An Introduction to the Material Point Method

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1 Introduction

The Material Point Method (MPM) as described by Sulsky, et al. [1, 2] is a particle method for structural mechanics simulations. Solid objects are represented by a collection of particles, or "material points." Each of these particles carries with it information for that part of the solid object that it represents. This includes the mass, volume, position, velocity and stress of that material. MPM differs from other so called "mesh-free" particle methods in that, while each object is primarily represented by a collection of particles, a computational mesh is also an important part of the calculation. Particles do not interact with each other directly, rather the particle information is interpolated to the grid, where the equations of motion are integrated forward in time. This time advanced solution is then used to update the particle state. An example of two disks initially approaching each other represented by material points on an overlying mesh is show in Figure 1.

The method usually uses a regular structured grid as a computational mesh. While this grid, in principle, deforms as the material that it is representing deforms, at the end of each timestep, it is reset to it's original undeformed position, in effect providing a new computational grid for each timestep. The use of a regular structured grid for each time step has a number of computational advantages. Computation of spatial gradients is simplified. Mesh entanglement, which can plague fully Lagrangian techniques, such as the Finite Element Method (FEM), is avoided. MPM has also been successful in solving problems involving contact between colliding objects, having an advantage over FEM in that the use of the regular grid eliminates the need for doing costly searches for contact surfaces[3].

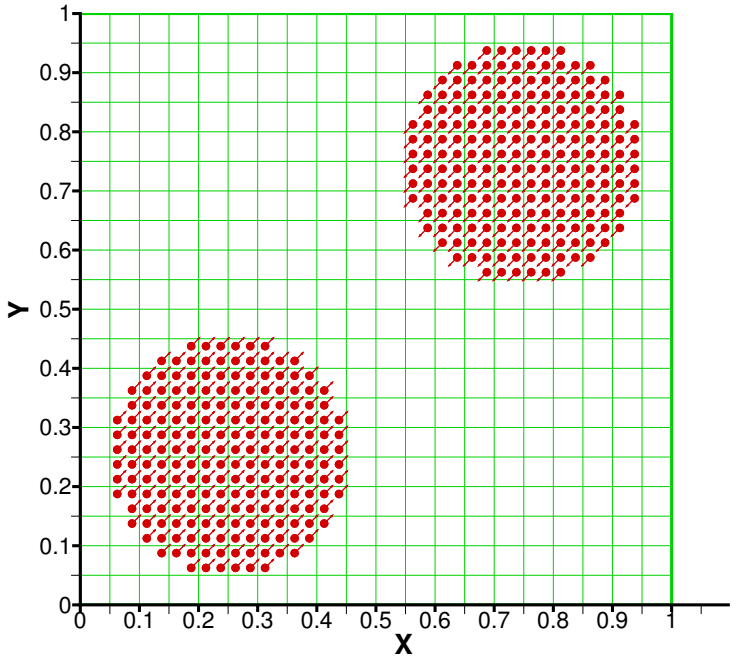


Figure 1: Initial particle representation of two colliding disks on an overlying mesh.

The choice of MPM over FEM as the C-SAFE structural mechanics method was only in small part for the above mentioned criteria. The primary motivation was the ability to use MPM together with a multimaterial CFD algorithm for solving tightly coupled fluid-structure interaction problems. This capability was first demonstrated in the CFDLIB codes from Los Alamos by Bryan Kashiwa and co-workers. There, as in Uintah, MPM serves as the Lagrangian description of the solid material in a multimaterial CFD code. Certain elements of the solution procedure are based in the Eulerian CFD algorithm, including intermaterial heat and momentum transfer as well as satisfaction of a multimaterial equation of state. The use of a Lagrangian method such as MPM to advance the solution of the solid material eliminates the diffusion typically associated with Eulerian methods.

