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ON THE NUMERICAL ANALYSIS OF SOLID DYNAMICS USING THE MOVING PARTICLE SEMI-IMPLICIT (MPS) METHOD

Koji Uenishi[1)]

Abstract: We examine the validity of the moving particle semi-implicit (MPS) method as applied to solid dynamics. Numerical simulations are performed for wave propagation in a two-dimensional linear elastic plate with stress-free boundaries. We shall compare the dynamic particle displacements obtained by the MPS method with those calculated by the finite difference method using the wave- fracture simulator SWIFD. The advantages and disadvantages of the use of the MPS method will be pointed out.

Key words: Wave propagation, moving particle semi-implicit (MPS) method, boundary conditions, large deformation

1. INTRODUCTION

As mentioned in our previous report[1)], recent progress in computational technologies has enabled us to simulate rather complex physical phenomena even on a PC basis[2-4)]. In solid dynamics, besides the typical numerical techniques – finite difference method (FDM), finite element method (FEM) and boundary element method (BEM) – particle methods are extensively used for problems involving large deformations and complex geometries. The idea of connecting "particle" to "deformation" is rather classical: The smallest part of a body studied in continuum mechanics is called a particle in general, and a deformation is expressed by a displacement field, which is an array of displacement vectors connecting the positions of particles before and after deformation[5)]. As shown in Figure 1, a deformation can be expressed as the sum of four different types of movement: rigid-body translation; rigid-body rotation, elongation (or contraction) and pure shear. The German physiologist and physicist Hermann Ludwig Ferdinand von Helmholtz (1821-1894) demonstrated in 1858 that this summation is true of any deformation and each type of movement is independent of the others[5)]. The particle methods are essentially based on this classical idea and evaluate the four independent movements explicitly or implicitly. The MPS (Moving Particle Semi-implicit) method discussed here is one of these "particle" methods, and the influence of a neighboring particle is evaluated with the "weight" inversely proportional to the particle distance. It has been reported that simulations involving large deformations and fracture may be performed rather simply[6,7)] by using the MPS method, but its validity in simulating wave phenomena in solids has not been clearly demonstrated. In this study, we shall perform simulations of two-dimensional wave propagation in a

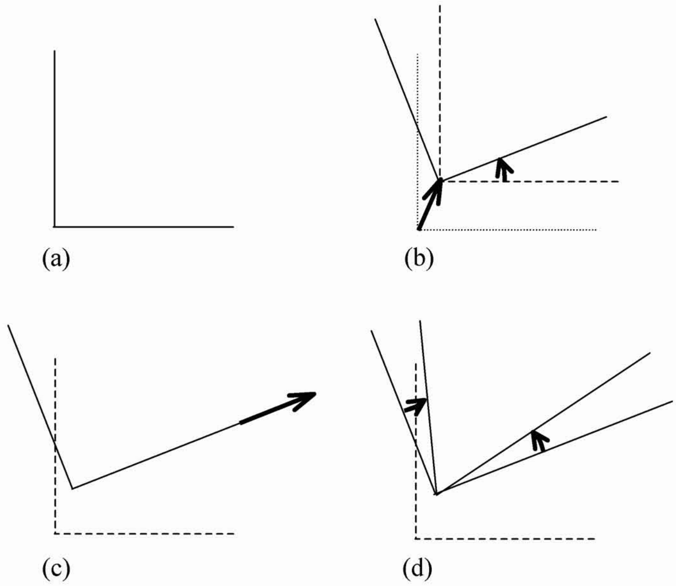


Figure 1   Deformation represented by two lines: (a) Original location; (b) Shifted and rotated; (c) One line segment elongated; and (d) Sheared (Modified after [5]).

linear elastic plate using the MPS method and FDM, compare their numerical results, and discuss the capability of the MPS method in wave dynamics.

2. THE MPS METHOD[6,7]

Here, a linear elastic body is assumed to be consisting of particles. The position, velocity, rotational angle and angular velocity associated with the particle i are denoted by $\mathbf{r}_i$, $\mathbf{v}_i$, $\mathbf{q}_i$ and ω_i, respectively. The relative position of the particle j with respect to i, initially $\mathbf{r}_{ij}^0$ and currently $\mathbf{r}_{ij}$, is given by (see Figure 2)

$$\mathbf{r}_{ij}^0 = \mathbf{r}_j^0 - \mathbf{r}_i^0,$$
$$\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i. \tag{1}$$

For the two-dimensional case, the relative displacement $\mathbf{u}_{ij}$ can be expressed as

$$\mathbf{u}_{ij} = \mathbf{r}_{ij} - \mathbf{R}\mathbf{r}_{ij}^0, \tag{2}$$

where the rotation matrix $\mathbf{R}$ is

$$\mathbf{R} = \begin{bmatrix} \cos\theta_{ij} & -\sin\theta_{ij} \\ \sin\theta_{ij} & \cos\theta_{ij} \end{bmatrix}, \tag{3}$$

with $\theta_{ij} = (\theta_i + \theta_j)/2$, and θ_i (θ_j) being the rotational angle of the particle i (j), respectively.

