Augmented Lagrangain SPH Method for Incompressible Flows

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***Abstract*—Incompressibility is a challenge in the context of Smoothed Particle Hydrodynamics (SPH). There are two major approaches to handle the Incompressibility; weakly compressible and fully incompressible SPH methods. In the present work, a SPH method based on the augmented Lagrangian method is proposed. In this method, it is assumed that the density is constant. However, the pressure is obtained from an equation of state. To achieve the divergence-free velocity field, the calculation of velocity and pressure are repeated iteratively. So, it is categorized as density-based method. Here, a new augmented Lagrangian SPH method is developed and the results are compared with those of a recent modified version of the weakly compressible SPH method in two illustrative 1D and 2D incompressible flow problems. It has been observed that the results of the proposed method overcome the pressure oscillations much better in comparison with those of the weakly compressible method.**

I. Introduction

As it is well known, the weakly compressible Smoothed Particle Hydrodynamics (WCSPH) method suffers from some difficulties especially in simulation of incompresible flows. One of them is non-physical oscillations especially in the pressure field. This is known as the *checker-board* problem and may arise in collocated methods [1]. High frequency (short wave length) spurious oscillations are preventable using suitable spatial discretization schemes [2]–[4].

In the present work, a new augmented Lagrangian SPH methods is proposed and compared with a recent modified version of the WCSPH method for unsteady incompressible flows. The proposed SPH method is based on the Augmented Lagrangian method [5], [6], an alternative to the aforementioned approaches, which is situated between the two others. In this method, it is assumed that the density is constant, however, the pressure is obtained from an equation of state. To achieve the divergence-free velocity field, the calculation of velocity and pressure are repeated iteratively [7].

In the following, the proposed augmented Lagrangian SPH method is introduced and the results are compared in two illustrative 1D and 2D incompressible flow problems.

II. SPH Methods

In this paper, the first derivative of an arbitrary field function u at particle (point) i is approximated using

$$\langle \nabla u \rangle_i = \sum_j \omega_j \mathbf{B}_i \cdot \nabla W_{ij} \left(u_j - u_i \right), \tag{1}$$

where j denotes the neighboring particles (points) including the particle i, u_j is the (estimated) value of u at particle j, and ω_j is the infinitesimally small volume for particle j. Also, $W_{ij} = W(r_{ij}, h)$ is the smoothing or kernel function which is a smoothed version of the Dirac delta function and is positive for $r_{ij} = |\mathbf{r}_{ij}| < h$ with a compact support of radius h [8].

Further,

$$\mathbf{B}_i = -\left[\sum_j \omega_j \nabla W_{ij} \mathbf{r}_{ij} \right]^{-1}, \tag{2}$$

is the (first derivative) renormalization tensor introduced by Randles and Libersky [9].

Here, also, the second derivative is approximated by the scheme proposed in [10] *i.e.*

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \psi_{ij} \left(u_j - u_i \right), \tag{3}$$

where,

$$\psi_{ij} = 2\hat{\mathbf{B}}_i : \Psi_{ij}, \tag{4}$$

and

$$\Psi_{ij} = \omega_j \left(\frac{\mathbf{e}_{ij}}{r_{ij}} \nabla W_{ij} + \mathbf{S}_{e2} \cdot \mathbf{B}_i \cdot \nabla W_{ij} \right), \tag{5}$$

in which $\mathbf{e}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}}$ and $\mathbf{S}_{e2} = \sum_j \omega_j \mathbf{e}_{ij} \mathbf{e}_{ij} \nabla W_{ij}$. Also, $\hat{\mathbf{B}}$ is the Laplacian renormalization tensor given by

$$\hat{\mathbf{B}}_i : \mathbf{Z}_i = \mathbf{I}, \tag{6}$$

where

$$\mathbf{Z}_i = \sum_j \Psi_{ij} \mathbf{r}_{ij} \mathbf{r}_{ij}. \tag{7}$$

A. Weakly compressible method

Here, we uses a modified form of the algorithm in [3] which also resolves the checker-board problem. The procedure is as follows.

