

Continuous Gradient Method to Cell Crossing Instability

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Material Point Method

Material point method has its unique advantages on avoiding the numerical diffusion and mesh distortion issues suffered by pure Eulerian and Lagrangian methods.

Because of these advantages, it has been used to many problems involving multimaterial interactions, multiphase flows, fluid-structure interactions,

We **believe** that material point method can be used to simulate large deformation of materials, but, there is an issue: the stress noise as particles move across cell boundaries.

My experience suggests that this issue does not hurt overall performance of MPM if the problem is continuous, such as ductile failures of the material, but for a problem with brittle damage, this issue can be a real problem. The material can fail purely due to numerical noise.

Noise due to Cell Crossing of Particles

- The momentum equation:

$$\rho \frac{d\mathbf{u}}{dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}$$

- MPM discretization:

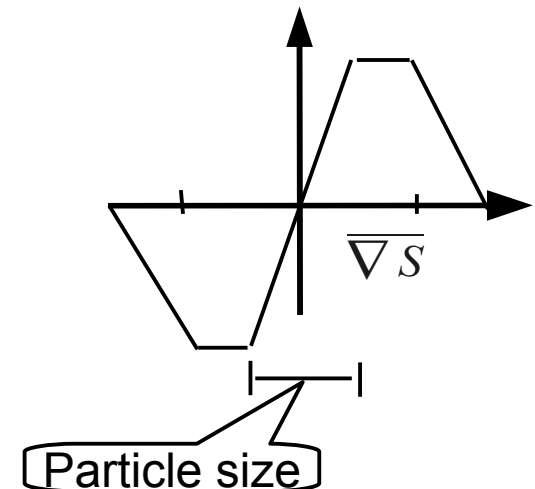
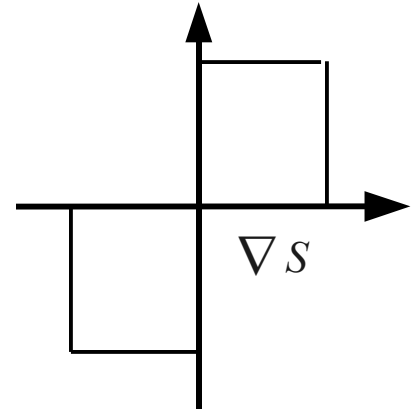
$$m_{ij} \frac{d\mathbf{u}_j}{dt} = - \int \boldsymbol{\sigma} \cdot \nabla S_i(\mathbf{x}) dv + \dots$$

$$\int \boldsymbol{\sigma} \cdot \nabla S_i(\mathbf{x}) dv \approx \sum_p v_p \boldsymbol{\sigma}_p \cdot \nabla S(\mathbf{x}_p)$$

- The discontinuity of the gradient of the shape function causes the noise.

- Solutions:

- Using higher order shape functions.
 - Has been tried in FEM. Mostly abandoned today because of enlarged support.
- Introducing particle size Bardenhagen and Kober (2004).
 - Works for moderate deformations.
 - Need to track particle size or shape for large deformations.



Seeking a solution....

- The problem starts with the use of

$$\int \boldsymbol{\sigma} \cdot \nabla S_i(\mathbf{x}) dv \approx \sum_p v_p \boldsymbol{\sigma}_p \cdot \nabla S(\mathbf{x}_p)$$

- We don't have to perform the numerical integral this way. Here is another way:

- Define stress on nodes:

$$\boldsymbol{\sigma}_j = \frac{1}{V_j} \sum_p v_p \boldsymbol{\sigma}_p S_j(\mathbf{x}_p), \quad \boldsymbol{\sigma}(\mathbf{x}) = \sum_j \boldsymbol{\sigma}_j S_j(\mathbf{x})$$

- and then integrate:

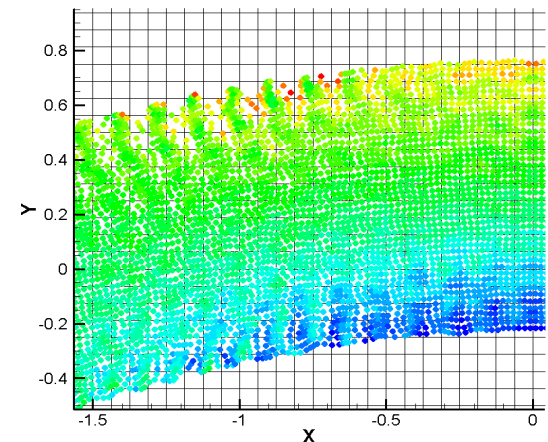
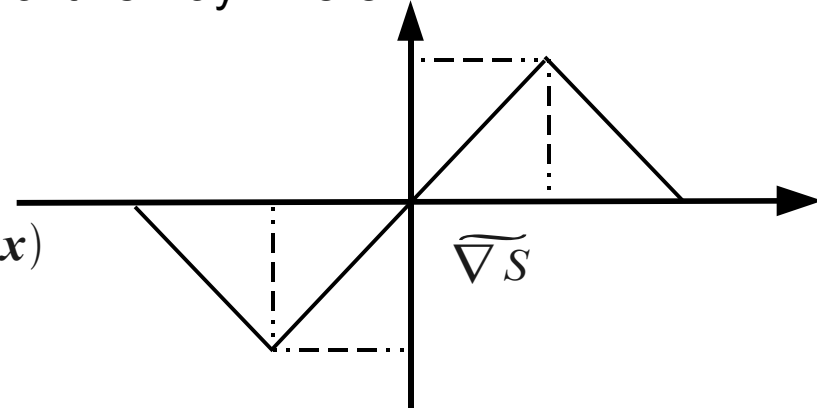
$$\int \boldsymbol{\sigma} \cdot \nabla S_i(\mathbf{x}) dv = \sum_j \boldsymbol{\sigma}_j \int S_j(\mathbf{x}) \nabla S_i(\mathbf{x}) dv = \sum_p v_p \boldsymbol{\sigma}_p \widetilde{\nabla} S(\mathbf{x}_p)$$

