Modeling Continuum to Disperse State Transitions

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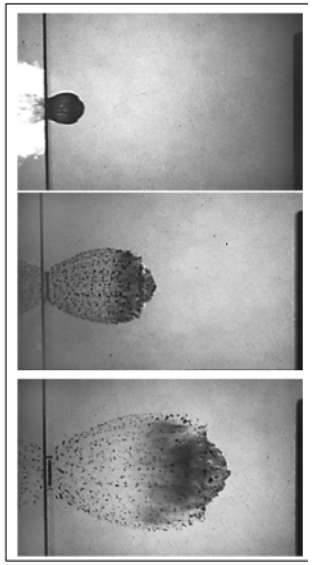
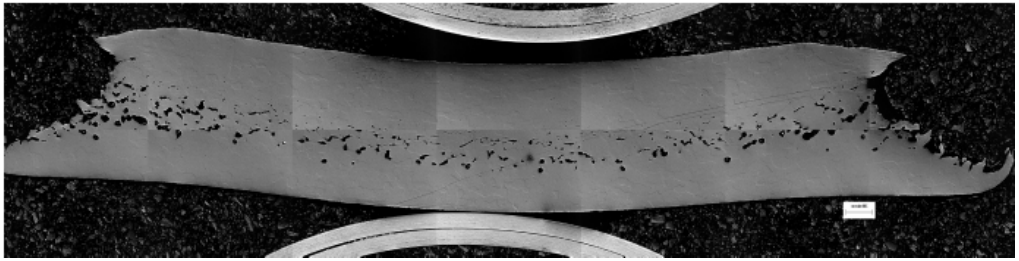
Applicability of Continuum Theory

Can the continuum theory be used to model void growth, fragmentation, pulverization, and debris flows?

- Applicability of the equation form?
- Applicability of material models?
- What are the suitable numerical methods for such complex material motion?





Microscopic Picture and Continuum Equations

In principle, a system can be completely and uniquely determined by the atom positions and velocities (represented by a point: $\mathcal{C} = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n; \mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n\}$, in the position-velocity phase space).

The evolution of the probability density function $P(\mathcal{C}, t)$ satisfies the Liouville equation.

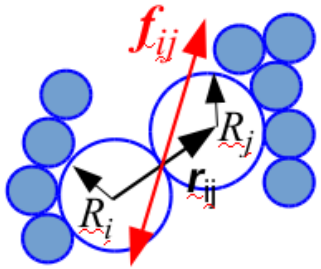
$$\frac{\partial P}{\partial t} + \sum_{p=1}^{N} \nabla_{x_p} \cdot (\mathbf{v}_p P) + \sum_{p=1}^{N} \nabla_{v_p} \cdot (\dot{\mathbf{v}}_p P) = 0.$$

Continuum quantities are moments of this probability density function, e.g. $\rho(\mathbf{x}, t) = \int \sum_{p=1}^{N} m_p \delta[\mathbf{x} - \mathbf{x}_p(\mathcal{C})] P(\mathcal{C}, t) d\mathcal{C}$.

Taking moments of this equation, one finds the continuum equations, e.g.

$$\frac{\partial \rho \overline{\mathbf{v}}}{\partial t} + \nabla \cdot (\rho \overline{\mathbf{v}}\ \overline{\mathbf{v}}) = \nabla \cdot \boldsymbol{\sigma},$$
$$\boldsymbol{\sigma} = \frac{1}{2} \int \sum_{p=1}^{N} \sum_{q=1}^{N} \delta(\mathbf{x} - \mathbf{x}_p) \mathbf{r}_{pq} \mathbf{f}_{pq} P(\mathcal{C}, t) d\mathcal{C} - \overline{(\rho \mathbf{v}' \mathbf{v}')}.$$

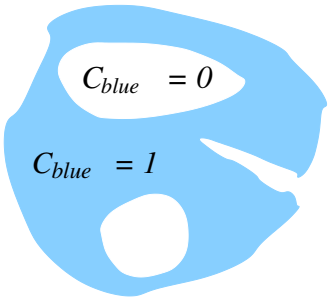
No assumption of continuum is necessary.