First, estimate an intermediate velocity field $\mathbf{V}^*$ by omitting the pressure term

$$\rho\left(\frac{\mathbf{V}^* - \mathbf{V}^n}{\Delta t}\right) = \mu\left\langle\nabla\cdot\nabla\mathbf{V}^n\right\rangle + \rho\mathbf{g}, \tag{8}$$

where, $\mathbf{g}$ is the acceleration due to a body force, and ρ, μ, and $\mathbf{V}$ are density, viscosity, and velocity vector of the fluid, respectively.

Then, find the new pressure

$$\frac{P^{n+1} - P^n}{\Delta t} = -\rho c^2\left(\left\langle\nabla\cdot\mathbf{V}^*\right\rangle - \Delta t\frac{\left\langle\nabla\cdot\nabla P^n\right\rangle}{\rho}\right), \tag{9}$$

where, P and c are fluid pressure and speed of sound.

Next, the new velocity is calculated using

$$\mathbf{V}^{n+1} = \mathbf{V}^* - \Delta t\frac{\left\langle\nabla P^{n+1}\right\rangle}{\rho}. \tag{10}$$

Finally, update the positions

$$\frac{\mathbf{r}^{n+1} - \mathbf{r}^n}{\Delta t} = \frac{1}{2}\left(\mathbf{V}^n + \mathbf{V}^{n+1}\right). \tag{11}$$

Although the above formulation resolves the difficulties of the standard form of weakly compressible method, however, there is still non-physical oscillations in the results because of the acoustic waves propagating at a velocity higher than the speed of sound. The next method is proposed to resolve this issue.

B. Augmented Lagrangian method

The augmented Lagrangian approach [5], [6] may be also used in the Lagrangian particle-based methods. In this method, At each time step, assuming constant density, beginning from $\mathbf{V}^{n+1,0} = \mathbf{V}^n$, $P^{n+1,0} = P^n$, and $\mathbf{r}^{n+1,0} = \mathbf{r}^n$, at each iteration m, first, estimate the intermediate velocity $\mathbf{V}^*$ by

$$\begin{aligned}\mathbf{V}^* - \mathbf{V}^n =& r_{AL}\Delta t\left\langle\nabla\left(\nabla\cdot\mathbf{V}^{n+1,m}\right)\right\rangle \\ &+\frac{\Delta t}{\rho}\left(\mu\left\langle\nabla\cdot\nabla\mathbf{V}^{n+1,m}\right\rangle + \rho\mathbf{g}\right).\end{aligned} \tag{12}$$

The firs term in the right-hand side of (12) is a penalty term and r_{AL} is the augmented Lagrangian parameter. This term in physical sense, acts like the bulk viscosity term.

Then, find the new pressure from

$$\begin{aligned}&P^{n+1,m+1} - P^{n+1,m} = \\ &-r_{AL}\rho\left(\left\langle\nabla\cdot\mathbf{V}^*\right\rangle - \Delta t\frac{\left\langle\nabla\cdot\nabla P^{n+1,m}\right\rangle}{\rho}\right),\end{aligned} \tag{13}$$

and the new velocity from

$$\mathbf{V}^{n+1,m+1} = \mathbf{V}^* - \Delta t\frac{\left\langle\nabla P^{n+1,m+1}\right\rangle}{\rho}. \tag{14}$$

It is noteworthy that in (13) despite of the WCSPH method the speed of sound c did not appear.

TABLE I
SUMMARY OF THE AUGMENTED LAGRANGIAN SPH ALGORITHM.

```
for each time-step n do
  for each pseudo-time-step m do
    find the neighboring particles;
    for each internal particle i do
      compute V*_i using (12);
    end for
    for each internal particle i do
      compute P_i^{n+1} using (13);
    end for
    update the pressure for wall particles
    for each internal particle i do
      compute V_i^{n+1} using (14);
    end for
    for each internal particle i do
      update r_i^{n+1,m} using (15);
    end for
    check for convergence by (16) or (17)
  end for
  for each internal particle i do
    shift the position by Δr_i evaluated from (18);
    correct the velocities and pressures using (19) and (20);
  end for
end for
```

At the end of each iteration, calculate the new position using

$$\frac{\mathbf{r}^{n+1,m+1} - \mathbf{r}^n}{\Delta t} = \frac{1}{2}\left(\mathbf{V}^n + \mathbf{V}^{n+1,m}\right). \tag{15}$$

The iteration converges at each time-step when the tolerance is less than a threshold ϵ, *i.e.*

$$\parallel P^{n+1,m+1} - P^{n+1,m} \parallel\leqslant \epsilon, \tag{16}$$

or

$$\parallel \left\langle\nabla\cdot\mathbf{V}^{n+1,m+1}\right\rangle \parallel\leqslant \epsilon. \tag{17}$$

The above method may be treated as an iterated form of the method described in the previous section II-A. However, it costs more computations than the WCSPH method because of repeating all operations such as searching for neighbours and updating ∇W_{ij}, $\mathbf{B}_i$, $\hat{\mathbf{B}}_i$, and other computations at each iteration.

