An Introduction to the Material Point Method using a Case Study from Gas Dynamics.

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Abstract. The Material Point Method (MPM) developed by Sulsky and colleagues is currently being used to solve many challenging problems involving large deformations and/or fragementations with considerable success as part of the Uintah code created by the CSAFE project. In order to understand the properties of this method an analysis of the considerable computational properties of MPM is undertaken in the context of model problems from gas dynamics. One aspect of the MPM method in the form used here is shown to have first order accuracy. Computational experiments using particle redistribution are described and show that smooth results with first order accuracy may be obtained.

Keywords: PIC, Material Point Method, Error Analysis
PACS: 02.60.Lj 02.70.Ns

INTRODUCTION TO MPM

The need to solve problems involving large deformations in materials has led to the development of a number of new computational methods. Examples of such methods are meshfree and particle methods, one of which is the relatively new Material Point Method of Sulsky et al., [7], which may, perhaps, be described as a quasi-meshless method. This method (MPM) has evolved from the particle-in-cell (PIC) and FLIP methods originally developed by Brackbill et al. see [1] and the references within. The method has also been used extensively in large-scale complex fluid-structure interactions, [5], arising from the modeling of safety studies involving explosions. Given the use of the method on such important and challenging problems it is important to under how accurate the method is. In this paper, the MPM procedure is considered in the context of a shock propagation problem. This problem has also been studied by Brackbill and York et al. [9] and very recently in the context of a comparison between MPM and SPH methods by Ma et al. [3]. Sod's gas dynamics problem, [6] consists of a shock tube, where a diaphragm is located in the middle of the tube. Two sides of the diaphragm have different pressure and density, which make the fluid flows when the diaphragm is broken. The left side of density is 1 and pressure is also 1. The right side of density is 0.125 and pressure is 0.1, and the initial velocities of both regions are zero. At time t=0, the diaphragm is removed the motion of the compressible and inviscid These equations ifor internal energy and density on a moving mesh may be written in the form given by [9] as:

$$\frac{\partial \varepsilon}{\partial t} + v\frac{\partial \varepsilon}{\partial x} + \frac{p}{\rho}\frac{\partial v}{\partial x} = 0 \tag{1}$$

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} + \rho\frac{\partial v}{\partial x} = 0 \tag{2}$$

Standard boundary conditions are used as well as the state equation for pressure:

$$p = (\gamma - 1)\rho\varepsilon. \tag{3}$$

At the start of a timestep, the mass of particle p at position x_p in a cell $[x_i, x_{i+1}]$ of width h_j is calculated from the density,ρ_p, and the volume of the particle, V_p, as

$$m_p = \rho_p V_p. \tag{4}$$

The volume of the cell is given in terms of the cell width, h_i, the number of particles in that cell, N_p^i, by:

$$V_p = \frac{h_i}{N_p^i}. \tag{5}$$

While this is a reasonable approximation for compressible flows, it represents a departure from the standard MPM approach for solid mechanics, in which the volumes associated with particles are tracked. The mass at each grid point is calculated from the projection of the particle properties:

$$m_i = \sum_{p=1}^{np} \bar{S_{ip}} \rho_p V_p, \; i = 1, ..., nv, \tag{6}$$

and the momentum at a grid node is given by

$$P_i = \sum_{p=1}^{n_p} \bar{S_{ip}} \rho_p V_p v_p, i = 1, ..., nv, \tag{7}$$

where $\bar{S_{ip}} = S_i(x_p)$ for the linear basis function $S_i(x)$ with value one at x_i and zero at other grid points. The nodal velocity is calculated from the mass and the momentum of the node as

$$v_i = \frac{P_i}{m_i}. \tag{8}$$

The ith nodel force depends on the jump between the averaged particle pressures in the intervals containing x_i:

$$F_i^{int} = \sum_{p:x_p \in I_i} p_p \frac{1}{N_p^i} - \sum_{p:x_p \in I_{i+1}} p_p \frac{1}{N_p^{i+1}} \tag{9}$$

The acceleration at a node is calculated from the force and the mass at the node.