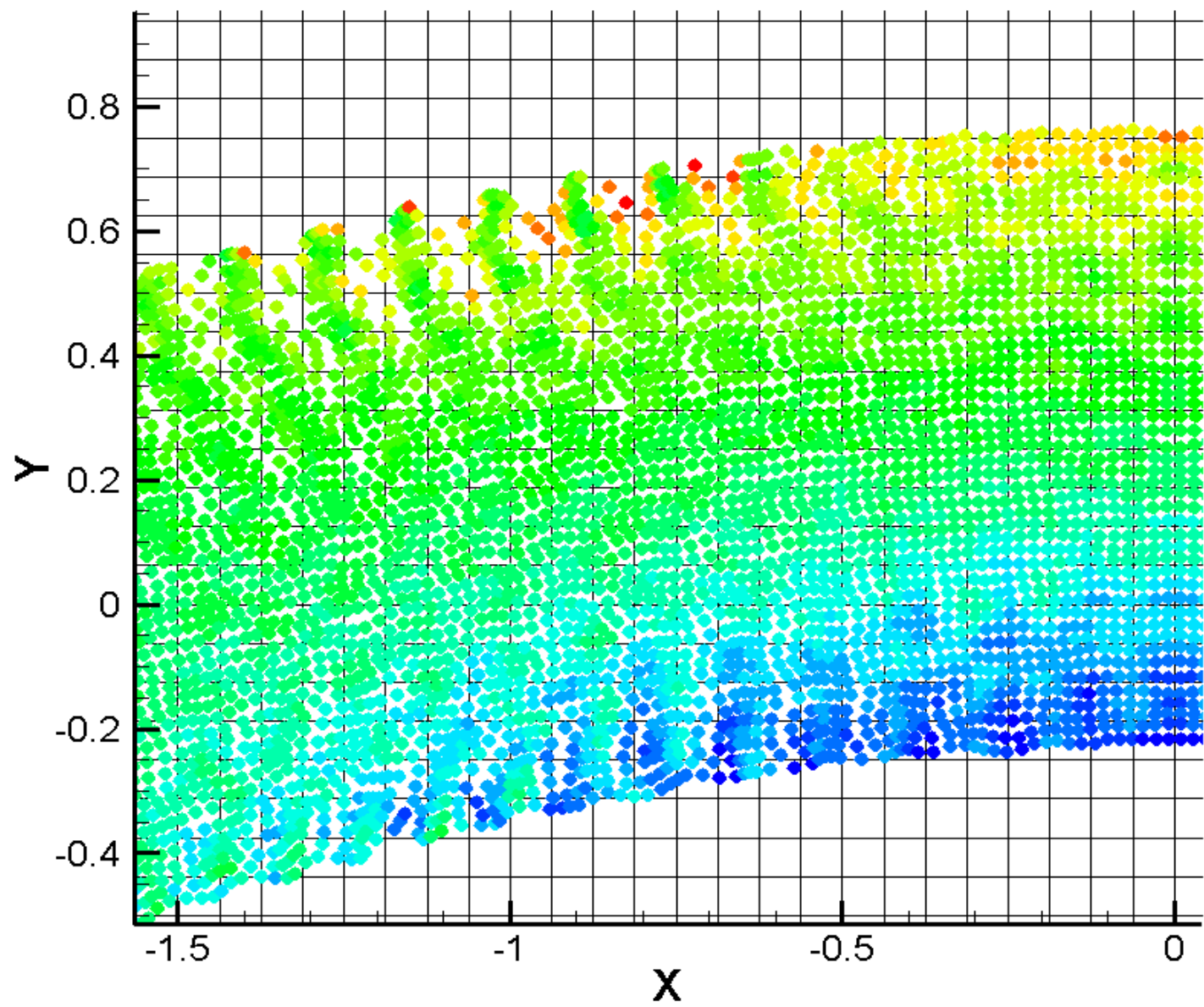
(discussed with Prof. Deborah Sulsky)

- Defined a new gradient of the shape function:

$$\widetilde{\nabla} S(\mathbf{x}_p) = \sum_j S_j(\mathbf{x}_p) \frac{1}{V_j} \int S_j(\mathbf{x}) \nabla S_i(\mathbf{x}) dv$$

This scheme also enlarges the influence region of a particle. It works for moderate deformation. **It becomes unstable for large deformation.**





Cause of the instability

We note that the zig-zag velocity field illustrated on the right is the highest frequency can be represented at this spatial discretization.

For systems with large deformation, one expects generation of high frequency components from nonlinear interactions. Therefore there are plenty of sources for this spatial mode.

With this spatial mode, the node force

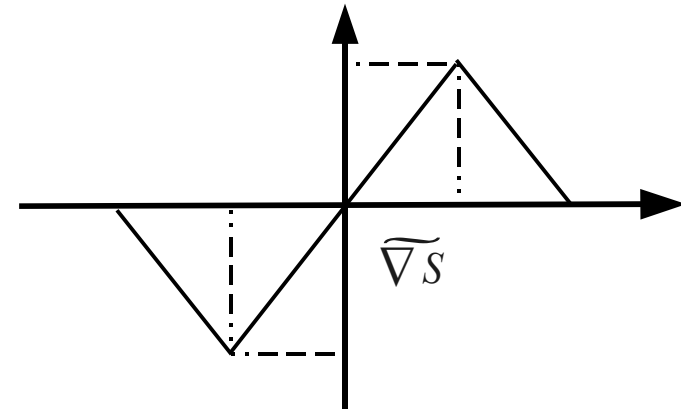
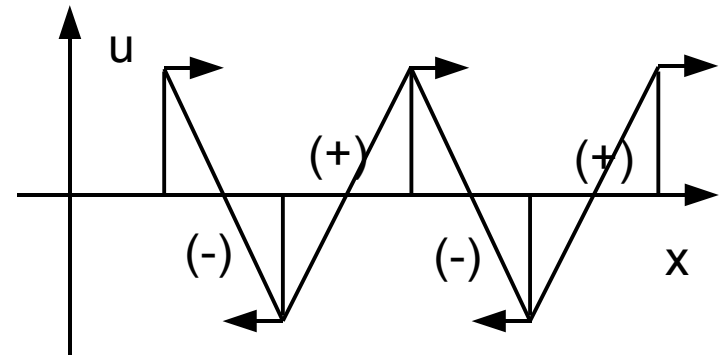
$$\int \boldsymbol{\sigma} \cdot \nabla S_i(\mathbf{x}) dv = \sum_p v_p \boldsymbol{\sigma}_p \widetilde{\nabla} S(\mathbf{x}_p)$$

calculated this way is zero. This difficulty is similar to the collocated pressure calculations in the finite volume method.

$$\boldsymbol{\sigma}(\mathbf{x}) = \sum_j \boldsymbol{\sigma}_j S_j(\mathbf{x}) + \mathbf{A}(\mathbf{x}),$$

$$\mathbf{A}(\mathbf{x}) = \sum_p \alpha(\mathbf{x}_p) v_p \boldsymbol{\sigma}_p \delta(\mathbf{x} - \mathbf{x}_p) - \sum_j \frac{1}{V_j} \sum_p \alpha(\mathbf{x}_p) v_p \boldsymbol{\sigma}_p S_j(\mathbf{x}_p) S_j(\mathbf{x})$$

It can be proven that $\mathbf{A}(\mathbf{x}) = O(\Delta x)^2$ for any bounded $\alpha(\mathbf{x})$ in the sense of weak convergence.