Summary of the above algorithm is shown in Table I.

Based on the idea of by Xu et al. [11] and also Shadloo et al. [12] especially for WCSPH, at the end of each time-step, all internal particles are shifted slightly by $\Delta\mathbf{r}_i$ which is defined by

$$\Delta\mathbf{r}_i = \epsilon V_i\Delta t\sum_j\left(\frac{d_0}{r_{ij}}\right)^3\mathbf{e}_{ij}, \tag{18}$$

where d_0 is the initial particles' spacing and ϵ is a constant which ranges from 0 to 0.1. Then, the velocity and pressure of the particles are interpolated at the modified position according to

$$\Delta\mathbf{V}_i = \Delta\mathbf{r}_i\cdot\left\langle\nabla\mathbf{V}\right\rangle_i, \tag{19}$$

$$\Delta P_i = \Delta\mathbf{r}_i\cdot\left\langle\nabla P\right\rangle_i, \tag{20}$$

III. Results and Discussions

To compare the behavior and the performance of the different methods described in the previous section, carefully determined illustrative test problems have been solved and here, their numerical results are presented.

A. 1D problem

First, a simple but stiff problem is considered, which is a 1D tank filled by a single phase fluid with $\rho = 1kg/m^3$ and $\mu = 0.001Pa.s$ initially at rest *i.e.* $u = 0$ and $P = 0$ where u is the x-component of the fluid velocity. The tank extends from $x = 0$ to $x = 1m$. At $t > 0$, a constant acceleration $g = -1m/s^2$ in x-direction is applied on the tank.

For this problem, assuming that the fluid is incompressible, the momentum and mass conservations can be written as

$$\rho \frac{du}{dt} = -\frac{\partial P}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2} + \rho g, \tag{21}$$

and

$$\frac{\partial u}{\partial t} = 0, \tag{22}$$

with boundary conditions

$$@x = 0, 1 \begin{cases} u = 0 \\ \frac{\partial P}{\partial x} = \rho g \end{cases} \tag{23}$$

Combining boundary condition for velocity with continuity (22) leads to $u \equiv 0$ for every $t > 0$. Thus,

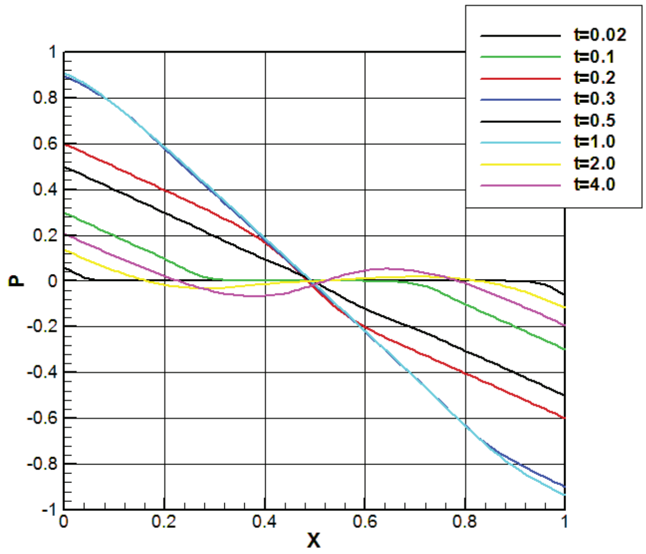
$$P = P_L + \rho g x, \tag{24}$$

where P_L is an integration constant. Since both conditions for the pressure are of Neumann type, here, the value of P_L is arbitrary.