2 Algorithm

While a more detailed description of MPM can be found in [2], the algorithm is laid out here. The equations of motion are cast in the form:

$$\mathbf{M}_g \cdot \mathbf{a}_g \quad = \quad \mathbf{Fext}_g - \mathbf{Fint}_g \tag{1}$$

where $\mathbf{M}_g$ is the mass matrix, $\mathbf{a}_g$ is the acceleration vector, $\mathbf{Fext}_g$ is the external force vector (sum of the body forces and tractions), and $\mathbf{Fint}_g$ is the internal force vector resulting from the divergence of the material stresses. In general, $\mathbf{M}_g$ is a large, sparse matrix. In practice, and in what follows here, a “lumped” mass matrix is used, which only has entries on the diagonal, and is thus represented as a column matrix.

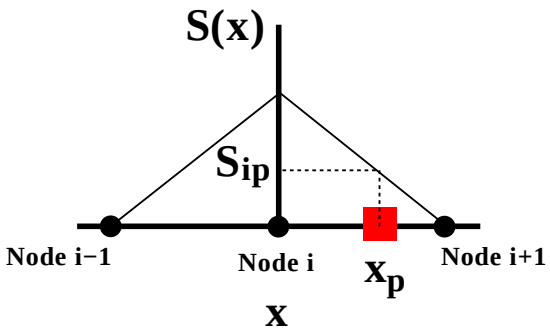
The solution procedure begins by interpolating the particle state to the grid, to form $\mathbf{M}_g$, $\mathbf{Fext}_g$, and to get a velocity on the grid $\mathbf{v}_g$. These quantities are calculated at each grid node by the following equations:

$$\mathbf{M}_i = \sum_p S_{ip} m_p \tag{2}$$

$$\mathbf{v}_i = \frac{\sum_p S_{ip} m_p \mathbf{v}_p}{\mathbf{M}_i} \tag{3}$$

$$\mathbf{Fext}_i = \sum_p S_{ip} \mathbf{Fext}_p. \tag{4}$$

m_p is the particle mass, $\mathbf{v}_p$ is the particle velocity, and $\mathbf{Fext}_p$ is the external force on the particle. The external force on the particle is generally an applied load of some type. In Equation 3, the numerator is the nodal momentum, which is then divided by the nodal mass to get a velocity. S_{ip} is a "shape function" for the ith node evaluated at $\mathbf{x}_p$. Traditionally, the shape functions are multiplicative combinations of one dimensional tent functions, as shown in Figure 2. The shape functions serve to distance weight the contribution of each particle to the grid nodes.



$$\mathbf{S(x) = (x - x_{i-1})/(x_i - x_{i-1})} \qquad \mathbf{x_{i-1} < x < x_i}$$

$$\mathbf{S(x) = (x_{i+1} - x)/(x_{i+1} - x_i)} \qquad \mathbf{x_i < x < x_{i+1}}$$

$$\mathbf{S(x) = 0} \qquad \mathbf{x < x_{i-1}} \qquad \mathbf{x > x_{i+1}}$$

Figure 2: One dimensional linear shape function, $S(x)$.

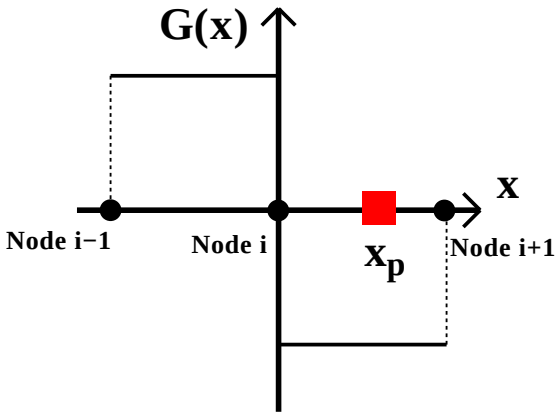
At this point, a velocity gradient, $\nabla \mathbf{v}_p$ is computed at each particle using the grid velocities $\mathbf{v}_g$:

