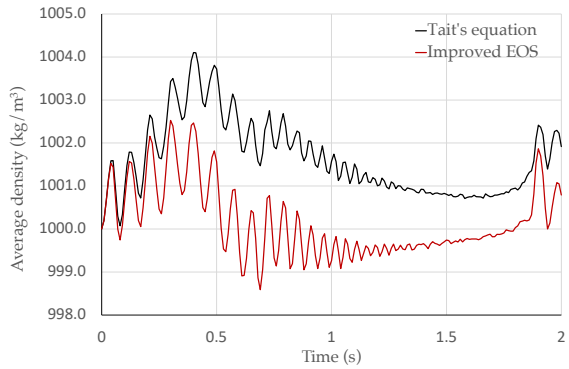

Figure 6. Average density of the fluid particles in the function of time.

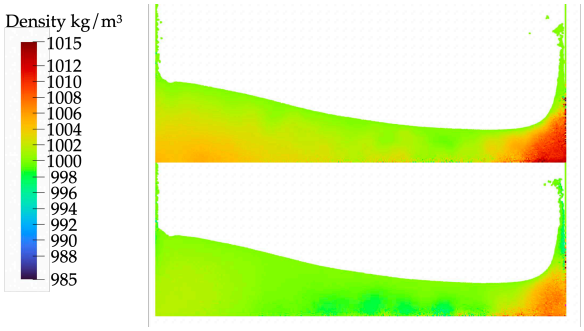

Figure 7. Instantaneous density distribution of the fluid after the collision with the right hand side of the tank wall at t=0.8 s. Top: Tait's equation, bottom: Modified eqaution of state.

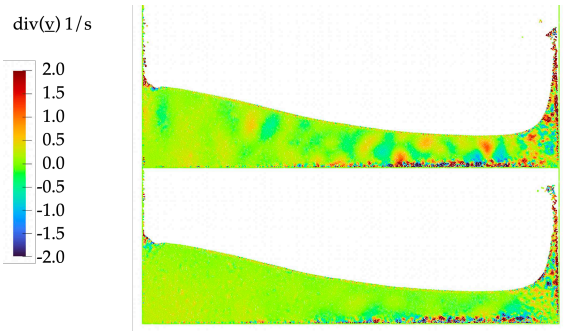

Figure 8. Divergence of the velocity at t=0.8 s. Top: Tait's equation, bottom: Modified eqaution of state.

density distribution after the collision with the tank wall is shown in Figure 7. Another valuable marker of the incompressibility is the divergence of the velocity field, which is presented at the same time instant in Figure 8. Apart from the near-wall fluctuations, it can be seen that the oscillations with long wavelengths are almost completely eliminated in the fluid. Although the constant density and divergence-free velocity field cannot be achieved by an explicit scheme, both of them are significantly improved without any additional computational time.

5. CONCLUSIONS

Motivated by the PID control theory, the present paper introduces a simple improvement of the weakly compressible SPH scheme by implying an integral and differential term in the conventional Tait's equation of state. Since the additional terms only use collocation-dependent quantities that are already computed in most SPH solvers, the computational requirement of the proposed modification is negligible. We present the efficiency of the improvement by two simple test cases of a hydrostatic and a dam break problem. Although the simulations are not truly incompressible, as in the case of an ISPH technique, the density and velocity divergence fields are considerably closer to the desired distributions in both cases. Moreover, in the case of the hydrostatic problem, the fluid reaches the desired reference density over the whole fluid domain. Since the motion of the particles is dependent on the instantaneous local configuration, the model could be further improved by choosing the differential and integral gains adaptively.

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