Continuous Gradient Scheme

After adding $A(x)$ to the stress, the force on node i can be calculated as

$$\int \boldsymbol{\sigma} \cdot \nabla S_i(\mathbf{x}) dV = \sum_p v_p \boldsymbol{\sigma}_p \overline{\nabla S}(\mathbf{x}_p),$$

where

$$\overline{\nabla S}_i(\mathbf{x}) = \alpha(\mathbf{x}) \nabla S_i(\mathbf{x}) + [1 - \alpha(\mathbf{x})] \widetilde{\nabla S}_i(\mathbf{x})$$

is the redefined gradient of the shape function. This redefined gradient of the shape function is continuous if $\alpha(x) = 0$ on the cell boundaries. We call this method as the material point method with continuous gradient (MPMCG). The redefined gradient of the shape function satisfies

$$\sum_{i=1} \overline{\nabla S}_i(\mathbf{x}) = 0, \quad \sum_{i=1} \mathbf{x}_i \overline{\nabla S}_i(\mathbf{x}) = \mathbf{I}.$$

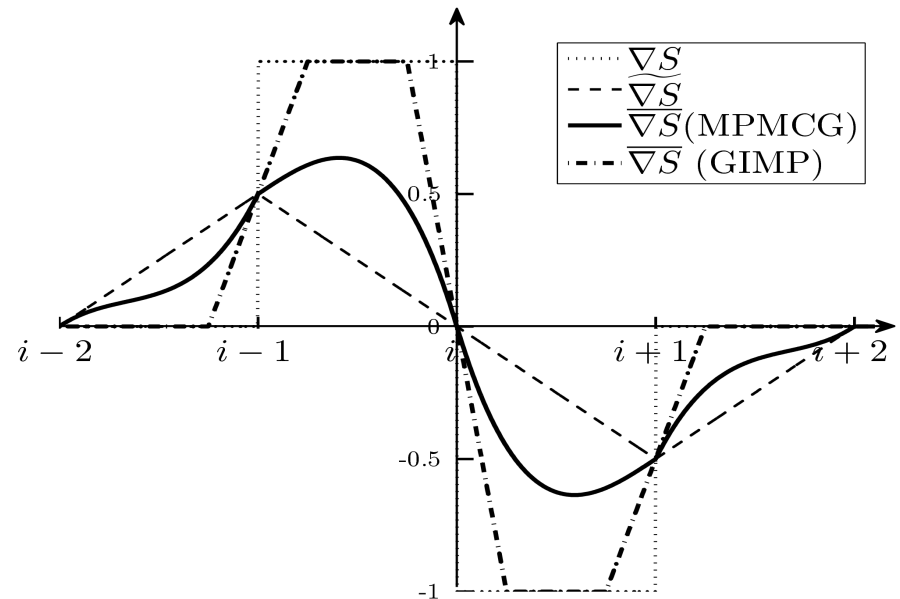
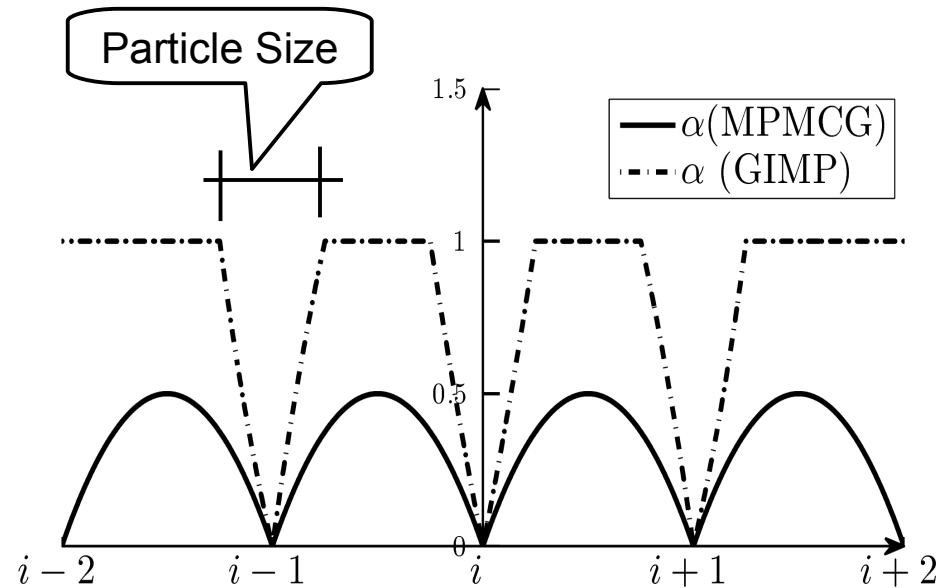
These properties can be used to prove mass, momentum and energy conservation properties.

The mass and momentum conservations are satisfied exactly. The error in energy conservation is second order both in time and spatial discretization as in the original MPM, if the velocity gradient is calculated using the same redefined gradient of the shape function.

$$\overline{\nabla \mathbf{u}}(\mathbf{x}_p) = \sum_{i=1} \mathbf{u}_i \overline{\nabla S}_i(\mathbf{x}_p).$$

