

Computation of Multi-Material Interactions Using Material Point Method

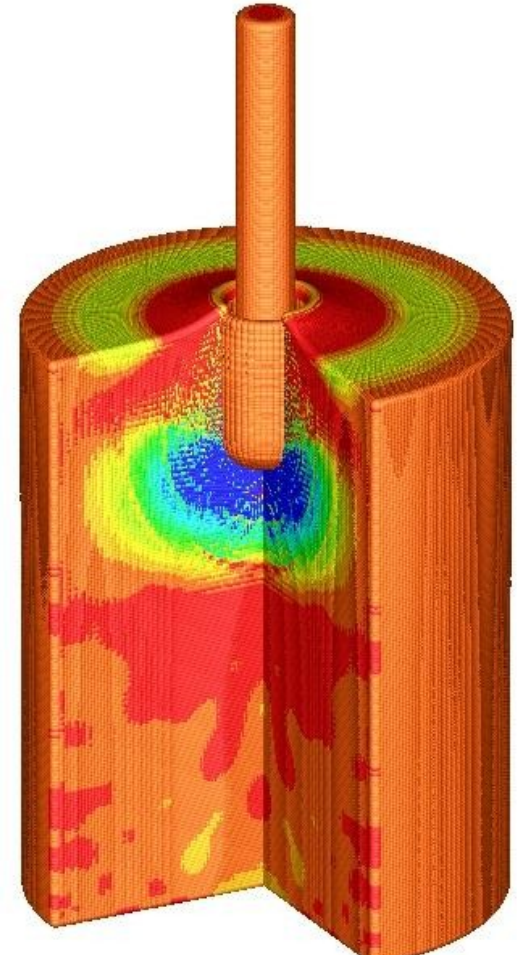
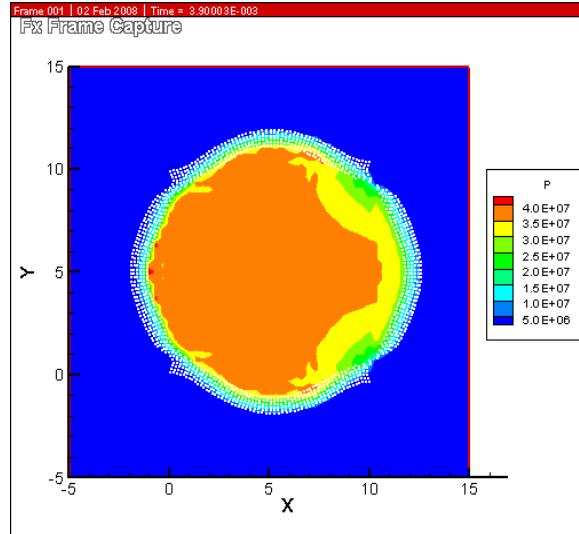
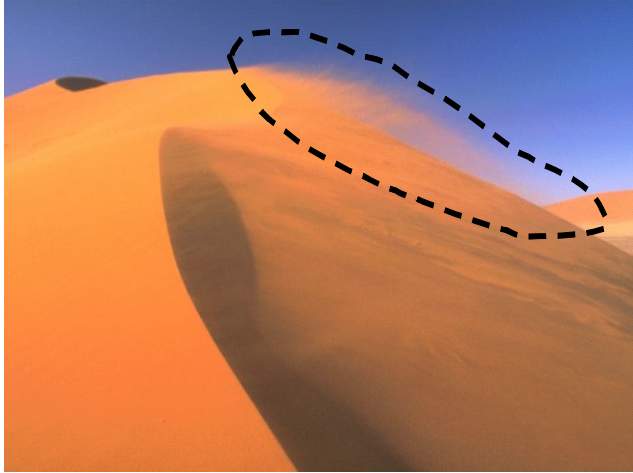
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<http://www.lanl.gov/projects/CartaBlanca>

Multi-material interactions



These interactions of materials can be described by:

$$\frac{\partial \rho_i \bar{\mathbf{u}}_i}{\partial t} + \nabla \cdot (\rho_i \bar{\mathbf{u}}_i \bar{\mathbf{u}}_i) = \theta_i \nabla p + \dots$$

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \bar{\mathbf{u}}_i) = 0$$

where θ_i is the volume fraction, ρ_i is the macroscopic density.