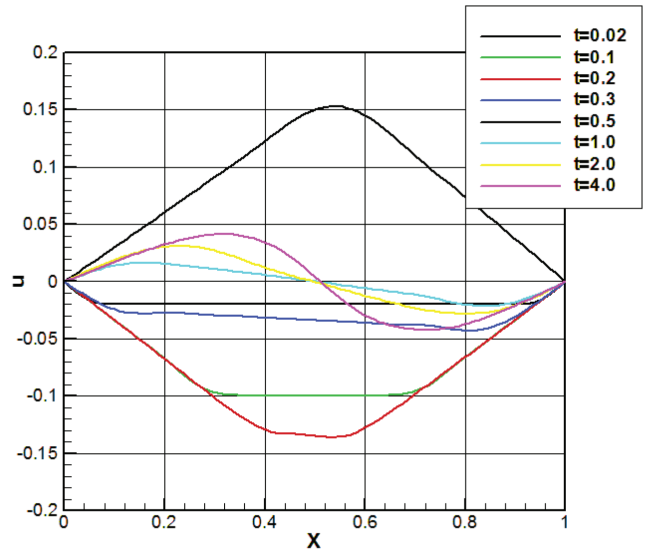
This is a stiff problem because the exact solution of the velocity is zero while for a weakly compressible method, the speed of sound c has a finite value. So, the method described in II-A is expected to encounter major difficulties. To asses the performance of the methods, a set of 101 SPH particles with equidistant initial arrangement is considered. The first and the last particles are fixed (wall particles) and the other 99 (fluid) particles move with the flow. Here, the quintic Wendland [13] kernel function with $h = 3\Delta x$ is used. In all methods, the density is assumed constant.

1) Weakly compressible SPH: The results of the problem obtained by the weakly compressible SPH method of the section II-A with $c = 3m/s$ and $\mu = 0.001Pa.s$ are shown in Fig. 1. The time-step size is limited to $\Delta t = 3.3e-4s$ for the sake of stability.

In Fig. 1 (a), at early times, two pressure waves initiate from wall boundaries and propagate in the domain in apposite directions. At about $t = 0.18s$, the waves reach each other and continue to move to the other boundary. After this time, some asymmetry appear in the velocity field (see Fig. 1 (b)). This is related to the non-linearity of the convection term in the momentum equation. Although the convection term does not exist explicitly in the Lagrangian form of the



(a)

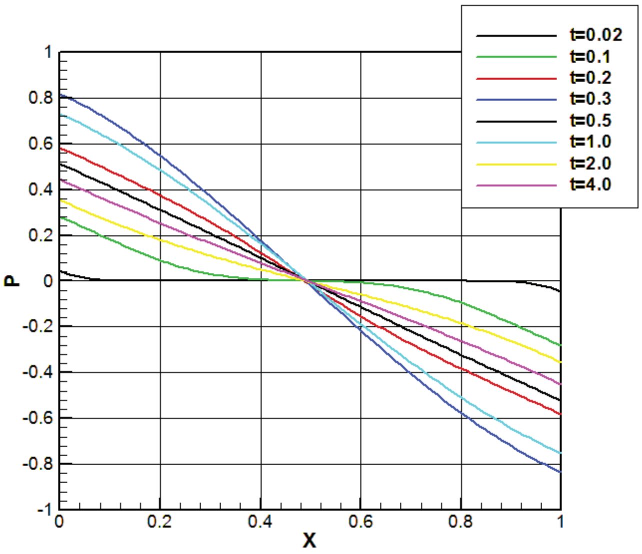


(b)

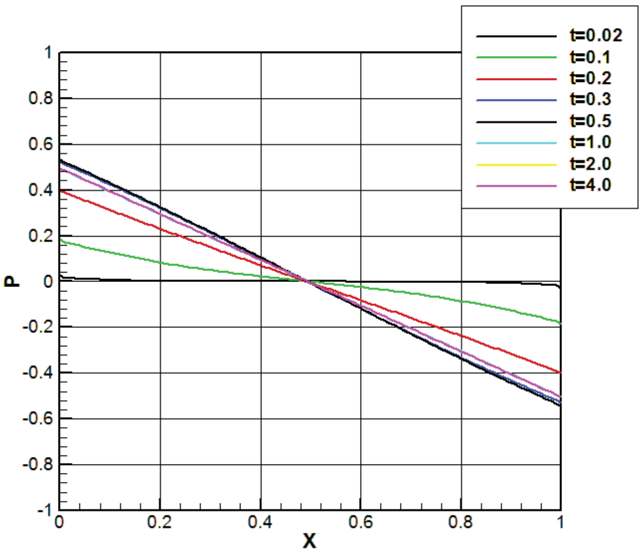
Fig. 1. Results of weakly compressible SPH method of the section II-A with $c = 3m/s$ and $\mu = 0.001Pa.s$ for selected times; (a) pressure and (b) velocity distributions.

momentum equation ((21)), its effect is present implicitly due to the motion of particles. Nonetheless, the asymmetry is not significant in the pressure profile of Fig. 1 (a). After $t = 0.34s$, the waves arrive at the walls and are reflected back.