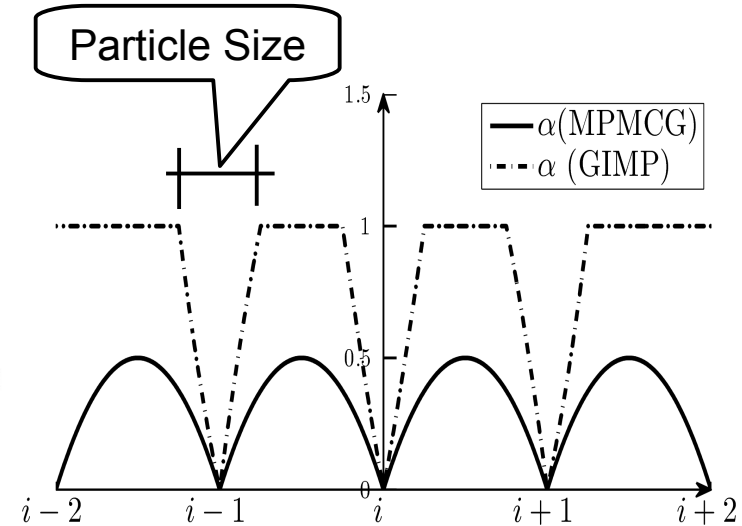
Relation to GIMP

- GIMP enlarges the support of the shape function, while in this scheme the shape function is unaltered from the original MPM.
- The gradient of the shape function used in GIMP can be obtained by a special choice of $\alpha(x)$ when particle “size” is introduced.
- In the current method (MPMCG), the concept of particle size or shape is not needed. Therefore no need to track them.
- The function $\alpha(x)$ is not periodic in GIMP.
- In MPMCG, function $\alpha(x)$ is periodic and can be calculated as products of shape functions.
- With this property, in MPMCG the non-local effects due to enlarged support of the gradient of the shape function can be accounted for by two steps of local operations.



α for GIMP

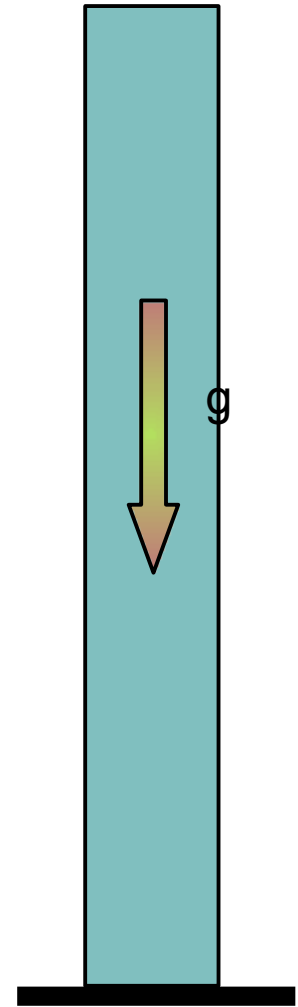
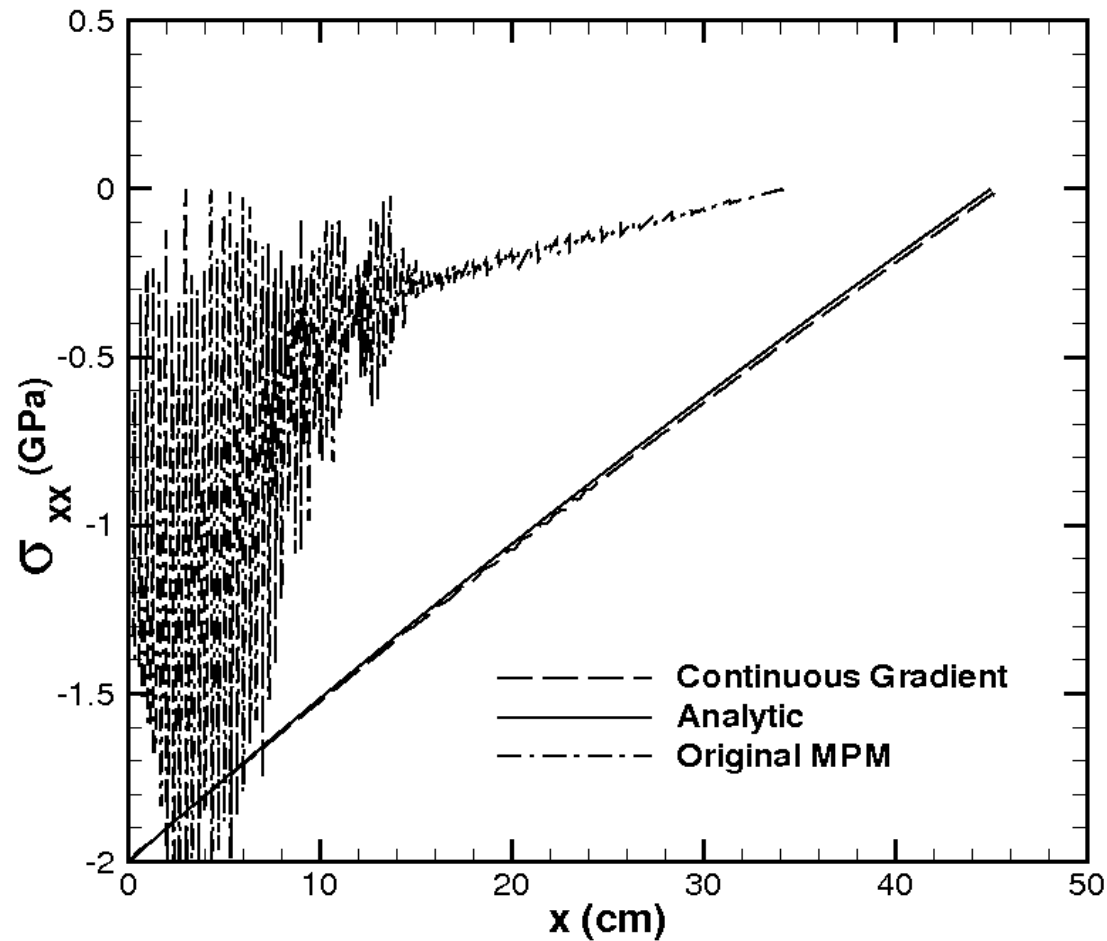
$$\alpha(x) = \begin{cases} 1, & x < x_{i-1} - \ell_p \\ 1 - \frac{\Delta x}{\ell_p} \cdot \frac{x - x_{i-1} + \ell_p}{x - x_{i-1} + \Delta x}, & x_{i-1} - \ell_p \leq x < x_{i-1} \\ \left(1 + \frac{\Delta x}{\ell_p}\right) \frac{x - x_{i-1}}{x - x_{i-1} + \Delta x}, & x_{i-1} \leq x < x_{i-1} + \ell_p \\ 1, & x_{i-1} + \ell_p \leq x < x_i - \ell_p \\ \left(1 - \frac{2\Delta x}{\ell_p}\right) \frac{x - x_i}{x - x_i + 2\Delta x}, & x_i - \ell_p \leq x < x_i \\ \left(1 - \frac{2\Delta x}{\ell_p}\right) \frac{x - x_i}{x - x_i - 2\Delta x}, & x_i \leq x < x_i + \ell_p \\ 1, & x_i + \ell_p \leq x < x_{i+1} - \ell_p \\ \left(1 + \frac{\Delta x}{\ell_p}\right) \frac{x - x_{i+1}}{x - x_{i+1} - \Delta x}, & x_{i+1} - \ell_p \leq x < x_{i+1} \\ 1 - \frac{\Delta x}{\ell_p} \cdot \frac{x - x_{i+1} - \ell_p}{x - x_{i+1} - \Delta x}, & x_{i+1} \leq x < x_{i+1} + \ell_p \\ 1, & x_{i+1} + \ell_p < x \end{cases}$$