$$\nabla \mathbf{v}_p = \sum_i \mathbf{G}_{ip} \mathbf{v}_I \tag{5}$$

where $\mathbf{G}_{ip}$ is the gradient of the ith node's shape function, evaluated at $\mathbf{x}_p$. A one dimensional example of $\mathbf{G}_{ip}$ is shown in Figure 3. Note that in going to multiple dimensions, the $\mathbf{G}_{ip}$ are found by taking gradients of the multidimensional S_{ip} NOT by forming multiplicative combinations of the one-dimensional $\mathbf{G}_{ip}$.

This velocity gradient is used as input to a constitutive model (stress-strain relationship) which is evaluated at each particle. The specifics of this calculation are dependent on the constitutive model. An example of a simple elastic material model is described in the appendix. The result of this calculation is the Cauchy stress at each particle, $\boldsymbol{\sigma}_p$. With this, the internal force due to the divergence of the stress is calculated:

$$\mathbf{Fint}_g = \sum_p \mathbf{G}_{ip} \boldsymbol{\sigma}_p v_p \tag{6}$$



$$
\begin{aligned}
G(x) &= 1/(x_i - x_{i-1}) && x_{i-1} < x < x_i \\
G(x) &= -1/(x_{i+1} - x_i) && x_i < x < x_{i+1} \\
G(x) &= 0 && x < x_{i-1} \qquad x > x_{i+1}
\end{aligned}
$$

Figure 3: One dimensional linear shape function derivative, $G(x)$.

where v_p is the particle volume. The internal force can be thought of as the force that holds a material together. For a given deformation, this force is larger for stiffer materials.

Everything is now available to solve Equation 1 for $\mathbf{a}_g$. With that, the backward Euler method is used for all time integrations. A convective grid velocity $\mathbf{v}_g^L$ is computed:

$$\mathbf{v}_g^L = \mathbf{v}_g + \mathbf{a}_g dt \tag{7}$$

While the following calculation is never carried out, in principal, the nodes of the grid also move with that convective velocity:

$$\mathbf{x}_g^L = \mathbf{x}_g + \mathbf{v}_g^L dt \tag{8}$$

During this part of the computation, the particles move with the deforming grid. Their position and velocity is explicitly updated by:

$$\mathbf{v}_p(t+dt) = \mathbf{v}_p(t) + \sum_i S_{ip}\mathbf{a}_i dt \tag{9}$$

$$\mathbf{x}_p(t+dt) = \mathbf{x}_p(t) + \sum_i S_{ip}\mathbf{v}_i^L dt \tag{10}$$

This completes one timestep. Note that not carrying out the calculation in 8 explicitly has the effect of resetting the deformed grid to it's undeformed position at the end of the timestep cycle.

As with all explicit time integration methods, a timestep size limit must be enforced such that $dt < dx/(|\mathbf{v}_p| + c)$ for all particles, where dx is the computational grid spacing and c is the speed at which stress waves propagate through the material. Failure to adhere to this condition will cause the solution to become unstable and blow up. The material wavespeed depends on the material model used, as well as on the particular parameters chosen for that model. Specifics of calculating the wavespeed are given in the appendix.

References

[1] D. Sulsky, Z. Chen, and H.L. Schreyer. A particle method for history dependent materials. *Comput. Methods Appl. Mech. Engrg.*, 118:179–196, 1994.

[2] D. Sulsky, S. Zhou, and H.L. Schreyer. Application of a particle-in-cell method to solid mechanics. *Computer Physics Communications*, 87:236–252, 1995.

[3] S.G. Bardenhagen, J.U. Brackbill, and D. Sulsky. The material-point method for granular materials. *Comput. Methods Appl. Mech. Engrg.*, 187:529–541, 2000.