It is observed that after a relatively long time ($t = 4s$), there is still a strong wave moving in the domain. Otherwise stated, there is a pressure oscillation at each point with a period of approximately $T = L/c = 1/3s$ where L is the length of the tank. Since the viscosity coefficient is relatively low, this oscillation damps very slowly. Here, a non-dimensional group equivalent to the Reynolds number is $\rho\sqrt{gL^3}/\mu = 1000$. Also,



(a)



(b)

Fig. 2. Pressure results of weakly compressible SPH method of the section II-A for selected times with different viscosity coefficients; (a) $\mu = 0.1Pa.s$ and (b) $\mu = 1.0Pa.s$.

based on the maximum velocity in Fig. 1 (b), the maximum Mach number is abut 0.05.

The damping effect of the viscosity coefficient on the results of the weakly compressible SPH method in this problem is shown in Fig. 2. In this figure, the results of pressure obtained by three different viscosity coefficients and $c = 3m/s$ are plotted. For $\mu = 0.1Pa.s$, the same time-step size $\Delta t = 3.3e-4s$ is used. However, for $\mu = 1.0Pa.s$, Δt is set to $4.5e-5s$ because of the dominant effect of viscosity. In this case, the stability condition is $\Delta t < 0.5\Delta x^2/\nu$ instead of the CFL condition. The comparison of Fig. 1 (a) with Fig. 2 (a) shows a significant reduction in the amplitude of the oscillation, and it is obviously converging with time to the linear pressure profile solution. This damping effect is manifested clearly in Fig. 2 (b) with $\mu = 1.0Pa.s$. In this case, the linear profile is achieved after just $t = 0.3s$.

It should be noted that in physical sense, indeed, damping is caused by the bulk viscosity not by the shear viscosity. In this special 1D case, since $\nabla^2\mathbf{V}$ and $\nabla\left(\nabla\cdot\mathbf{V}\right)$ are both simplified to $\frac{\partial^2 u}{\partial x^2}$, the two aforementioned terms are the same.

2) Augmented Lagrangian SPH: Here, the results of augmented Lagrangian SPH based on the explicit iterative method in section II-B is presented. In this method, the Lagrange coefficient r_{AL} is uniformly set to $C_{BV}U_{r,max}^2\Delta t$ where $U_{r,max} = \max\left(V_{max}, \frac{\nu}{\Delta x}\right)$ is the reference velocity similar to the previous method. Also, C_{BV} is a tuning constant between 1 and 100. Although non-uniform r_{AL} may increase the convergence rate, however the algebraic adaptive method suggested in [7] is suited to the implicit method.

The results of the method with two different values of C_{BV} for early and late times are shown in Fig. 3 respectively. In these cases, the number of iterations per time-step N_{iter} is set to 10^3. By increasing C_{BV} from 1 to 10, the solution converges more rapidly. However, for $C_{BV} > 15$ the iteration diverges. The reason is that the increase of C_{BV} is equivalent to a greater viscosity coefficient as discussed in section III-A1. So, the time-step size may no longer satisfy the stability condition.