$$a_i = \frac{F_i^{int}}{m_i}. \tag{10}$$

This method of force calculation has been developed here as being more appropriate for compressible gas dynamics as it assumes that the particles within a cell have the same volume. Analysis and investigation of alternative methods for solid mechanics and different approaches to gas dynamics are provided by [7, 9]. The nodal velocity at the end of Lagrangian step is defined using the Euler method for time integration as:

$$v_i^{n+1} = v_i^n + a_i^n dt \tag{11}$$

where a_i^n is the acceleration at time t_n. The particle velocity and location are updated using these new values:

$$v_p^{n+1} = v_p^n + \sum_{i=1}^{n_v} S_{ip} a_i^n dt, \tag{12}$$

$$x_p^{n+1} = x_p^n + \sum_{i=1}^{n_v} S_{ip} v_i^{n+1} dt. \tag{13}$$

Tran et al. [8] show that the use of linear basis functions means that only first order time accuracy is possible because of discontinuities in high-order time derivatives of both particle position and velocity as particles cross mesh points. Once the nodal velocities are known as in equation (11), it is possible to update the velocity gradient and hence calculate the energy and a density of the particles at the next time step, as denoted by $\varepsilon_p^{n+1}, \rho_p^{n+1}$ by:

$$\varepsilon_p^{n+1} = \varepsilon_p^n - \frac{p_p^n}{\rho_p^n} \frac{\partial v_p^{n+1}}{\partial x} dt, \tag{14}$$

$$\rho_p^{n+1} = \rho_p^n (1 - \frac{\partial v_p^{n+1}}{\partial x} dt), \tag{15}$$

where the velocity gradient of each particle is calculated using nodal velocities and the gradients of the nodal basis functions. The pressure update is given by:

$$p_p^{n+1} = (\gamma - 1) \rho_p^{n+1} \varepsilon_p^{n+1} + a_v. \tag{16}$$

The term a_v is a standard artificial viscosity term which was was used by [4] with SPH methods. Given that the density, energy and pressure values are positive, their numerical approximations should also be positive. From equations (15)-(16) it may be seen that this occurs for the discrete density equation under a Courant-like condition:

$$dt\frac{\partial v_p^{n+1}}{\partial x} << 1, \tag{17}$$

although this shows that values of density and energy remain positive overshoots in pressure energy and density may be caused by use of velocity gradient from "old"cell. This may potentially result in new extrema being created. In order to prevent this further artificial diffusion is applied in the case when extrema occur in velocity $(v_{i-1}-v_i)(v_{i+1}-v_i) > 0$, the new value of velocity is then calculated by

$$v_i = v_i + \frac{v_{i-1}-2v_i+v_{i+1}}{3} \tag{18}$$

and the same approach applied if extrema are detected in density. Once particles move to an adjacent cell, the changed number of particles in a cell is used to calculate new particle volume and mass after the density calculation is completed. If there were too few particles per cell and some of these particles move from one cell to another cell, it is possible for a cell not to have any particles. This may cause stability problems and may be remedied by using an uneven distribution of particles that reflects the equidistribution of the density as described below for the Sod Problem.

MASS PROJECTION ERROR ANALYSIS.

An important result, Theorem 2.3 of Hickernell [2], helps in deriving the order of this MPM method. This result when mapped to the interval $[x_i, x_{i+1}]$, [8], proves for any function $f(x) \in X^p \equiv \left[f : \frac{df}{dx} \in L^p([x_i, x_{i+1}]) \right]$:

$$\left| \int_{x_i}^{x_{i+1}} f(y)dy - \frac{h_{i+1}}{N_p^{i+1}} \sum_{i=1}^{N_p^{i+1}} f(x_i) \right| \leq D_2(P, N_p^{i+1})\, h_{i+1}^2 \left| \frac{df}{dx}(\xi) \right| \tag{19}$$

for some $\xi \in I_{i+1}$ and where

$$D_2(P, N_p^{i+1}) = \sqrt{\frac{1}{12(N_p^{i+1})^2} + \frac{1}{N_p^{i+1}h^2} \sum_{i=1}^{N_p^{i+1}} \left((hz_i + x_i) - \left(x_i + \frac{(2i-1)h}{2N_p^{i+1}} \right) \right)^2}. \tag{20}$$