For the three-dimensional problems, we introduce the notation of quaternion rotation as

$$\mathbf{q} = (q_x, q_y, q_z, s) = \left(\nu_x \sin(\theta/2), \nu_y \sin(\theta/2), \nu_z \sin(\theta/2), \cos(\theta/2)\right), \tag{4}$$

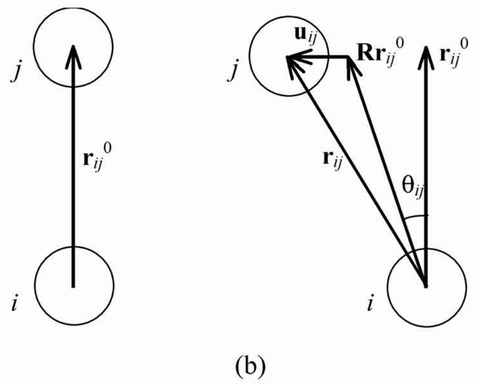


Figure 2　Relative displacement between two particles: (a) Initial state; and (b) Current position (Modified after [7]).

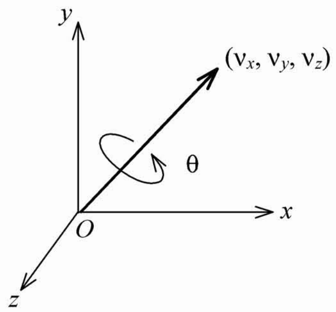


Figure 3　Rotation in a three-dimensional space, represented by quaternion rotation (Modified after [7]).

with the unit vector (ν_x, ν_y, ν_z) related to the rotational axis (Figure 3) satisfying

$$\nu_x^2 + \nu_y^2 + \nu_z^2 = 1, \tag{5}$$

i.e.,

$$q_x^2 + q_y^2 + q_z^2 + s^2 = 1. \tag{6}$$

Then, the rotation matrix **R** becomes

$$\mathbf{R} = \begin{bmatrix} 1-2q_y^2-2q_z^2 & 2q_xq_y-2sq_z & 2q_xq_z+2sq_y \\ 2q_xq_y+2sq_z & 1-2q_x^2-2q_z^2 & 2q_yq_z-2sq_x \\ 2q_xq_z-2sq_y & 2q_yq_z+2sq_x & 1-2q_x^2-2q_y^2 \end{bmatrix}, \tag{7}$$

and the relative displacement $\mathbf{u}_{ij}$ is written as

$$\mathbf{u}_{ij} = [(\mathbf{r}_{ij} - \mathbf{R}(\mathbf{q}_i)\mathbf{r}_{ij}^0) + (\mathbf{r}_{ij} - \mathbf{R}(\mathbf{q}_j)\mathbf{r}_{ij}^0)]/2. \tag{8}$$

Once obtaining $\mathbf{u}_{ij}$, we can calculate the normal and tangential stresses, σ_{ij}^n and σ_{ij}^s, respectively, based on

$$\begin{aligned} \boldsymbol{\sigma}_{ij}^n &= 2\mu\boldsymbol{\varepsilon}_{ij}^n = 2\mu\, \mathbf{u}_{ij}^n / |\mathbf{r}_{ij}^0|, \\ \boldsymbol{\sigma}_{ij}^s &= 2\mu\boldsymbol{\varepsilon}_{ij}^s = 2\mu\, \mathbf{u}_{ij}^s / |\mathbf{r}_{ij}^0|. \end{aligned} \tag{9}$$