Calculation of volume fractions

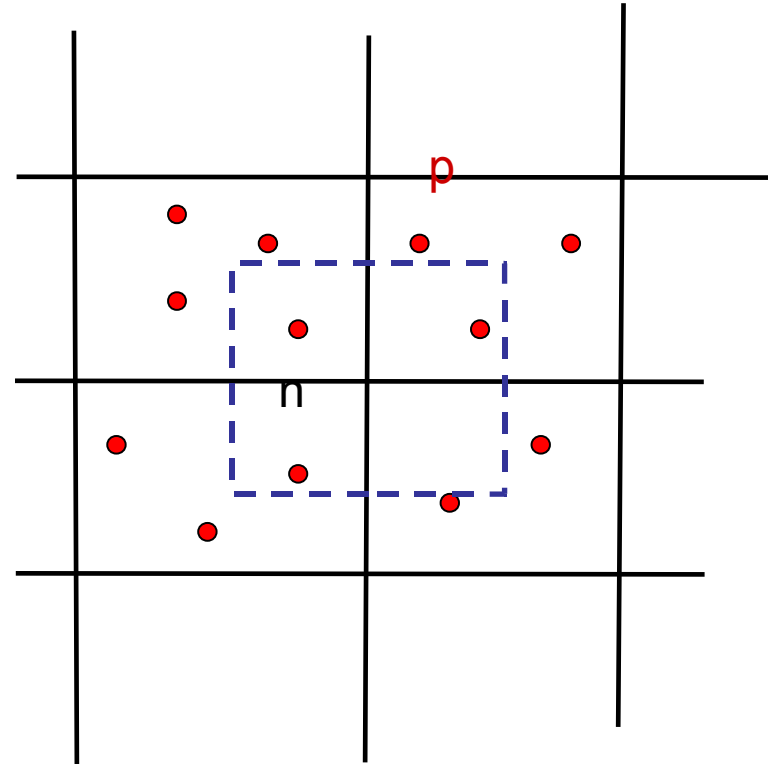
For Eulerian calculations, the pressure in the system is determined by satisfying the continuity equation:

$$\sum_{i=1}^m \theta_i = \sum_{i=1}^m \frac{\rho_i}{\rho_i^0(p)} = 1,$$

but this approach does **not** work for MPM calculations, because in MPM volume fraction is approximated as:

$$\theta_i = \frac{1}{V_{cell}} \sum_{p=1}^{N_p} V_p^i S(x_p).$$

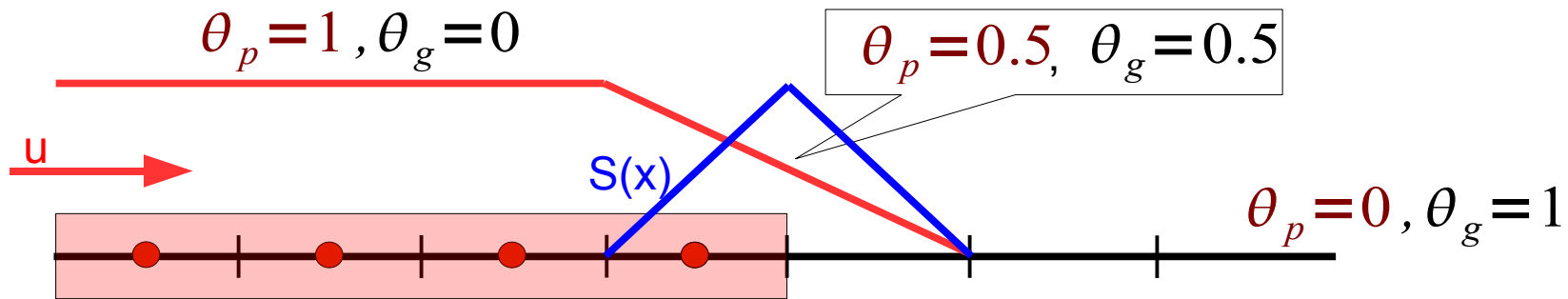
S is the shape function.