Multimaterial Formulation

In many practical problems, regions occupied by materials can be identified. For these cases, we introduce material indicator function:

$$C_i(\mathbf{x}, t, \mathcal{C}) = \begin{cases} 1, & \text{if } \mathbf{x} \in \text{material } i, \\ 0, & \text{otherwise.} \end{cases}$$



We can then define the volume fraction and averages $\langle \cdot \rangle$:

$$\theta_i(\mathbf{x}, t) = \int C_i(\mathbf{x}, t, \mathcal{C}) P(\mathcal{C}, t) d\mathcal{C}.$$

$$\langle \mathbf{v}_i \rangle(\mathbf{x}, t) = \frac{1}{\theta_i} \int C_i(\mathbf{x}, t, \mathcal{C}) \mathbf{v}_i(\mathbf{x}, t, \mathcal{C}) C_i(\mathbf{x}, t) P(\mathcal{C}, t) d\mathcal{C}.$$

$$\langle \nabla \mathbf{v}_i \rangle(\mathbf{x}, t) = \frac{1}{\theta_i} \int C_i(\mathbf{x}, t, \mathcal{C}) \nabla \mathbf{v}_i(\mathbf{x}, t, \mathcal{C}) C_i(\mathbf{x}, t) P(\mathcal{C}, t) d\mathcal{C}.$$

$$\nabla \langle \mathbf{v}_i \rangle = \langle \nabla \mathbf{v}_i \rangle + \frac{1}{\theta_i} \int (\mathbf{v}_i - \langle \mathbf{v}_i \rangle) \nabla C_i P(\mathcal{C}, t) d\mathcal{C},$$

Macroscopic velocity gradient = average material velocity gradient
+ interface effects, (crack opening, void growth, $\cdots$).

Multi-velocity Description

Conservation equations:
The ensemble phase averaged equations can be derived from these definitions.

- volume:

$$\frac{d\theta_i}{dt} = \theta_i(\langle \nabla \cdot \mathbf{v}_i \rangle - \nabla \cdot \langle \mathbf{v}_i \rangle)$$

$$= -\int (\mathbf{v}_i - \langle \mathbf{v}_i \rangle) \cdot \nabla C_i P(\mathcal{C}) d\mathcal{C}.$$

- mass:

$$\frac{d\rho_i}{dt} = -\rho_i \langle \nabla \cdot \mathbf{v}_i \rangle$$

- momentum:

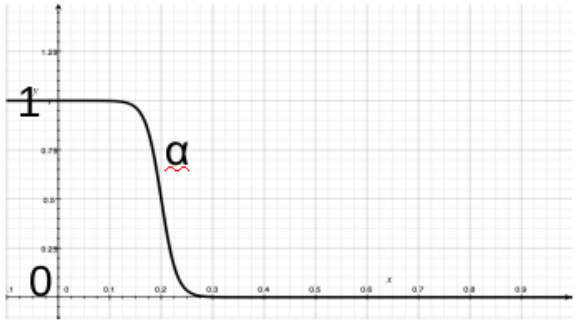
$$\theta_i \rho_i \frac{d\langle \mathbf{v}_i \rangle}{dt} = \theta_i \nabla \cdot \langle \boldsymbol{\sigma}_i \rangle + \sum_j \mathbf{F}_{ij},$$

where $\mathbf{F}_{ij}$ is the interaction force between materials i and j.

Multipressure model:
(Zhang, et al. 2007 Int. J. Multiphase Flow)

$$\theta_i(\nabla \langle \mathbf{v}_i \rangle - \langle \nabla \mathbf{v}_i \rangle) = \theta_i(a_i \mathbf{I} + \mathbf{D}_i + \boldsymbol{\Omega}_i).$$

- $\boldsymbol{\Omega}_i = \mathbf{0}$.
- $\mathbf{D}_i = (1 - \alpha_i) \times$ the deviatoric part of $\nabla \langle \mathbf{v}_i \rangle$.
- $a_i = \theta_i[(1 - \alpha_i) \nabla \cdot \langle \mathbf{v}_i \rangle - B_i]$,
- $\langle \nabla \cdot \mathbf{v}_i \rangle = \alpha_i \nabla \cdot \langle \mathbf{v}_i \rangle + B_i$
- B_i is related to compressibility of other materials to ensure continuity ($\sum_i \theta_i = 1$).