Here, μ is the shear modulus, and $\boldsymbol{\varepsilon}_{ij}^n$ and $\boldsymbol{\varepsilon}_{ij}^s$ ($\mathbf{u}_{ij}^n$ and $\mathbf{u}_{ij}^s$) are the relative strains (displacements) normal and tangential to $\mathbf{r}_{ij}$, respectively. The "pressure" p_i

$$p_i = -\lambda \,\mathrm{div}(\mathbf{u})_i = -\lambda \frac{d}{n^0} \sum_{j \neq i} |\boldsymbol{\varepsilon}_{ij}^n| \, w(|\mathbf{r}_{ij}^0|), \tag{10}$$

is equivalent to the thermodynamic pressure in fluid mechanics, determined by the thermodynamic equation of state. In equation (10), λ is Lamé's constant, $\mathrm{div}(\mathbf{u})_i$ is the divergence of relative displacement related to the particle i, $d = 2$ for a two-dimensional problem and 3 for three-dimensional calculations, and the particle density n^0 and the weight w, a function of the distance r, are

$$n^0 = \sum_{j \neq i} w(|\mathbf{r}_{ij}^0|), \tag{11}$$

$$w(r) = \begin{cases} r_e / r - 1, & \text{for } r < r_e \\ 0, & \text{for } r \geq r_e \end{cases} \tag{12}$$

respectively. In the calculations performed in the next chapter, we assume $r_e = 2.1\ l_0$, with l_0 being the initial distance between the nearest particles.

Using the above relations, the acceleration of the particle i at time k is given by

$$\dot{\mathbf{v}}_i^k = \frac{2d}{\rho_i n^0} \left[\sum_{j \neq i} \frac{\boldsymbol{\sigma}_{ij}^n}{|\mathbf{r}_{ij}^0|} w(|\mathbf{r}_{ij}^0|) + \sum_{j \neq i} \frac{\boldsymbol{\sigma}_{ij}^s}{|\mathbf{r}_{ij}^0|} w(|\mathbf{r}_{ij}^0|) - \sum_{j \neq i} \frac{p_{ij} \mathbf{r}_{ij}}{|\mathbf{r}_{ij}^0| |\mathbf{r}_{ij}|} w(|\mathbf{r}_{ij}^0|) \right], \tag{13}$$

with ρ_i is the mass density of the particle i, $p_{ij} = (p_i + p_j)/2$, $\dot{(\,)}$ is a partial derivative with respect to time, and $\mathbf{v}_i^k$ is the velocity of the particle i at time k. Then, the velocity and position of the particle i at time $k + 1$, $\mathbf{v}_i^{k+1}$ and $\mathbf{r}_i^{k+1}$, respectively, are

$$\begin{aligned} \mathbf{v}_i^{k+1} &= \mathbf{v}_i^k + \dot{\mathbf{v}}_i^k \,\Delta t, \\ \mathbf{r}_i^{k+1} &= \mathbf{r}_i^k + \mathbf{v}_i^{k+1} \,\Delta t. \end{aligned} \tag{14}$$

The particle j renders the shearing force acting on the particle i

$$\mathbf{F}_{ij} = m_i \frac{2d}{\rho_i n^0} \sum_{j \neq i} \frac{\boldsymbol{\sigma}_{ij}^s}{|\mathbf{r}_{ij}^0|} w(|\mathbf{r}_{ij}^0|) = \frac{2d\, l_0^d}{n^0} \sum_{j \neq i} \frac{\boldsymbol{\sigma}_{ij}^s}{|\mathbf{r}_{ij}^0|} w(|\mathbf{r}_{ij}^0|), \tag{15}$$

and the torque

$$\mathbf{T}_{ij} = \mathbf{F}_{ij} \times \mathbf{r}_{ij}, \tag{16}$$

is induced on both particles i and j. Using the moment of inertia of the particle i, I_i (= $m_i l_0^2/6$ for 2D square and for 3D cube particles with sides of length l_0), the angular acceleration may be evaluated by summation of half of each induced torque as

$$I_i \dot{\boldsymbol{\omega}}_i^k = -\frac{1}{2} \sum_{j \neq i} \mathbf{T}_{ij}, \tag{17}$$

and, the angular velocity of the particle i at time $k + 1$ is

$$\boldsymbol{\omega}_i^{k+1} = \boldsymbol{\omega}_i^k + \dot{\boldsymbol{\omega}}_i^k \,\Delta t. \tag{18}$$

For a two-dimensional model, the rotational angle of the particle i at time $k + 1$ may be written as

$$\theta_i^{k+1} = \theta_i^k + |\boldsymbol{\omega}_i^{k+1}| \Delta t. \tag{19}$$