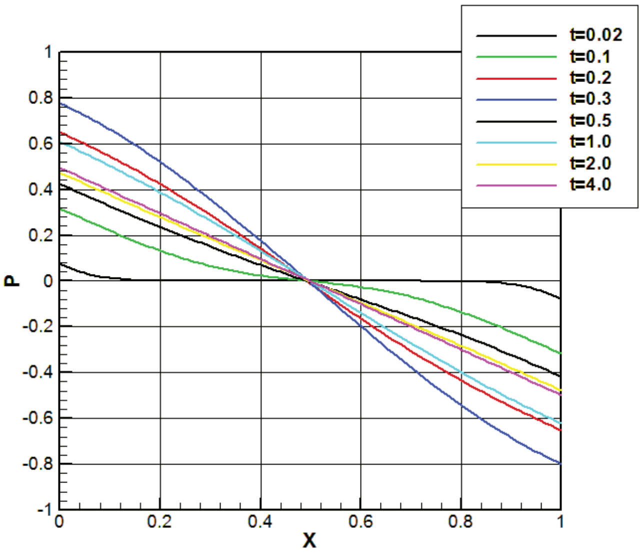
B. 2D pressure jump

To evaluate the performance of the methods in two dimensions, here, a pressure-jump in a fluid container is considered. The container is a $1m \times 1m$ square with periodic boundaries, which in this problem, may also considered as symmetric conditions. At initial time, the fluid is at rest and has uniform -1 Pa pressure except for a circle of radius 0.17 m in which the pressure is 10 Pa.

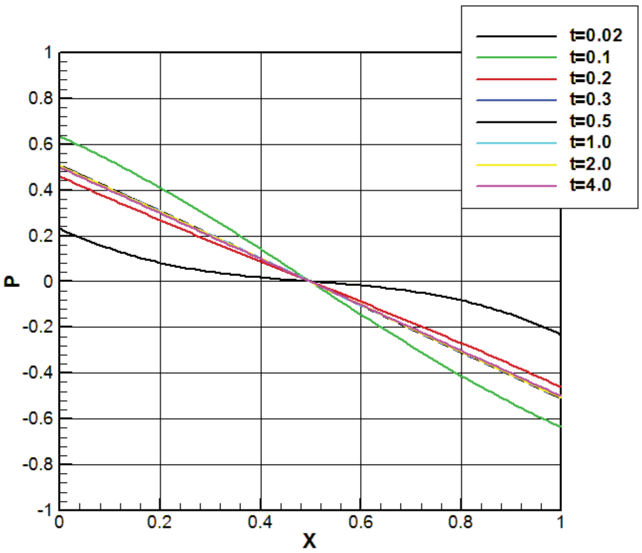
As discussed in the previous test case, at any time after the initial condition, the solution of pressure is expected to be uniform due to the incompressibility of the fluid. However, for the density-based solvers, this is impossible. Thus, any deviations in the results from the uniform solution can be regarded as numerical errors.

The pressure contours of the numerical results of the aforementioned methods are shown in Fig. 4. In this figure, two first rows belong to the results of the presented weakly compressible SPH method with two different speeds of sound. For the upper row (a) the speed of sound is c=10 m/s at which the maximum Mach number during the simulation is slightly less than 0.1. For the next row (b) the speed of sound is set to be c=35 m/s. At this condition, the value of $\Delta P/\rho c^2$ is less than 0.01 where ΔP is the magnitude of the initial pressure jump *i.e.* 11 Pa. This guaranties that the relative changes of the density are less than one percent during the simulation.

The next row (c) in Fig. 4 show the pressure evolution results of the augmented Lagrangian SPH method. Noting the scale of pressure in the different times, it can be seen that the



(a)



(b)

Fig. 3. Pressure results of the 1D problem with $\mu = 0.001 Pa.s$ using the augmented Lagrangian SPH method of the section II-B for selected times; (a) $C_{BV} = 1$ and (b) $C_{BV} = 10$.

results of this method overcome the pressure oscillations much better in comparison with those of the weakly compressible method.

IV. Conclusion

In this paper, a new density-based SPH method for incompressible flows was introduced and compared with a modified version of the well-known weakly compressible SPH method. The proposed method is based on a successful iterative density-based formulation which is in use in the grid-based method to handle the stiffness of the nearly incompressible problem. In the augmented Lagrangian method, the divergence-free velocity field is produced by adding a penalty term to the momentum equation. This term acts like a bulk viscosity term.

The performance of the proposed method was investigated in two incompressible flow problems. The cases were 1D and 2D stiff problems in which the exact solutions of the pressure field at any time after the initial condition are smooth distribution that are not reachable for a density based method. The augmented Lagrangian SPH method gives smooth pressure results that converge to the exact solution after some reasonable time-steps while at the same conditions, the pressure results of the weakly compressible SPH method oscillates even after long time. For the WCSPH method, the increase of the speed of sound dose not have significant effect on the magnitude of the pressure oscillation. However, the time-period of these oscillations changes.