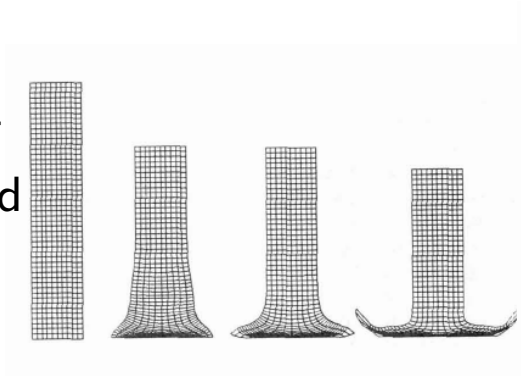


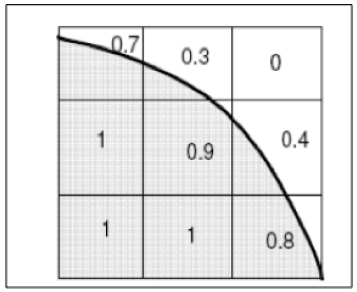
Effective plastic strain

Numerical Solution Methods

Material in these types of problems usually undergo extreme deformation, and the material models are often history dependent.

Mesh distortion of Lagrangian method

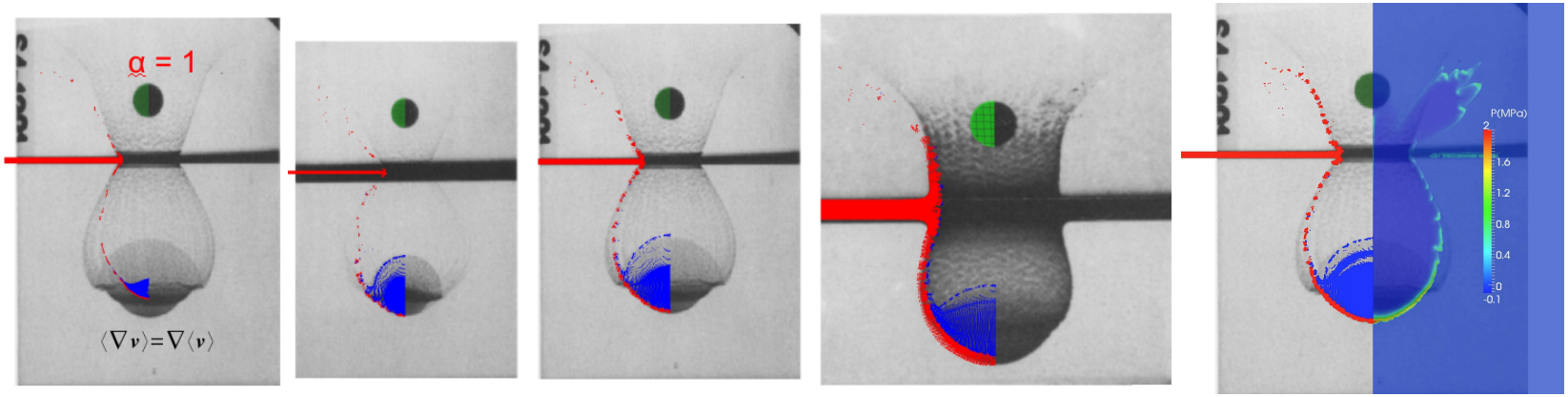




failure = 0.9 ?!

Numerical diffusion of Eulerian method

From the Dual Domain Material Point Method:



Material Point Methods

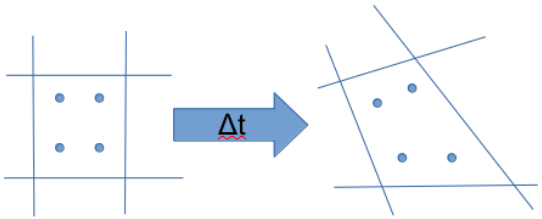
- Particle-in-cell (PIC) method was first used by Frank Harlow in the 1960s. Nearest grid point interpolation was used.
- In the late 1980s, shape functions were introduced. The method is then called FLuid Implicit Particle (FLIP) method.
- In the 1990s particle-in-cell method was re-formatted based on weak solutions to partial differential equations (or the virtual work theory). Since then the method is called the material point method (MPM).
- The Dual Domain Material Point (DDMP) method is introduced (Zhang et al., 2011, JCP) to reduce numerical noise caused by particles moving across cells.
- DDMP is applicable for history dependent problems with extreme material deformation. The method has very little numerical diffusion.
- It is more computationally expensive than typical finite volume method and finite element method combined per cell, but not as many cells are needed for a given problem.

Material Point and Finite Element Methods

Weak solution: For node k, $m_k \frac{d\mathbf{v}_k}{dt} = -\int \boldsymbol{\sigma} \cdot \nabla S_k dv + \cdots$.

FEM

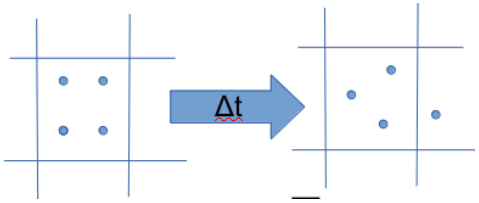
$$\int \boldsymbol{\sigma} \cdot \nabla S_k dv = \sum_{g=1}^{N} J_g W_g \boldsymbol{\sigma}_g \nabla S_k(\mathbf{x}_g),$$



- Gauss points are fixed on elements.
- Elements are Lagrangian. They can be distorted for large material deformations.

Original MPM

$$\int \boldsymbol{\sigma} \cdot \nabla S_k dv = \sum_{p=1}^{N_p} v_p \boldsymbol{\sigma}_p \nabla S_k(\mathbf{x}_p)$$



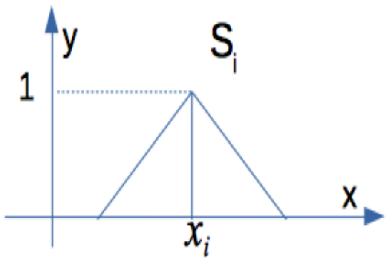
- Mesh is fixed. No mesh distortion.
- Particles move (= advection).
- $\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \sum_k \Delta \mathbf{v}_k S_k(\mathbf{x}_p)$
- $\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \sum_k \mathbf{v}_k^{n+1/2} S_k(\mathbf{x}_p)$
- $m_k \mathbf{v}_k^{n+1} = \sum_p m_p \mathbf{v}_p^{n+1} S_k(\mathbf{x}_p)$

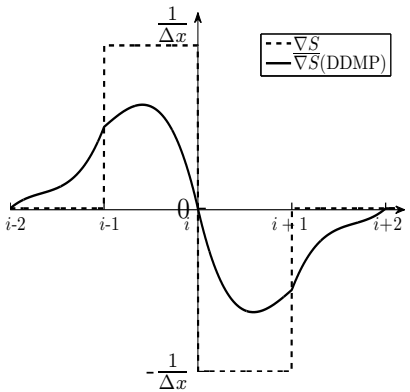
MPM gains the freedom of moving integration points, but there is a price to pay.

Dual Domain Material Point Method

Zhang et al., 2011, JCP

$$\int \boldsymbol{\sigma} \cdot \nabla S_k dv = \sum_{p=1}^{N} v_p \boldsymbol{\sigma}_p \overline{\nabla S_k}(\mathbf{x}_p)$$





In original MPM, ∇S_k is discontinuous, causing numerical noises.

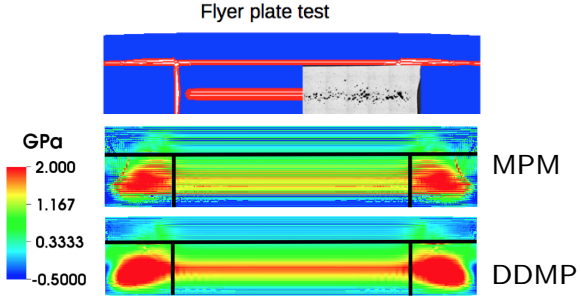
DDMP replaces it with a continuous one, while ensuring:

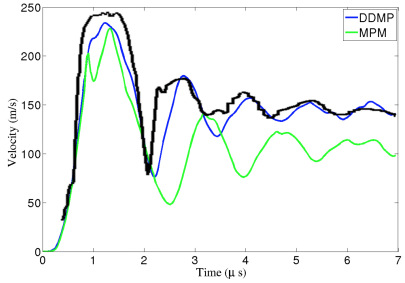
$\sum S_k = 1$, mass conservation.