In the three-dimensional case, the associated changes are expressed as

$$\begin{aligned}
&\mathbf{v}_i'^{k+1} = (v_x', v_y', v_z')_i^{k+1} = \frac{1}{|\boldsymbol{\omega}_i^{k+1}|}(\omega_x, \omega_y, \omega_z)_i^{k+1}, \\
&\theta_i'^{k+1} = |\boldsymbol{\omega}_i^{k+1}| \Delta t, \\
&\mathbf{q}_i'^{k+1} = (q_x', q_y', q_z', s')_i^{k+1} = \left(v_x' \sin(\theta'/2), v_y' \sin(\theta'/2), v_z' \sin(\theta'/2), \cos(\theta'/2)\right)_i^{k+1},
\end{aligned} \tag{20}$$

and the quaternion rotation at time $k + 1$ is obtained by

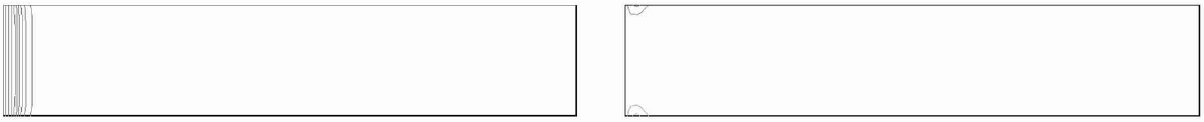
$$\mathbf{q}_i^{k+1} = \begin{pmatrix} q_x^{k+1} \\ q_y^{k+1} \\ q_z^{k+1} \\ s^{k+1} \end{pmatrix}_i^T = \begin{pmatrix} s'^{k+1} q_x^k + q_x'^{k+1} s^k + q_y'^{k+1} q_z^k - q_z'^{k+1} q_y^k \\ s'^{k+1} q_y^k + q_y'^{k+1} s^k + q_z'^{k+1} q_x^k - q_x'^{k+1} q_z^k \\ s'^{k+1} q_z^k + q_z'^{k+1} s^k + q_x'^{k+1} q_y^k - q_y'^{k+1} q_x^k \\ s'^{k+1} s^k - q_x'^{k+1} q_x^k - q_y'^{k+1} q_y^k - q_z'^{k+1} q_z^k \end{pmatrix}_i^T. \tag{21}$$

From the expressions given above, we can calculate the position, velocity, rotational angle and angular velocity of each particle at each time step.

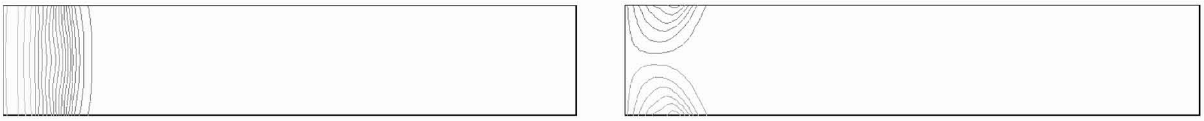
3. DISCUSSION: COMPARISON WITH THE FINITE DIFFERENCE METHOD

Now let us calculate the dynamic displacement field using the MPS method. Consider a two-dimensional linear elastic plate. Its dimensions are 0.19 m × 1 m, and the mass density, Young's modulus and Poisson's ratio are assumed to be 1000 kg/m^3, 1000 N/m^2, and 0.3, respectively. From the left side, an incident sinusoidal wave (length 0.64 m and amplitude 10^{-4} m in the horizontal direction) is propagated to the right. The other three sides are stress-free boundaries. Figure 4 shows the results numerically generated by the MPS method using 20 × 100 particles. The left (right) column corresponds to the horizontal (vertical) particle displacement, respectively. The effect of the upper, lower and right boundaries on wave propagation seems visible.

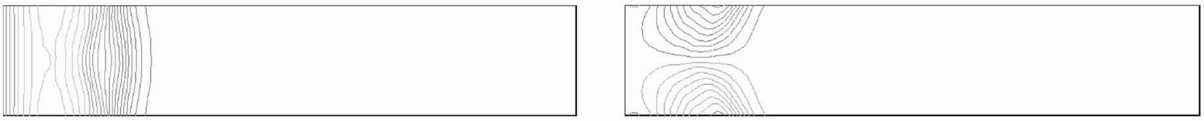
The same two-dimensional problem is solved by the finite difference simulator SWIFD[2,3)] and the snapshots of displacement distributions are found in Figure 5. The horizontal (left column) and vertical (right) particle displacements calculated using the 20 × 101 grid-point-system suggest that the boundary effect noted in Figure 4 is too weak. For example, at time 0.474 s, von Schmidt (head) waves and their interaction in the plate can be clearly identified in Figure 5 while in Figure 4 the MPS method *cannot* well reproduce the strong effect of propagation and interaction of head waves generated at stress-free boundaries. Also, the wave focusing effect at later stages, induced by the upper and lower (and right) boundaries, seems to be too little in Figure 4 compared with that in Figure 5 (see e.g., 1.164 s), and therefore, the results obtained by the MPS method may not be reliable, especially when the problem considered involves boundaries.