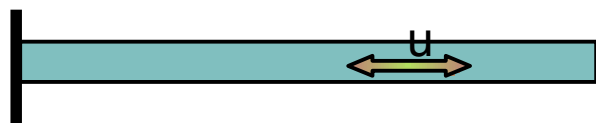
Near the cell boundaries, this function is not linear, but it is very close to linear functions.

Just a thought: **If we approximate it using linear functions near the boundaries, can we simplify GIMP?**

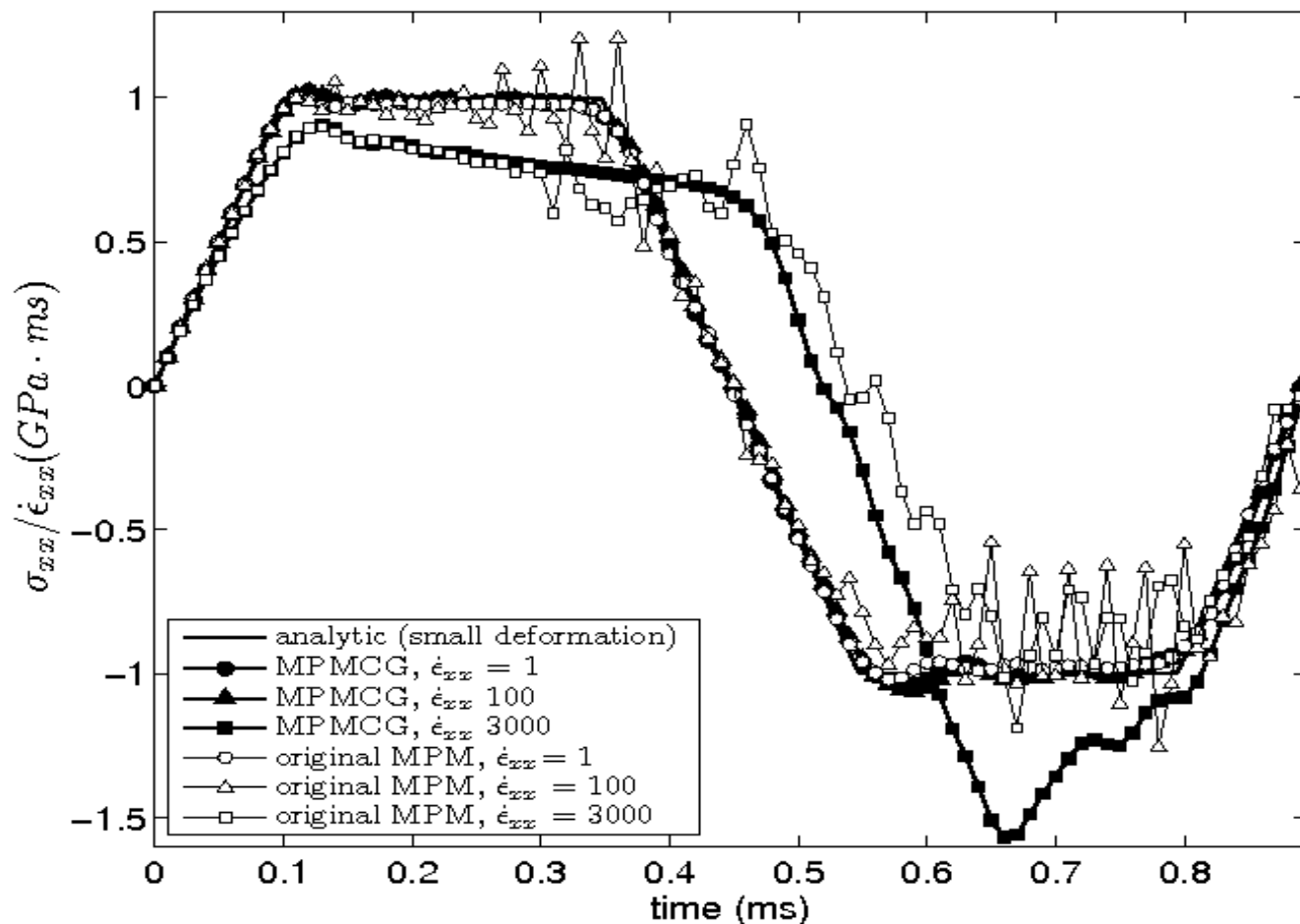
Examples from Continuous Gradient Method Implemented in CartaBlanca