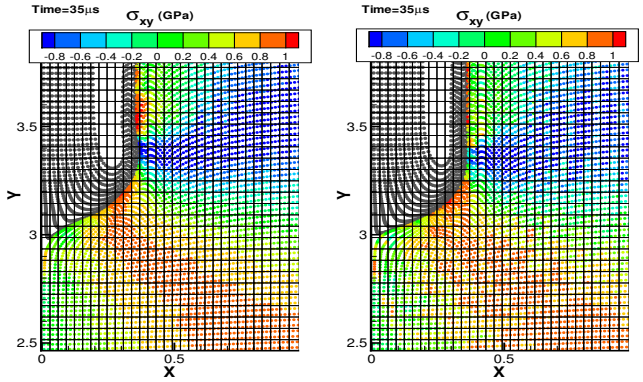
$\sum \overline{\nabla S_k} = 0$, momentum conservation.

$\sum \mathbf{x}_k \overline{\nabla S_k} = \mathbf{I}$, $O(\Delta x^2)$ error on energy conservation.

The nonlocal effects in DDMP can be calculated using two local operations.

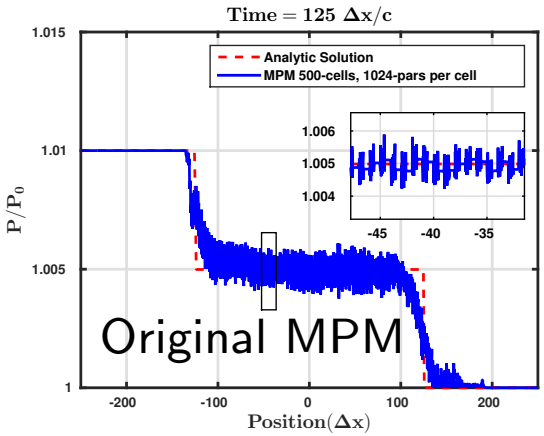


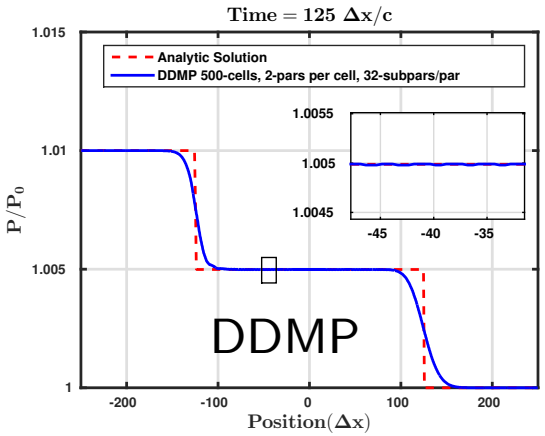


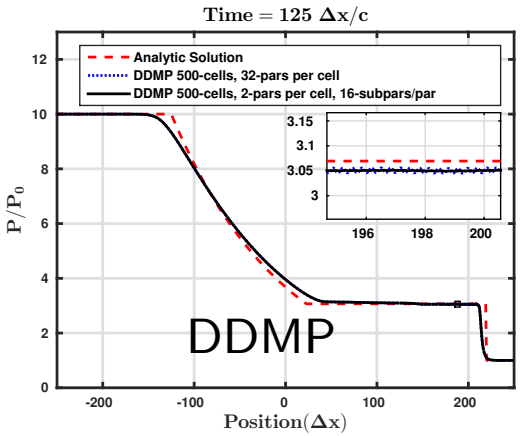


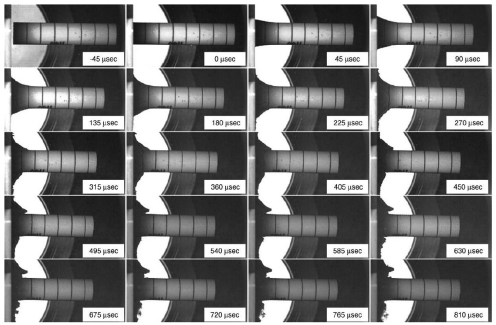
DDMP MPM

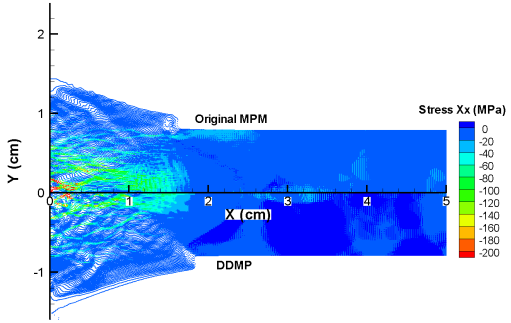
Extreme Deformations

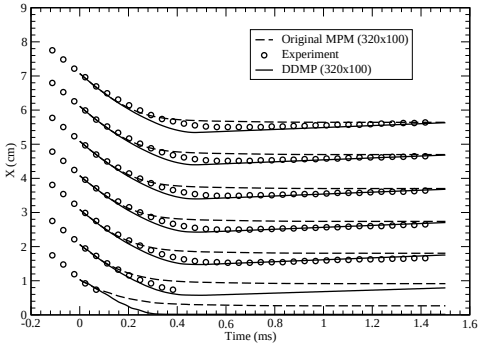


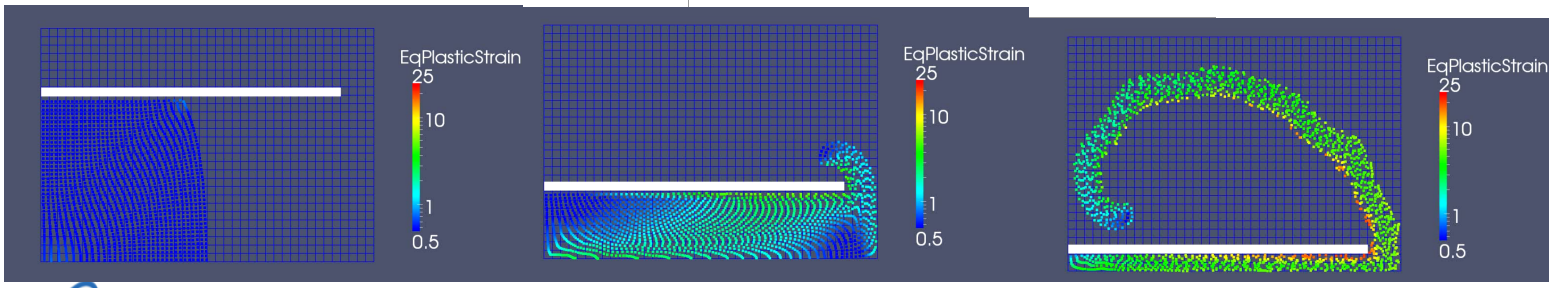


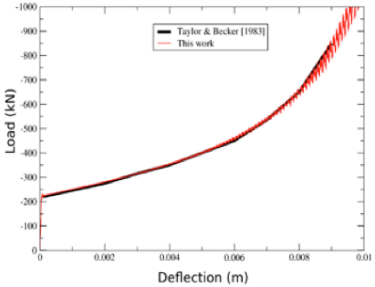












Conclusions

- Continuum description and the conservation equations are applicable in problems involving continuum to disperse state transitions, however the closure relations need to reflect the lower length scale interactions, including the loss of connectivity.
- We have developed a multi-velocity formulation for numerical simulation of shock propagation, material failure, fragmentation, pulverization, and transitions between continuous and disperse particulate states.
- DDMP method has been proven to be a reliable method with accurate conservation properties for these types of complex multi-material interactions. Numerical diffusion and mesh distortion are not issues in the DDMP method.
- Many material models have been implemented into the CartaBlanca code equipped with DDMP.