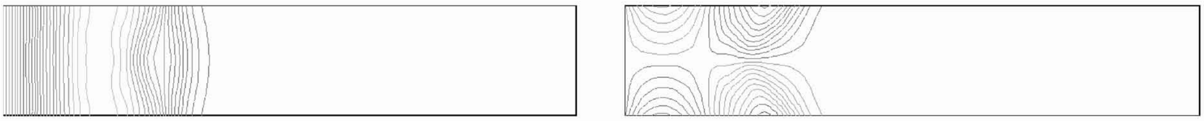
0.043 s (10 time steps)



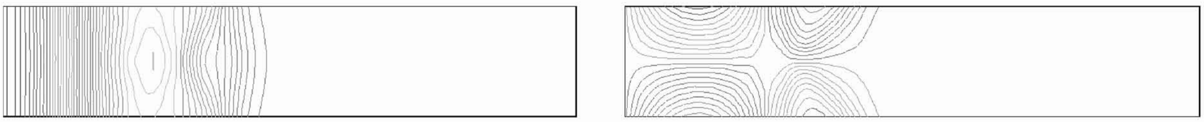
0.129 s (30 steps)



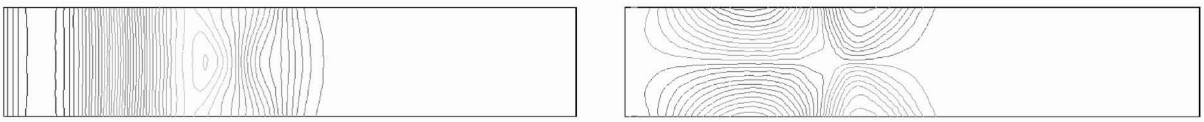
0.216 s (50 steps)



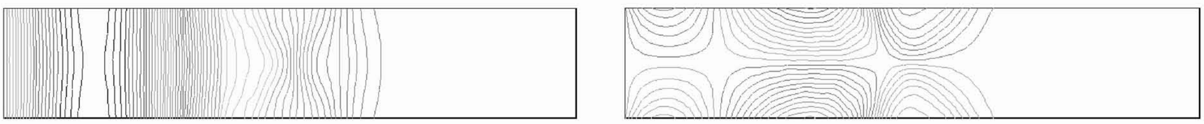
0.302 s (70 steps)



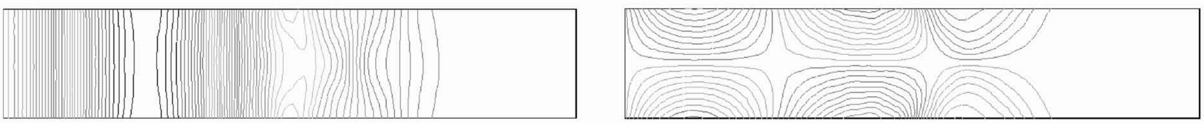
0.388 s (90 steps)



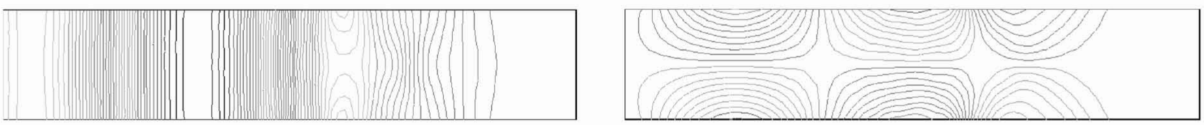
0.474 s (110 steps)



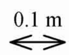
0.560 s (130 steps)



0.646 s (150 steps)



0.733 s (170 steps)