A Hyperelastic Material Models

The subject of modeling the response of materials to deformation is a subject that has filled numerous textbooks. Therefore, rather than attempt to condense these volumes, here the reader will be simply be given a simple material response model. Other more complex material response models can be interchanged in the framework discussed above quite readily.

The author has come to prefer a class of models known as hyperelastic models. What this means is that the stress response of these materials is derived from a strain energy function. A strain energy function gives a relationship between the state of deformation that a material is in, and the amount of stored strain energy that this material has. This is akin to the familiar relationship for the stored energy in a spring, $W = \frac{1}{2}kdx^2$ where k is the spring constant, and dx is the distance that the spring has been compressed or extended.

One such strain energy function is given by:

$$W = \frac{\lambda}{4}(J^2 - 1) - (\frac{\lambda}{2} + \mu)lnJ + \frac{\mu}{2}(trace(\mathbf{F}^T\mathbf{F} - 3) \tag{11}$$

from which the following relationship for the stress can be derived:

$$\boldsymbol{\sigma} = \frac{\lambda}{2}(J - \frac{1}{J})\mathbf{I} + \mu(\mathbf{F}\mathbf{F}^T) - \mathbf{I}) \tag{12}$$

where λ and μ are material constants, while J and $\mathbf{F}$ describe the state of deformation. These will be defined shortly.

In the Algorithm section, the calculation of the velocity gradient, $\nabla\mathbf{v}_p$ is given in Equation 5. Starting from there, we can then compute an increment in the deformation gradient, $\mathbf{F}(dt)$ by:

$$\mathbf{F}(dt) = \nabla\mathbf{v}_p dt + \mathbf{I}. \tag{13}$$

This increment in the deformation gradient can then be used to compute a new total deformation gradient using:

$$\mathbf{F}(t + dt) = \mathbf{F}(dt)\mathbf{F}(t). \tag{14}$$

Note that the initial (t=0) deformation gradient is simply the identity, i.e. $\mathbf{F}(0) = \mathbf{I}$. Now with the deformation gradient, one can compute J by:

$$J = det(\mathbf{F}(t + dt)). \tag{15}$$

Note that J represents the volumetric part of the deformation. Specifically, it is the ratio of the current volume of an element of material to it's original volume. Similarly, we can define an increment in J as:

$$J_{inc} = det(\mathbf{F}(dt)) \tag{16}$$

which is the ratio of the current volume of an element of material to it's volume at the previous timestep. Thus we can write:

$$v_p(t + dt) = J_{inc} v_p(t). \tag{17}$$

Elastic material properties are frequently given in terms of bulk and shear moduli, or κ and μ. The shear is sometimes denoted by G. The shear modulus μ appears in Equation 12 above. λ can be computed from κ and μ by:

$$\lambda = \kappa - \frac{2}{3}\mu. \tag{18}$$

Lastly, based on material properties λ and μ, a material wavespeed can be computed:

$$c^2 = (\lambda + 3\mu)\frac{m_p}{v_p}. \tag{19}$$

This wavespeed can be used in computing the timestep size as described above.

B Other Material Models In the UCF

Other material models implemented into the Uintah Computational Framework (UCF) have been chosen for three purposes:

- To verify the accuracy of the material point method (MPM) and to validate the coupling between the computational fluid dynamics code (ICE) and MPM.
- To model the elastic-plastic deformation of the steel container and the consequent damage in the regimes of both high and low strain rates and high and low temperatures.
- To model the polymer bonded explosive contained in the container under various strain rates and temperatures.

B.1 Material models for the validation of MPM

The models that have been implemented for the verification of MPM are:

- Isotropic hypoelastic model using the Jaumann rate of stress.
    1. MPM predictions have been compared with exact results for thick cylinders under internal pressure for small strains, three-point beam bending, etc.
    2. MPM predictions for the strain/stress contours for a set of disks in contact have been found to match experimental results.