Results of Continuous Gradient Method

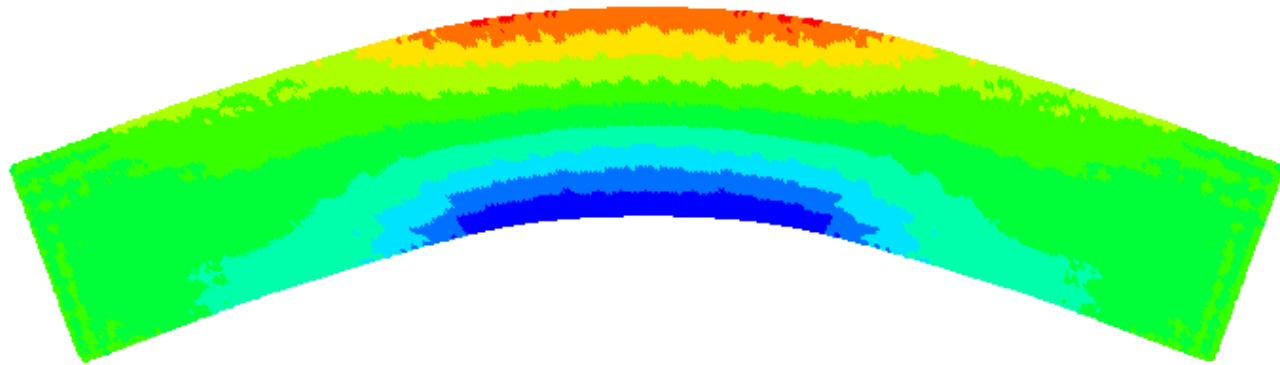


X = 27.7 cm

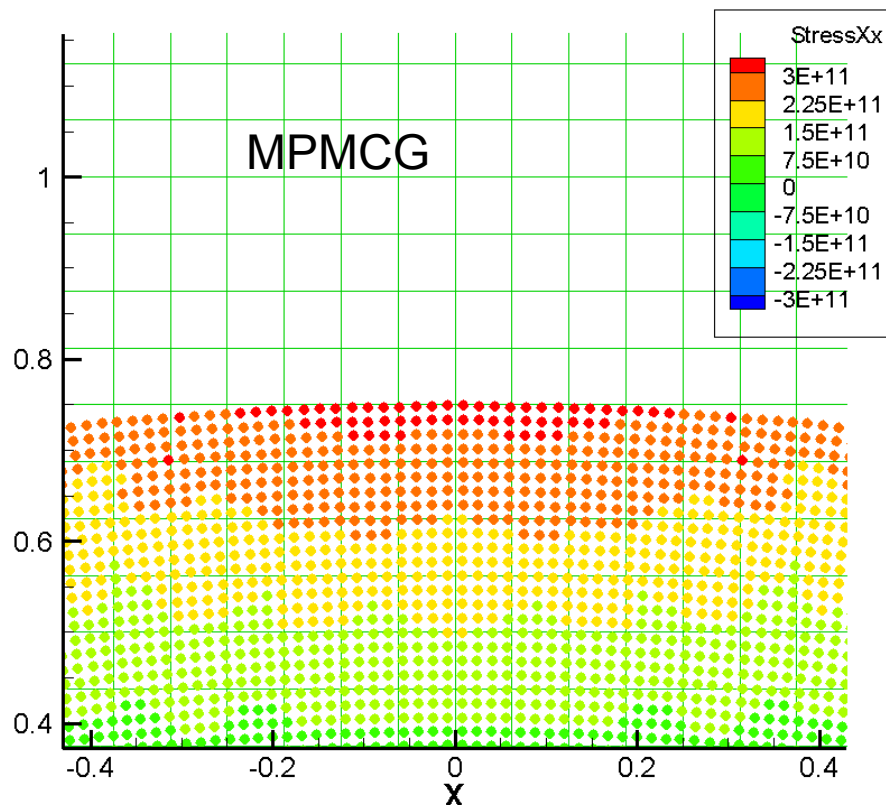


Results of Continuous Gradient Method

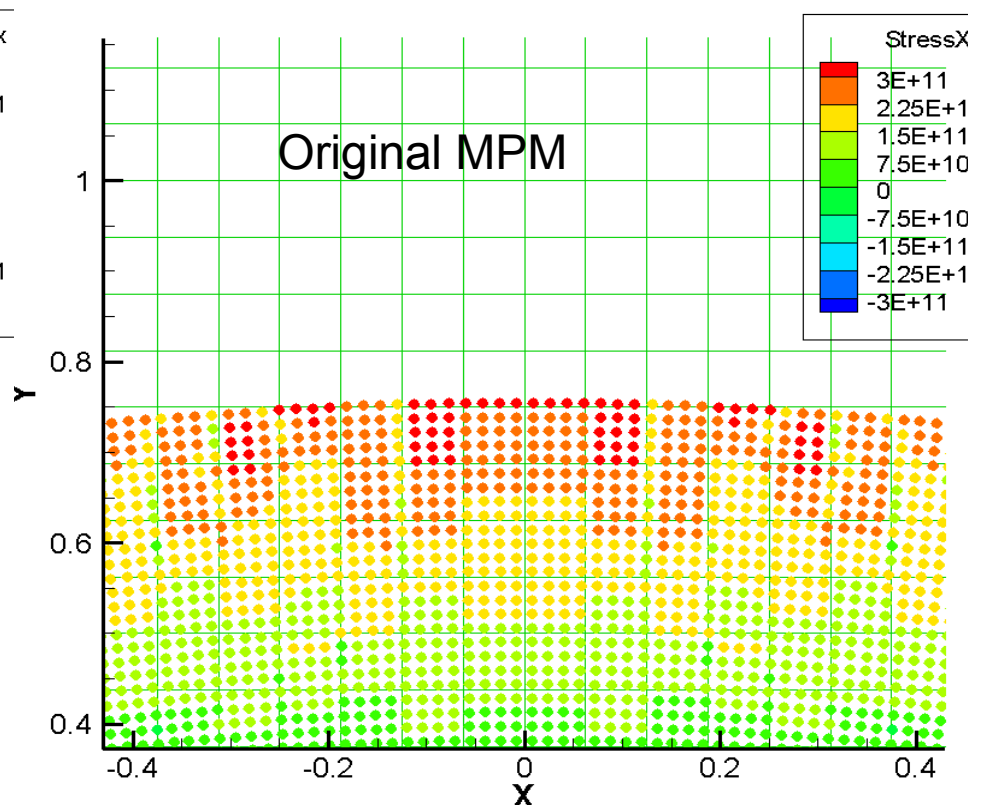
Bent beam:



MPMCG

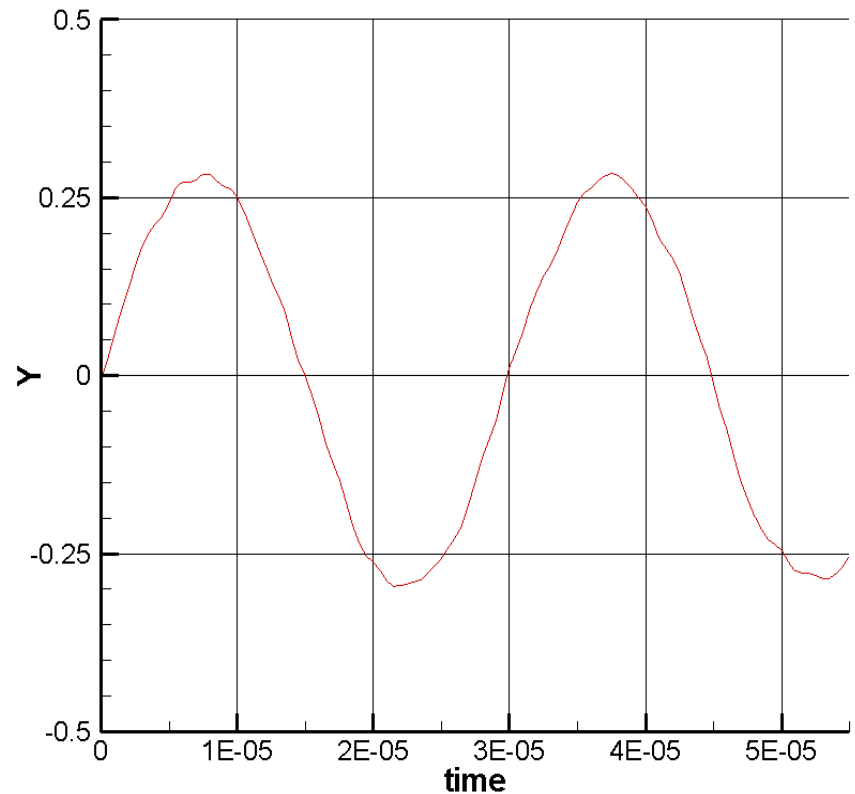
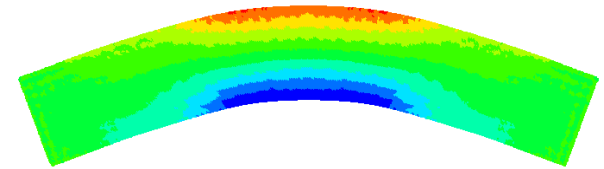
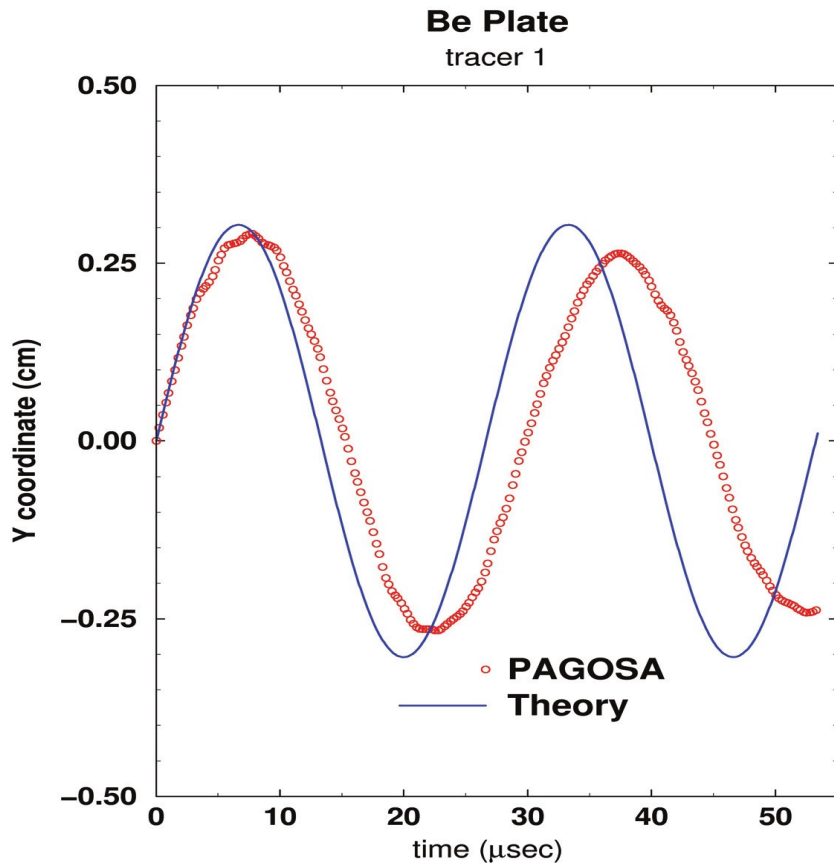


Original MPM



Comparison with PAGOSA

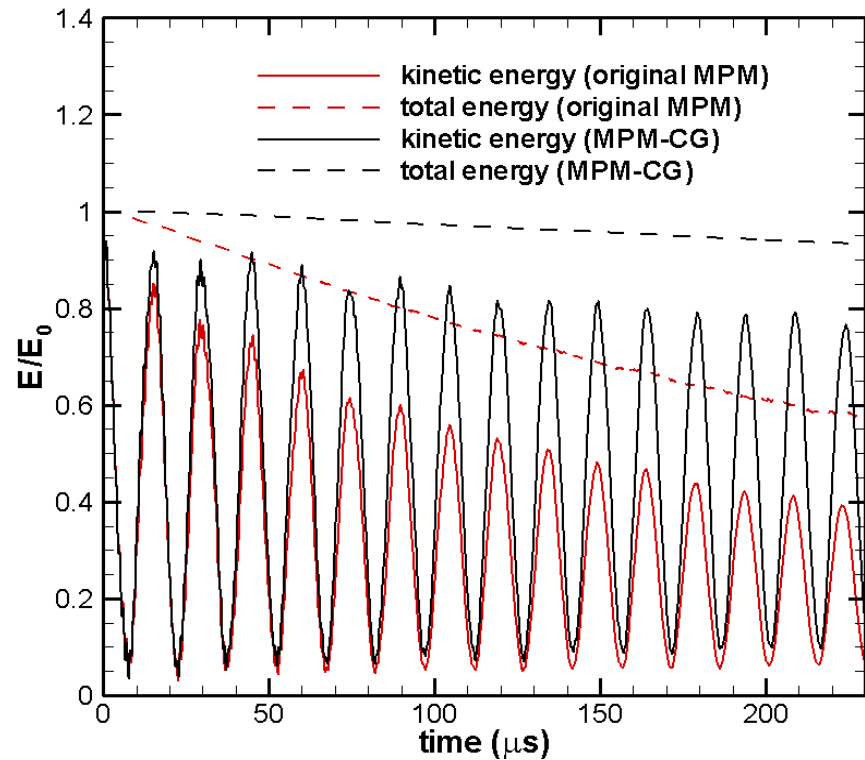
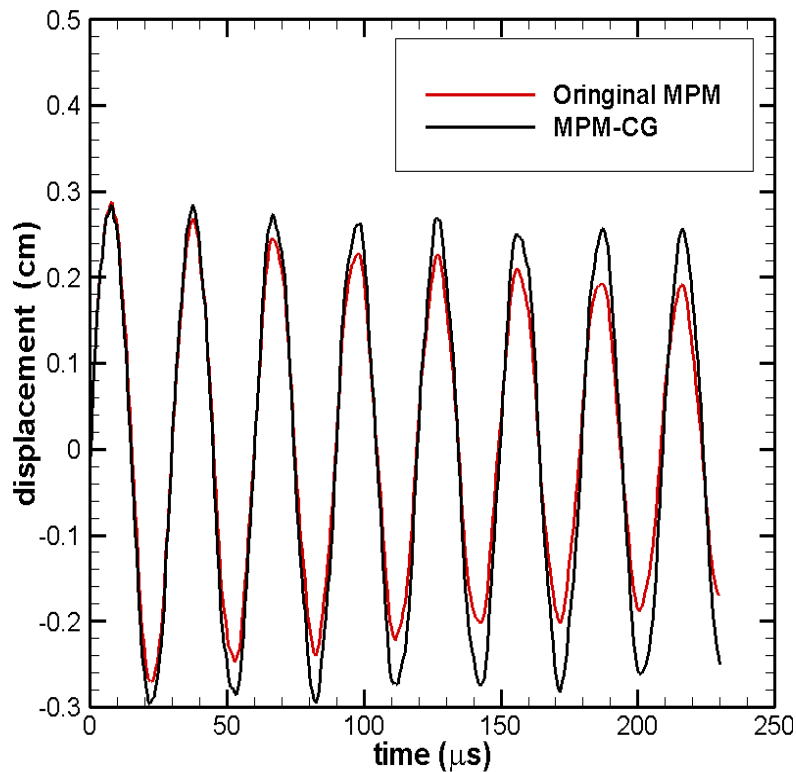
Comparing to PAGOSA code with interface reconstruction, our results are very similar, including small features.