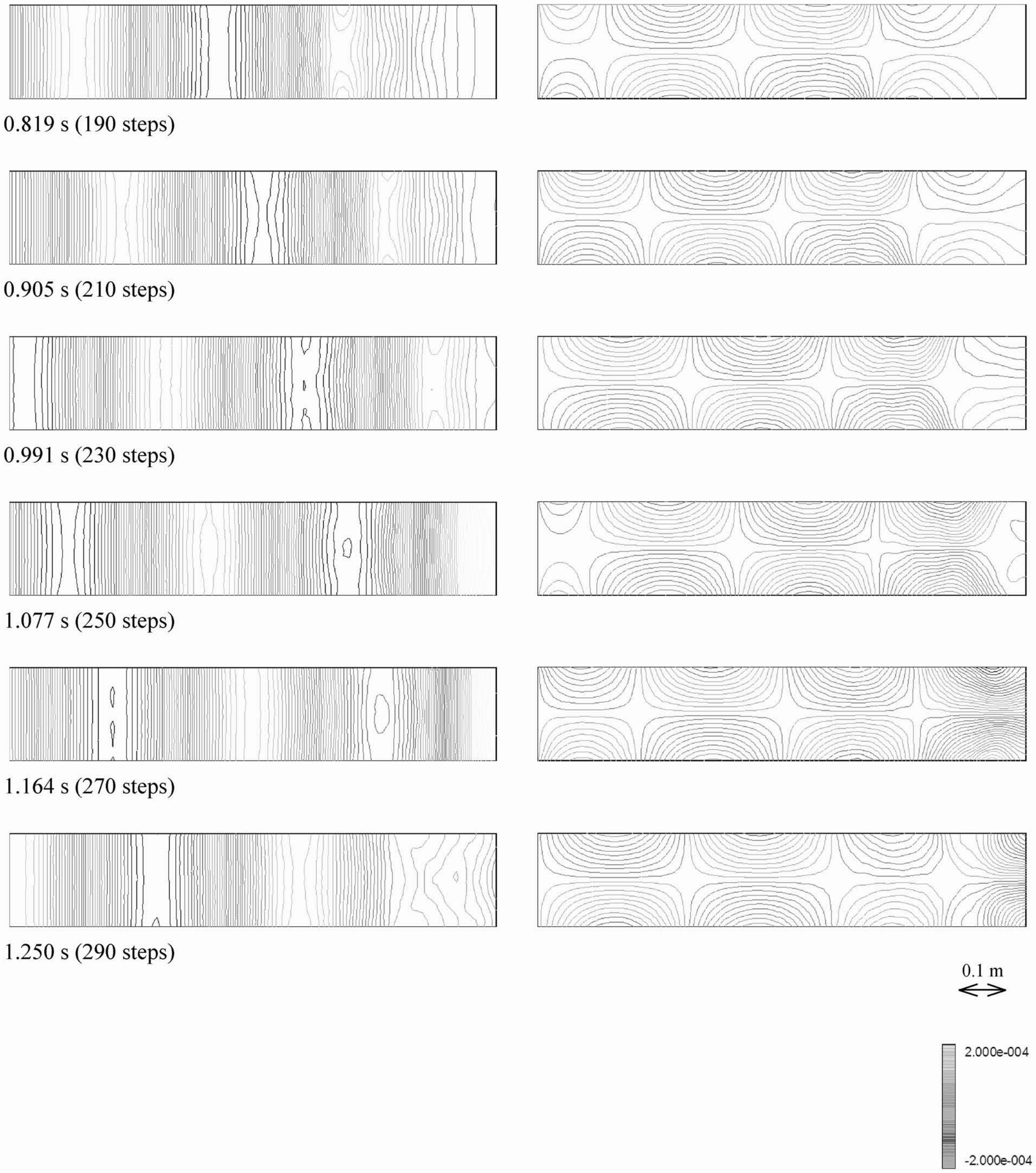
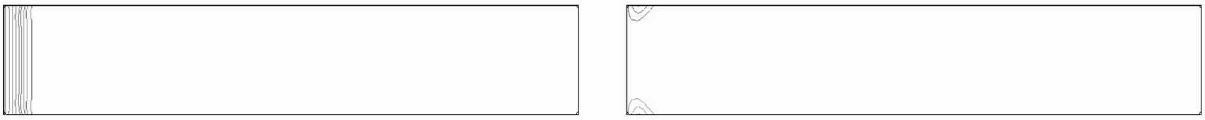
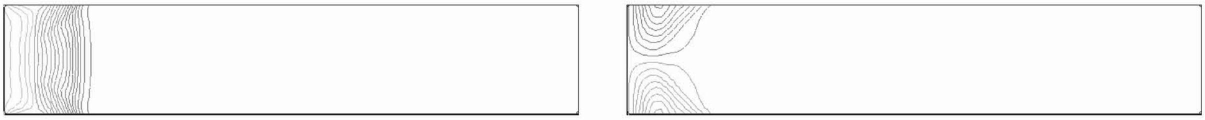
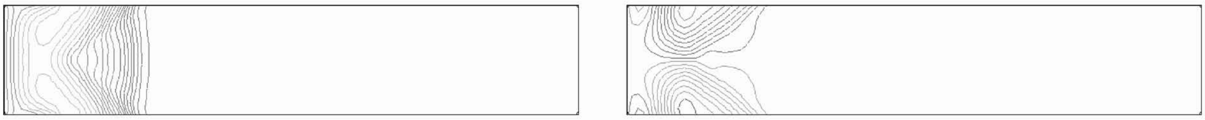
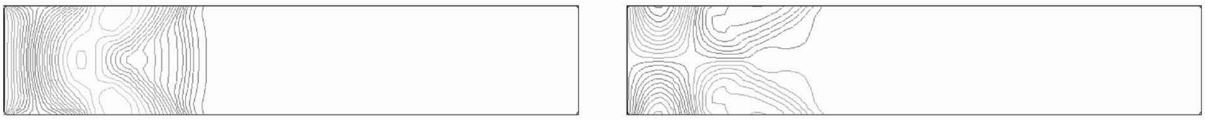