The values of $D_2(P, N_p^{i+1})$ clearly depend on the point distribution and thus in turn on the problem being solved. This result may be used to analyze the mass error associated with equation (6) as denoted by E_m^i and as defined by

$$E_m^i = \int_{x_{i-1}}^{x_{i+1}} \rho(x) S_i(x) dx - m_i \tag{21}$$

where there are N_p^j points in the interval I_j. This may be written in terms of the points in each interval as

$$E_m^i = \int_{x_{i-1}}^{x_i} \rho(x) S_i(x) dx - \frac{h}{N_p^i} \sum_{p:x_p \in I_i} S(x_{ip})\rho_p + \int_{x_i}^{x_{i+1}} \rho(x) S_i(x) dx - \frac{h}{N_p^{i+1}} \sum_{p:x_p \in I_{i+1}} S(x_{ip})\rho_p. \tag{22}$$

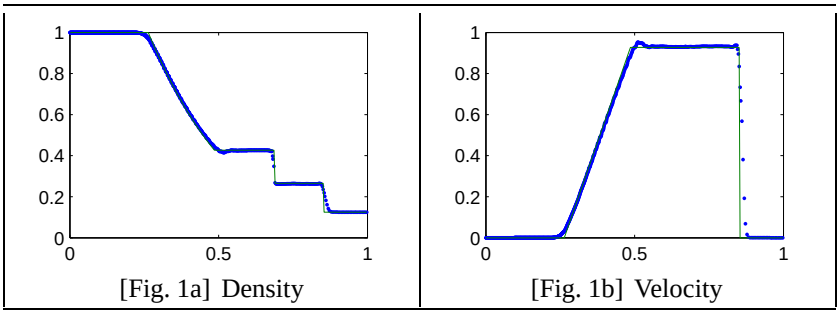
This error term is thus composed of two terms of the form of the right side of (19):

$$\left| E_m^i \right| \leq D_2(P, N_p^i) h^2 \left| \frac{d(\rho(x) S_i(x))}{dx}(\xi_1) \right| + D_2(P, N_p^{i+1}) h^2 \left| \frac{d(\rho(x) S_i(x))}{dx}(\xi_2) \right| \tag{23}$$

for some $\xi_1 \in I_i$ and some $\xi_2 \in I_{i+1}$. However as the first derivative of $S_i(x)$ depends on $\frac{1}{h}$ this experssion is only first order in h. The same approach may be used to show that the momentum projection error is only first order, too. The acceleration error is more difficult to analyze, see [8], and depends on the distribution of mesh points.

GAS DYNAMICS RESULT

The errors in the MPM method arise from the nodal projections of mass, momentum, internal force, velocity and acceleration and from the interpolation of nodal values back to the particles. These errors are shown by[8] to be of first order accuracy. Initially, the gas to the left and right of the diaphragm have densities of 1.0 and 0.125 . Hence eight particles per cell are assigned to the left and one particle to the right. This reflects the movement of left particles rightwards during the time integration process. The results of experiments, [8], show that the method has first order accuracy on smooth problems. The density and velocity profiles at the end of a run and the approximate norms in the density error for the Sod problem are shown below, and are of good quality for a particle method.



[Fig. 1a] Density [Fig. 1b] Velocity

TABLE 1. Density Errors at T=0.2

h	L1-Norm	L2-Norm	Mesh Point
0.01	0.00831	0.01587	0.148
0.005	0.00434	0.01046	0.154
0.0025	0.00231	0.00759	0.156
0.00125	0.00126	0.00576	0.138

An analysis of the error shows that, where the solution is smooth, there is first-order accuracy, but large errors in the shock and contact regions. As the width of these regions is h these errors are order h in L1-Norm and $h^{\frac{1}{2}}$ in L2-Norm.

ACKNOWLEDGEMENT

This work was supported by C-SAFE, U. of Utah, funded by the Department of Energy, subcontract B524196.

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