From Wayne Weseloh, XDT-1

Energy Conservation for Continuous Gradient Method (Large Deformation)

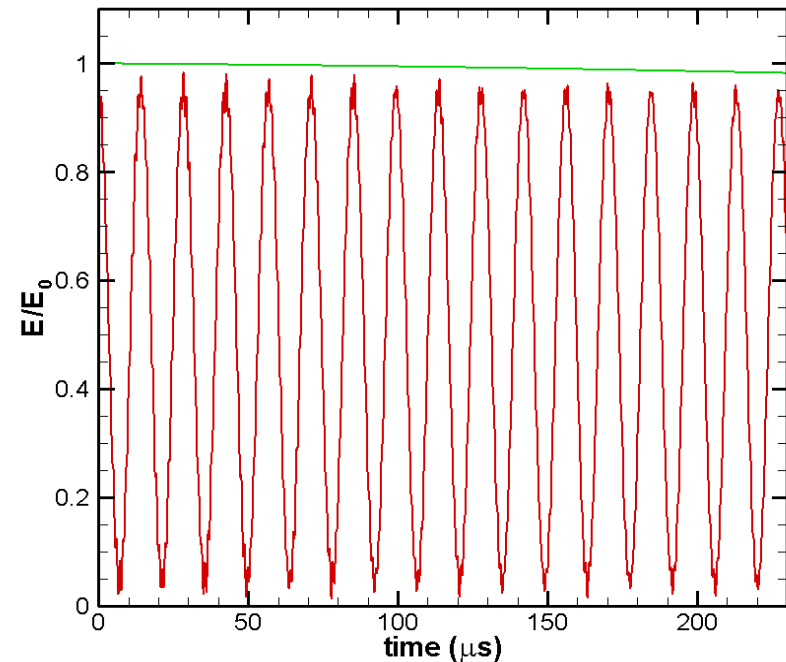
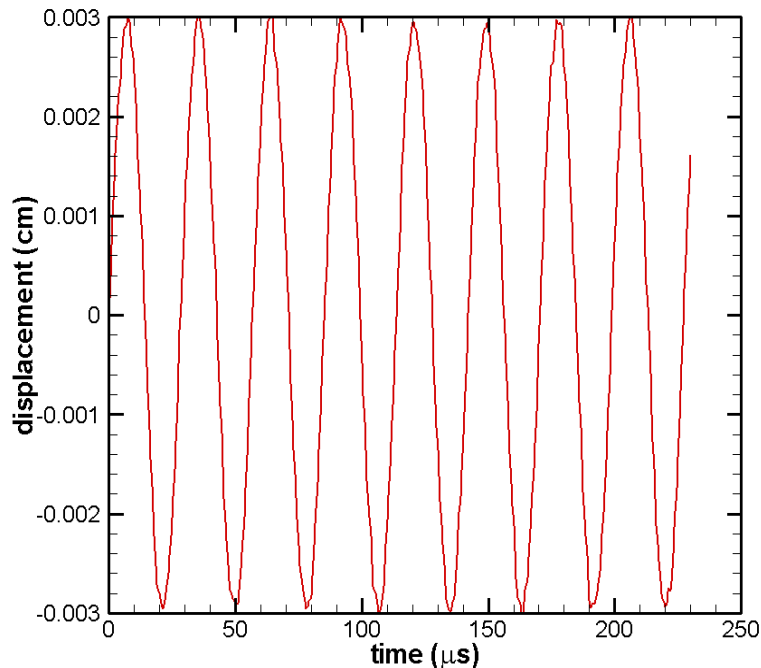
The motion of the beam is initiated by a prescribed velocity field. MPM with the continuous gradient method is less dissipative compared to the original MPM.



The difference between the total energy and the peak kinetic energy could be the effect of the higher order harmonics produced by nonlinear effects in the large deformation (energy cascade).

Energy Conservation for Continuous Gradient Method (Small Deformation)

With 1% of the deformation:



Comparing to that of large deformation, the difference between the total energy and the peak kinetic energy is much smaller for this small deformation case.

Summary

- The instability caused by cell crossing of particles can be eliminated by the material point method with continuous gradient for shape functions (MPMCG).
- MPMCG conserves mass and momentum. The error on energy conservation is second order on both time and spatial discretization, as in the original MPM.
- MPMCG only alters the gradient of the shape function, not the shape functions.
- With usual choices of the weight function α , MPMCG only requires local operations.
- GIMP is a special case of MPMCG when the weight function α is chosen according to particle size.
- Although more tests are needed, results from MPMCG implemented in CartaBlanca are very encouraging.