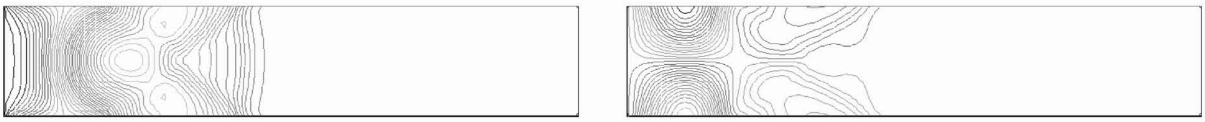
Figure 4 The horizontal (left column) and vertical (right) particle displacements associated with wave propagation in a two-dimensional plate (0.19 m × 1 m). The mass density, Young's modulus and Poisson's ratio of the plate are 1000 kg/m^3, 1000 N/m^2, and 0.3, respectively. The incident sinusoidal wave, having the length 0.64 m and amplitude 10^{-4} m in the horizontal direction, propagates from left to right. The results obtained by the MPS method with 20 × 100 particles are shown.

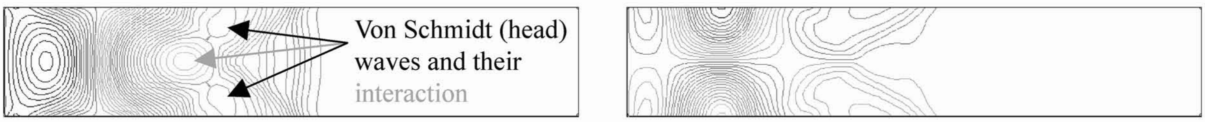

0.043 s (10 time steps)


0.129 s (30 steps)

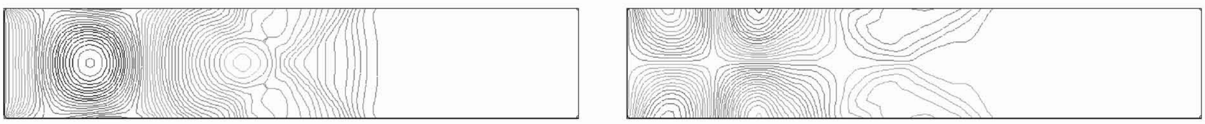

0.216 s (50 steps)

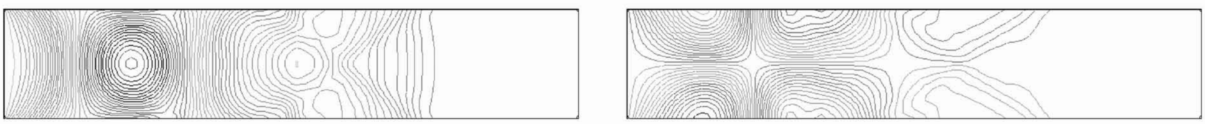

0.302 s (70 steps)

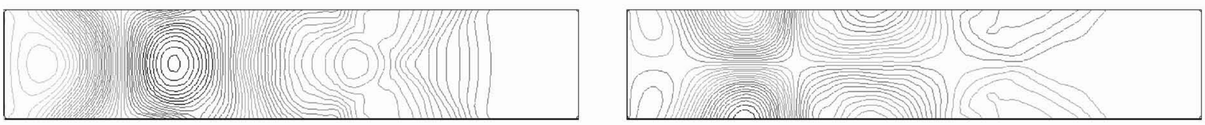

0.388 s (90 steps)



0.474 s (110 steps)


0.560 s (130 steps)


0.646 s (150 steps)


0.733 s (170 steps)