- Isotropic hyperelastic material models for Mooney-Rivlin rubber and a modified compressible Neo-Hookean material. Isotropic strain hardening plasticity for the Neo-Hookean material.

    1. A billet compression problem has been simulated using MPM and the results have been found to closely match finite element simulations.
    2. MPM simulations for a thick cylinder under internal pressure with plastic deformation (perfect plasticity) compare well with the exact solution.

B.2 Material models for the container

The material model for the steel container is used to determine the state of stress in the container for an applied deformation rate and deformation gradient at each material point. The strain rates can vary from 10^{-3}/s to 10^{6}/s and temperatures in the container can vary from 250 K to 1000 K. Plasticity dominates the deformation of the container during the expansion of the explosive gases inside. At high strain rates the volumetric response of the container is best obtained using an equation of state. After the plastic strain in the container has reached a threshold value a damage/erosion model is required to rupture the container.

Two plasticity models with strain rate and temperature dependency are the Johnson-Cook and the Mechanical Threshold Stress (MTS) models. The volumetric response is calculated using a modified Mie-Gruneisen equation of state. A damage model that ties in well with the Johnson-Cook plasticity model is the Johnson-Cook damage model. The erosion algorithm either removes the contribution of the mass of the material point or forces the material point to undergo no tension or shear under further loading.

The stress update at each material point is performed using either of the two methods discussed below.

- Isotropic Hypoelastic-plastic material model using an additive decomposition of the rate of deformation tensor.

    1. The rate of deformation tensor a material point is calculated using the grid velocities.
    2. An incremental update of the left stretch and the rate of rotation tensors is calculated.
    3. The stress and the rate of deformation are rotated into the material coordinates.
    4. A trial elastic deviatoric stress state is calculated.
    5. The flow stress is calculated using the plasticity model and compared with the vonMises yield condition.
    6. If the stress state is elastic, an update of the stress is computed using the Mie-Gruneisen equation of state or the isotropic hypoelastic constitutive equation.
    7. If the stress state is plastic, all the strain rate is considered to the plastic and an elastic correction along with a radial return step move the stress state to the yield surface. The hydrostatic part of the stress is calculated using the equation of state or the hypoelastic constitutive equation.
    8. A scalar damage parameter is calculated and used to determine whether material points are to be eroded or not.
    9. Stresses and deformation rates are rotated back to the laboratory coordinates.

- Isotropic Hyperelastic-plastic material model using a multiplicative decomposition of the deformation gradient.

    1. The velocity gradient at a material point is calculated using the grid velocities.
    2. An incremental update of the deformation gradient and the left Cauchy-Green tensor is calculated.
    3. A trial elastic deviatoric stress state is calculated assuming a compressible Neo-Hookean elastic model.
    4. The flow stress is calculated using the plasticity model and compared with the vonMises yield condition.
    5. If the stress state is elastic, an update of the stress is computed using the Mie-Gruneisen equation of state or the compressible Neo-Hookean constitutive equation.

6. If the stress state is plastic, all the strain rate is considered to the plastic and an elastic correction along with a radial return step move the stress state to the yield surface. The hydrostatic part of the stress state is calculated using the Mie-Gruneisen equation of state or the Neo-Hookean model.
7. A scalar damage parameter is calculated and used to determine whether material points are to be eroded or not.

The implementations have been tested against Taylor impact test data for 4340 steel and HY 100 steel as well as one-dimensional problems which have been compared with experimental stress-strain data. At large tensile strains, material points tend to separate from the main body. This issue is currently being explored and solutions are being sought in the framework of MPM.

B.3 Material models for the explosive

The explosive is modeled using the ViscoSCRAM constitutive model. Since large deformations or strains are not expected in the explosive, a small strain formulation has been implemented into the UCF. The model consists of five generalized Maxwell elements arranged in parallel, crack growth, friction at the crack interfaces and heating due to friction and reactions at the crack surfaces. The implementation has been verified with experimental data and found to be accurate.