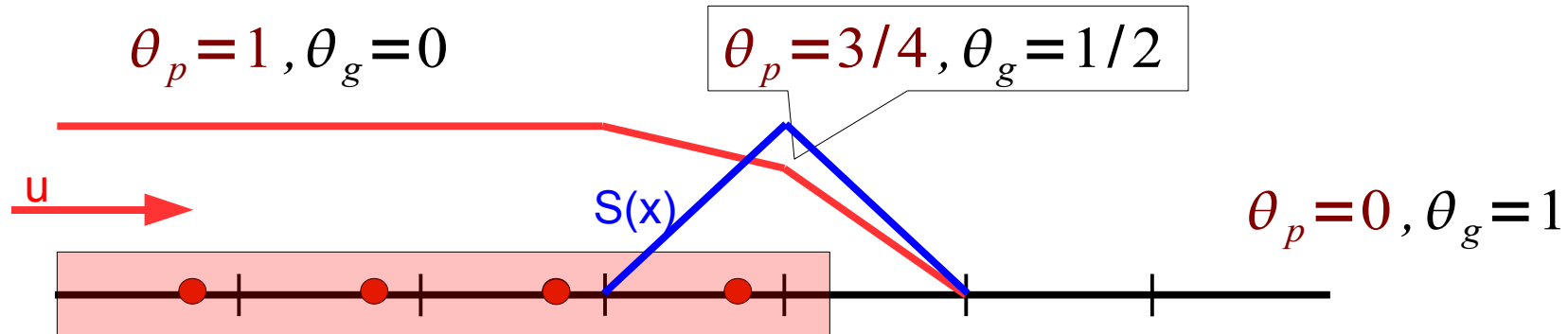
A simple example

Representing solid by MPM and gas by ordinary Eulerian mesh.

$$V_p = 1, V_{cell} = 1 \quad \theta_i = \frac{1}{V_{cell}} \sum_{p=1}^{N_p} V_p^i S(x_p)$$



- During a rigid translation, after advection we have:



Consequence of the volume fraction error

- To calculate pressure p^{n+1} at time step $n+1$ we solve

$$\sum_{i=1}^m \theta_i(p^{n+1}) = f(p^{n+1}, t) = \sum_{i=1}^m \frac{\rho_i(p^{n+1}, t)}{\rho_i^0(p^{n+1})} = 1$$

After the Taylor expansion:

$$f(p^n, t^n) + \frac{\partial f}{\partial t} \Delta t + \frac{\partial f}{\partial p} \Delta p = 1 \quad \longrightarrow \quad \frac{\partial f}{\partial t} + \frac{\partial f}{\partial p} \frac{\Delta p}{\Delta t} + O\left(\frac{\Delta x}{\Delta t}\right) = 0$$

1 + O(Δx)

In a calculation, time step is restricted by Δx . In a time explicit scheme,

$$\Delta t < \Delta x / C, \quad \Delta t < (\Delta x)^2 / D,$$

where C is the speed of sound. In every time step the error in Δp increases by $C\Delta t$ or $C/\Delta t$.

The accumulated pressure error will overwhelm the result in just a few time steps. **Even the rigid body translation problem cannot be calculated correctly.** For a given physical time, this error **cannot** be reduced by reducing mesh size or time step.

Fixing it — evolution equation approach

Developers of CFDLIB are aware of this issue. To fix it, evolution equation is used.

$$\frac{\partial \theta_i}{\partial t} + \nabla \cdot (\theta_i \bar{\mathbf{u}}_i) = \theta_i \langle \nabla \cdot \mathbf{u}_i \rangle,$$

where $\langle \nabla \cdot \mathbf{u}_i \rangle$ is related to material interaction model.

With this evolution equation approach, the error in volume fractions are of order of Δt . This results in pressure error to be of $O(\rho C_i^2 \Delta t / T)$, where T is the characteristic time scale of the problem, and C_i is the speed of sound.

$$\frac{\partial \rho_i \bar{\mathbf{u}}_i}{\partial t} + \nabla \cdot (\rho_i \bar{\mathbf{u}}_i \bar{\mathbf{u}}_i) = \theta_i \nabla [p + O(\rho_i C_i^2 \Delta t / T)] + \dots$$

In order for this approach to work, $\Delta t \ll M^2 T$, where M is the Mach number. **Trouble for low speed flows.** This is the reason in Eulerian calculations we use $\sum \theta_i = 1$, instead of the evolution equations.