0.1 m

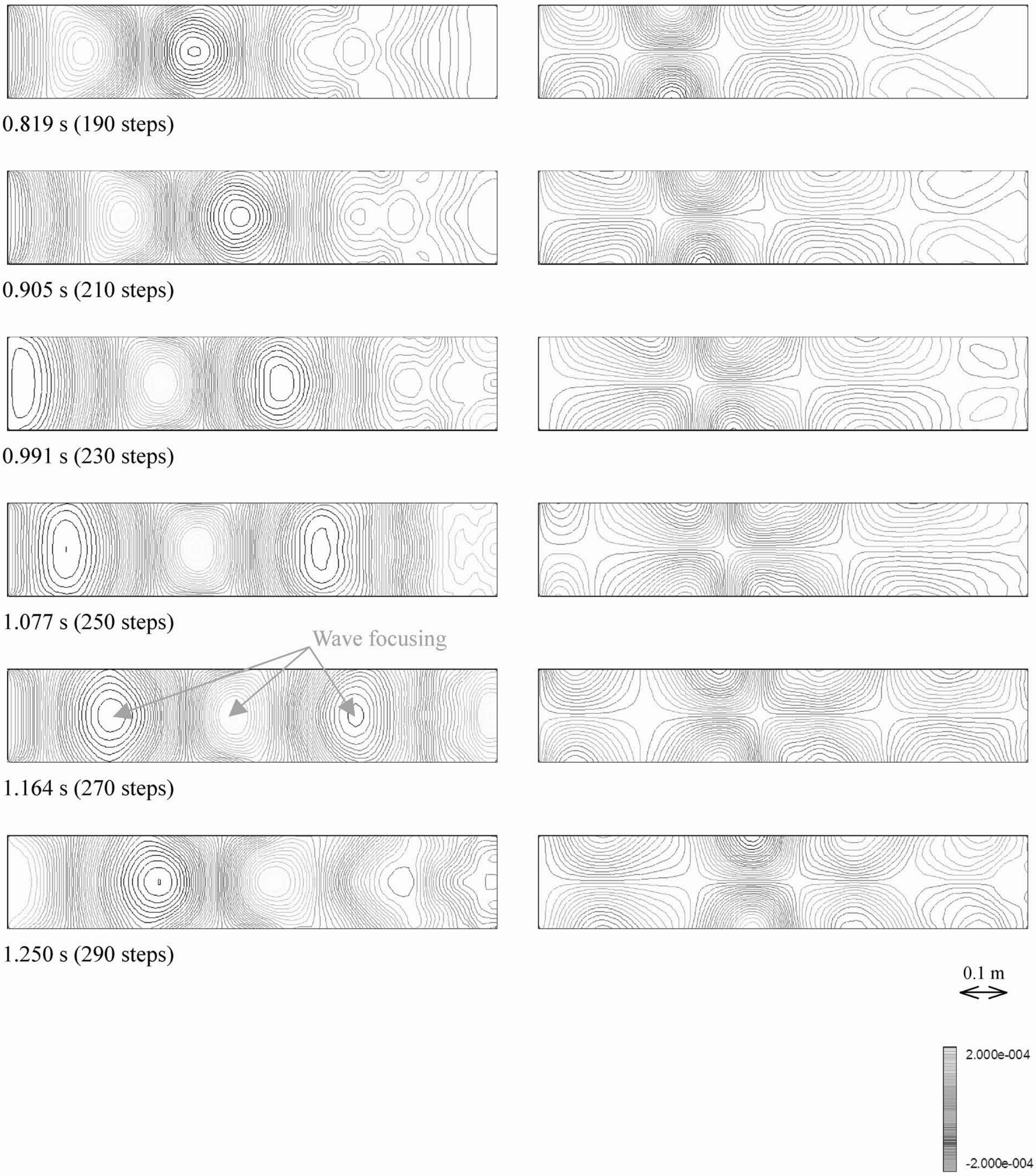


Figure 5 Wave propagation in a two-dimensional plate: Horizontal (left column) and vertical (right) particle displacements calculated by the finite difference method (SWIFD[2,3]) with 20 × 101 grid points. Material properties and boundary conditions remain the same as in Figure 4. We immediately notice that the MPS method *cannot* well reproduce the strong effect of propagation and interaction of head waves that are generated at stress-free boundaries.

4. CONCLUSIONS

By simulating two-dimensional wave propagation in a linear elastic plate, we have checked the capability of the MPS method. The comparison of the displacement fields numerically obtained by the MPS method with those of the finite difference method suggests the following merits and questions related to the MPS method: The advantages are (1) The algorithm itself is very simple; and (2) The CPU time needed by the MPS method is as little as that of finite difference method; The questionable points are <1> The MPS method has been originally developed in the field of fluid mechanics, and therefore, the effect of shearing in solid may not be correctly evaluated; and <2> Strains near surfaces may not be properly assessed and smaller values tend to be obtained, and hence boundary conditions may not be precisely satisfied; Careful attention should be paid in simulating fracture, impact, and near-surface wave phenomena when the MPS method is used.

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