Nevertheless, the smooth results of the proposed iterative methods need more than 1000 iteration per time-step. In these problems, increasing the number of iteration in each time-step has significant effect on the results.

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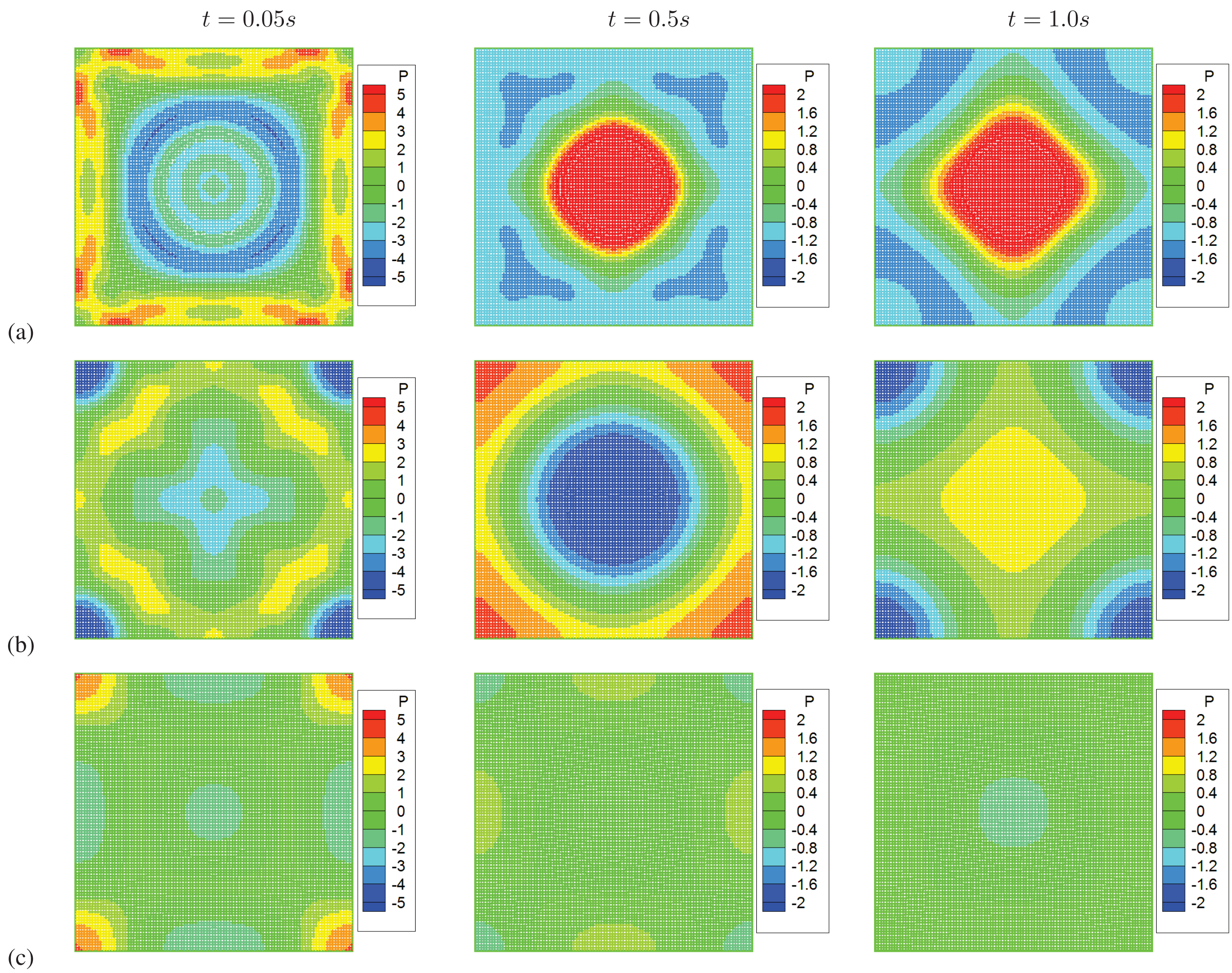

Fig. 4. Pressure distribution at different times obtained by using (a) weakly compressible with c=10 m/s, (b) weakly compressible with c=35 m/s, and (c) augmented Lagrangian SPH methods.

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