Seeking higher order accuracy

Summing $\frac{\partial \theta_i}{\partial t} + \nabla \cdot (\theta_i \bar{\mathbf{u}}_i) = \theta_i \langle \nabla \cdot \mathbf{u}_i \rangle$ over all phases we find that the continuity requirement $\sum_{i=1}^m \theta_i = 1$ is satisfied **if and only if** $\nabla \cdot \mathbf{u}_m = \sum_{i=1}^m \theta_i \langle \nabla \cdot \mathbf{u}_i \rangle$, where $\mathbf{u}_m = \sum_{i=1}^m \theta_i \bar{\mathbf{u}}_i$ is the mixture velocity.

The evolution equation approach only satisfy this relation to $O(\Delta t)$,

$$\nabla \cdot \mathbf{u}_m - \sum_{i=1}^m \theta_i \langle \nabla \cdot \mathbf{u}_i \rangle = O(\Delta t).$$

and leads to $O(\rho C_i^2 \Delta t / T)$ error in pressure.

We now seek a way to satisfy this equation to a higher order ($\Delta x \Delta t$).

By defining $\frac{d_m}{d_m t}(\cdot) = \frac{\partial}{\partial t}(\cdot) + \mathbf{u}_m \cdot \nabla(\cdot)$, and then adding and subtracting $\theta_i \nabla \cdot \mathbf{u}_m$ to the evolution equation for volume fraction, we have

$$\frac{d_m \theta_i}{d_m t} + \nabla \cdot [\theta_i (\bar{\mathbf{u}}_i - \mathbf{u}_m)] + \theta_i \nabla \cdot \mathbf{u}_m = \theta_i \langle \nabla \cdot \bar{\mathbf{u}}_i \rangle.$$

Weak solution approach

$$\frac{d_m \theta_i}{d_m t} + \nabla \cdot [\theta_i (\bar{\mathbf{u}}_k - \mathbf{u}_m)] + \theta_i \nabla \cdot \mathbf{u}_m = \theta_i \langle \nabla \cdot \bar{\mathbf{u}}_k \rangle.$$

We then seek weak solution for this equation. The trial function takes form $\delta \theta = \sum \delta \theta_n S_n(x)$ and the discretized form of the equation is

$$\frac{d_m V_{ni}}{d_m t} = \int S_n \nabla \cdot [\theta_i (\bar{\mathbf{u}}_i - \mathbf{u}_m)] dv + \int S_n \theta_i (\langle \nabla \cdot \mathbf{u}_i \rangle - \nabla \cdot \mathbf{u}_m) dv,$$

$$V_{ni} = \int \theta_i S_n dv \approx \sum_{p=1}^{N_p} V_{ip} S_p = \theta_{in} V_n [1 + O(\Delta x)].$$

Summing over all phases:

$$\frac{\partial}{\partial t} \sum V_{ni} + \mathbf{u}_m \cdot \nabla \sum V_{ni} = \int S_n \nabla \cdot \sum [\theta_i (\bar{\mathbf{u}}_i - \mathbf{u}_m)] dv + \int S_n (\theta_i \sum \langle \nabla \cdot \mathbf{u}_i \rangle - \nabla \cdot \mathbf{u}_m) dv,$$

The continuity requirement $\nabla \cdot \mathbf{u}_m - \sum \theta_i \langle \nabla \cdot \mathbf{u}_i \rangle = 0$ which is equivalent to $\sum_{i=1}^m \theta_i = 1$, can be satisfied to order $\Delta x \Delta t$, if

$$\frac{\partial}{\partial t} \sum V_{ni} + \mathbf{u}_m \cdot \nabla \sum V_{ni} - \int S_n \nabla \cdot \sum [\theta_i (\bar{\mathbf{u}}_i - \mathbf{u}_m)] dv = O(\Delta x \Delta t).$$

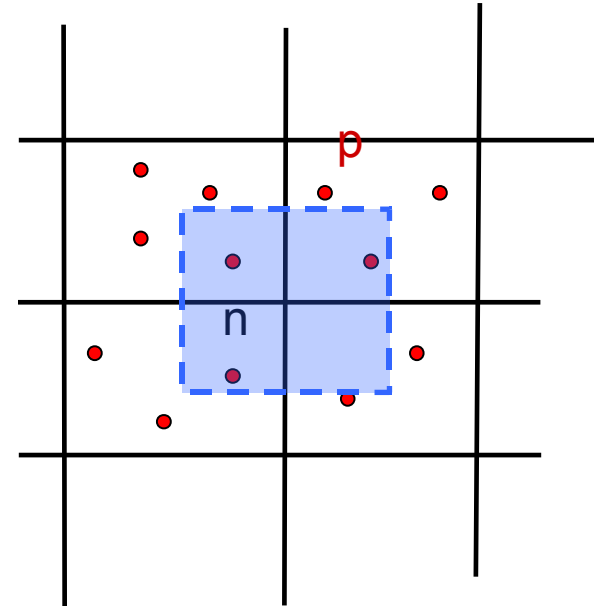
Weak solution to volume fraction equation

$$\frac{\partial}{\partial t} \sum V_{ni} + \mathbf{u}_m \cdot \nabla \sum V_{ni} - \int S_n \nabla \cdot \sum [\theta_i (\bar{\mathbf{u}}_i - \mathbf{u}_m)] dv = O(\Delta x \Delta t),$$

Noting $\sum \theta_i = 1 + O(\Delta x) \neq 1$ and using $V_{ni} \approx \sum_{p=1}^{N_p} V_{ip} S_p = \theta_{in} V_n [1 + O(\Delta x)]$ and then setting $\mathbf{u}_m = \sum \theta_i \bar{\mathbf{u}}_i / \sum \theta_i$, we find

$$\frac{\partial}{\partial t} (\sum \theta_{in}) + \mathbf{u}_m \cdot \nabla \sum \theta_{in} = O(\Delta x \Delta t).$$

When this equation is satisfied, the continuity equation is satisfied to $\Delta x \Delta t$; and the error in the pressure is then $O[\rho C_i^2 (\Delta x/L)(\Delta t/T)]$. The error is a factor of $\Delta x/L$ smaller than the evolution equation approach.



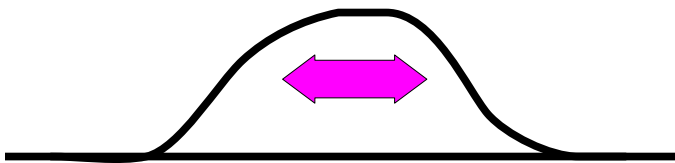
In this scheme, we designed a method to cancel the error in sum of volume fractions.

The sum $\sum \theta_i$ of “volume fractions” is “incompressible”.

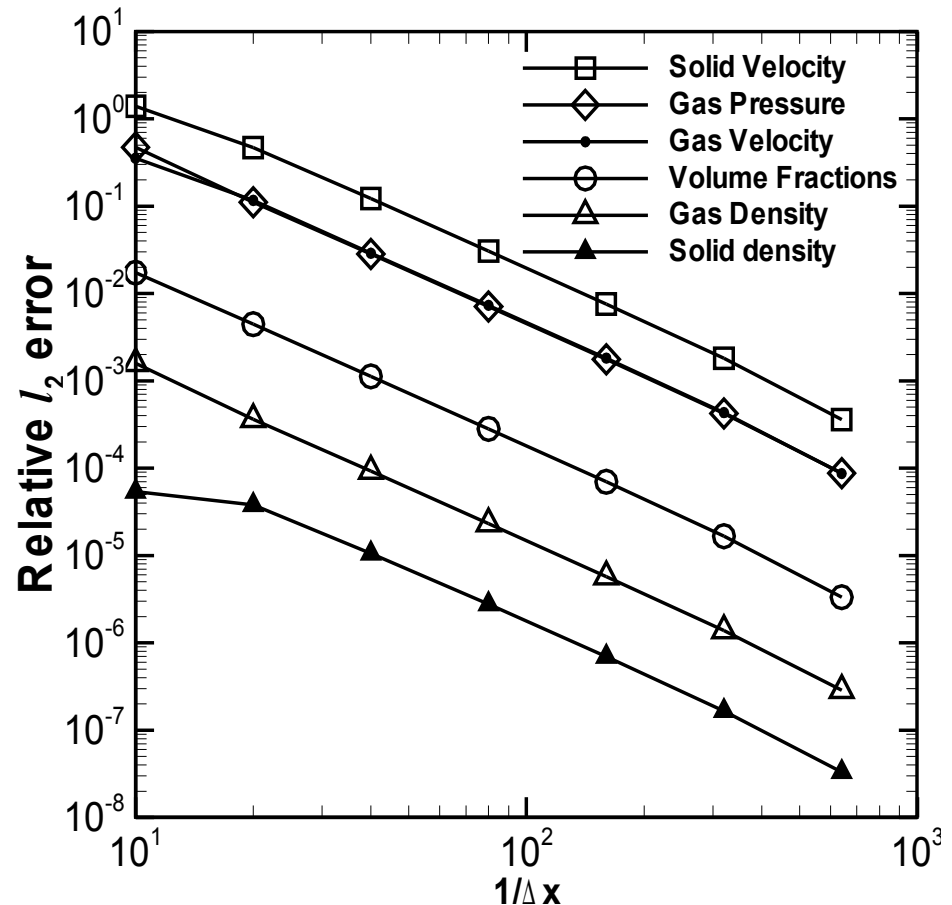
Numerical results

$$\frac{\partial}{\partial t} \left(\sum \theta_{in} \right) + \mathbf{u}_m \cdot \nabla \sum \theta_{in} = 0.$$

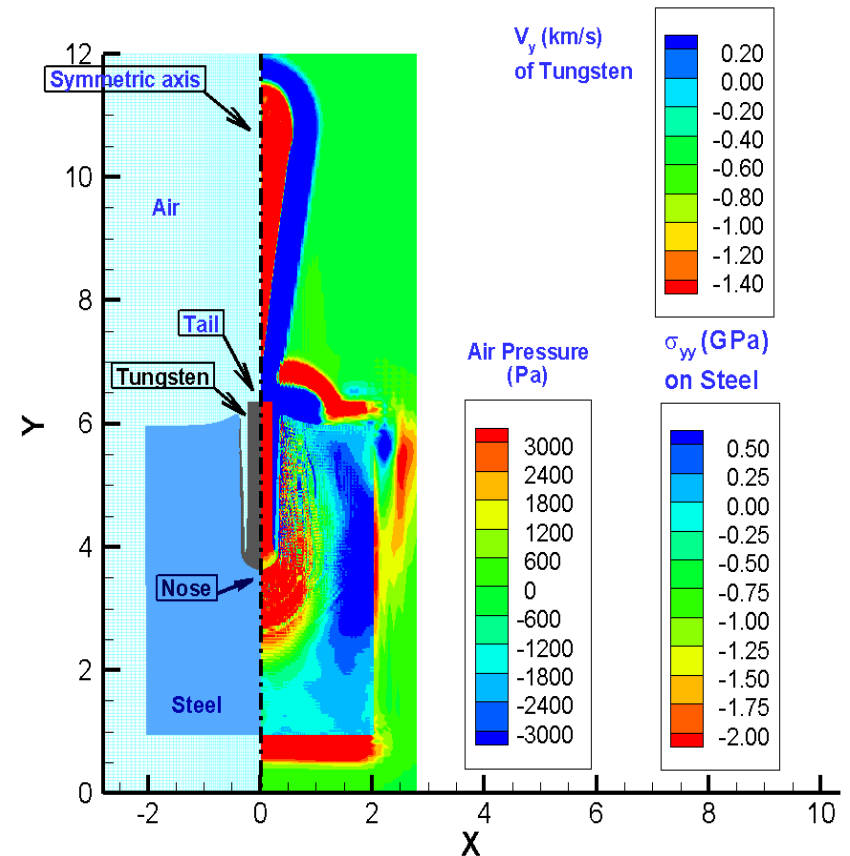
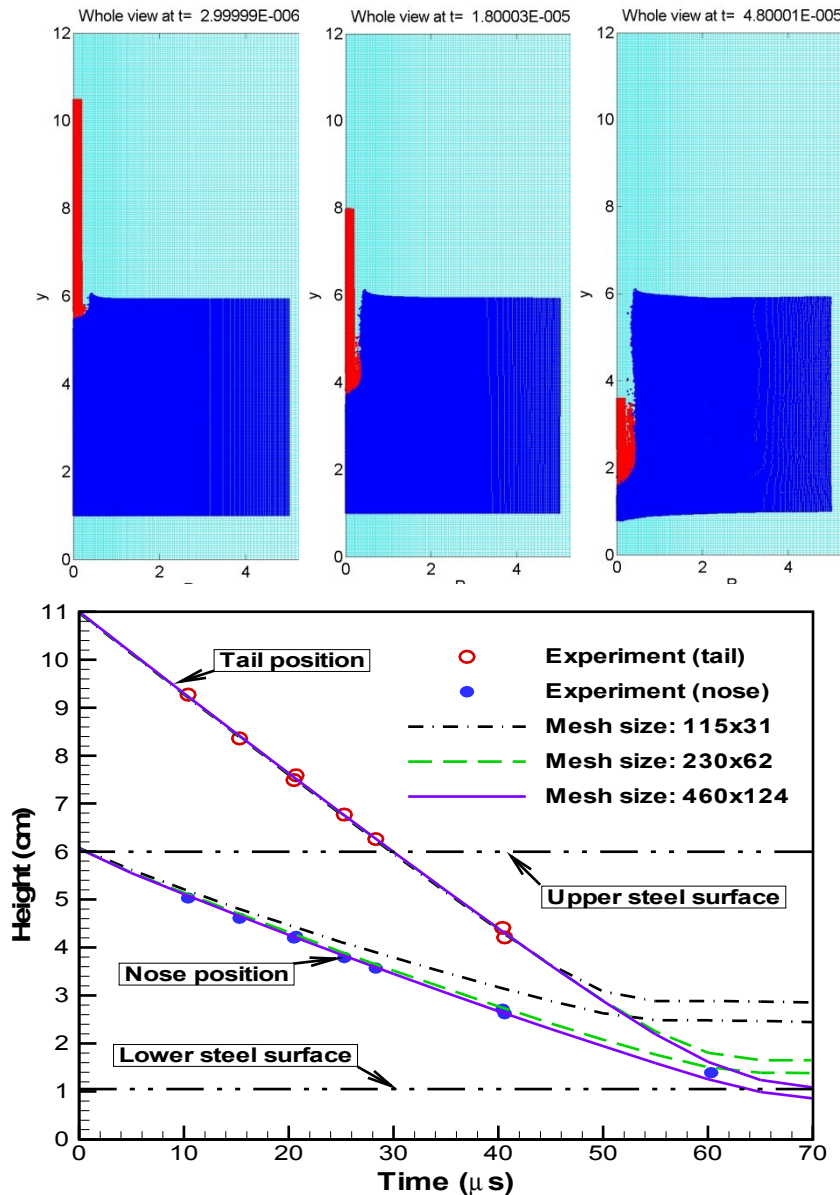
- For fields with discontinuity, we have proved that this scheme can satisfy the above continuity equation to $O(\Delta x \Delta t)$.
- For smooth fields, this scheme can satisfy the continuity equation to $O[(\Delta x)^2 \Delta t]$.



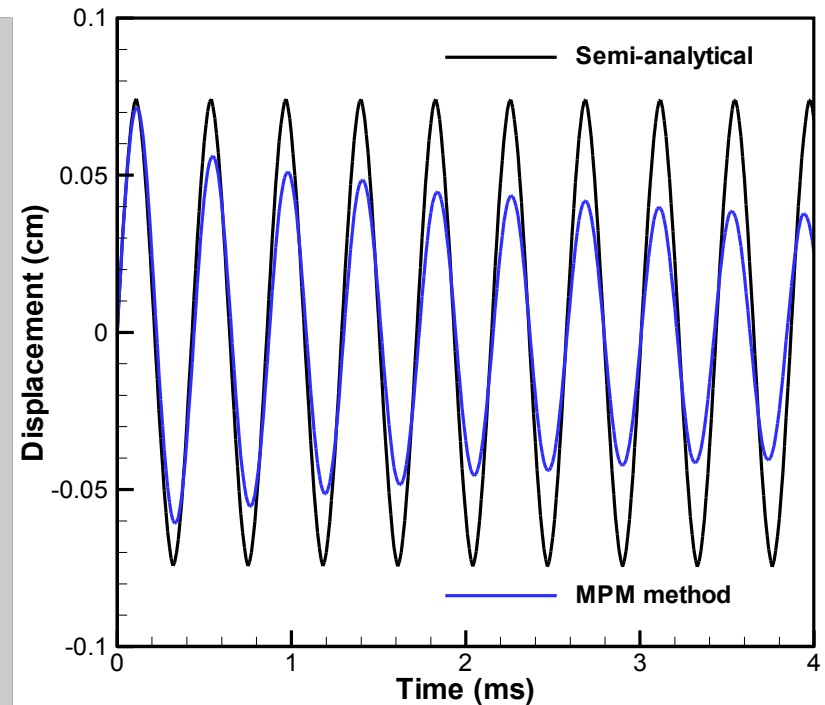
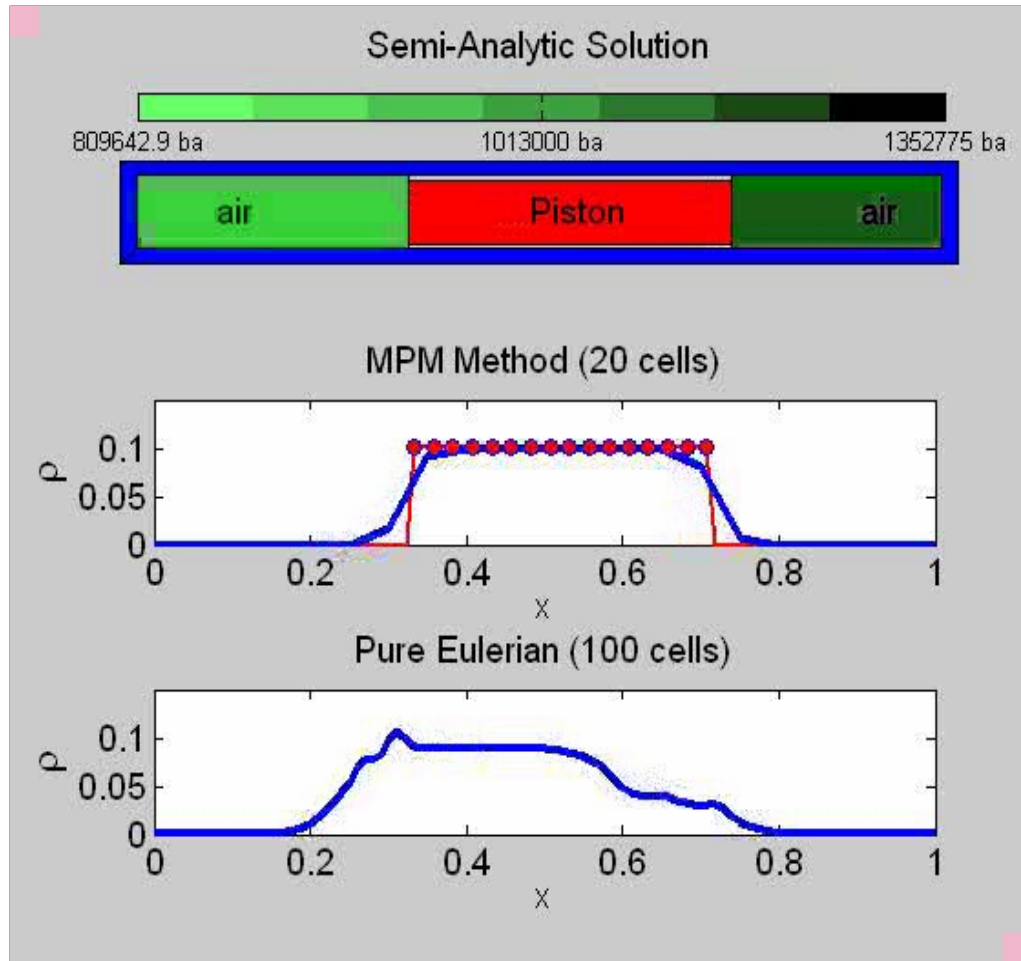
After implementing this new scheme in CartaBlanca, we find



Example 1 (projectile-target interaction)



Example 2



Conclusions

- Using MPM method for calculation of two-phase or multi-material interaction, the way of calculating pressure used in Eulerian methods **cannot** be used.
- The use of evolution equations for pressures or material densities leads to a significant error, especially for low Mach number motions.
- The correct approach is to allow the discretization error and treat the sum of the volume fraction as an “incompressible volume” following the mixture velocity.
- The implementation of the new scheme is similar to the one used in Eulerian methods.
- This new scheme is implemented in CartaBlanca. Significant improvements to accuracy and stability of calculations are seen.