LA-UR- 11-06617

Approved for public release;
distribution is unlimited.

Title:	Modeling Material Interactions Using Multiphase Point Method
Author(s):	D.Z. Zhang-T-3 X. Ma-T-3 P.T. Giguere-T-3 B. Jayaraman-T-3
Intended for:	3rd International Symposium of Computational Mechanics Taipei, Taiwan December 5-7, 2011

Form 836 (7/06)

Third International Symposium on Computational Mechanics (ISCM III)
Second Symposium on Computational Structural Engineering (CSE II)
December 5-7, 2011, Taipei, TAIWAN

Modeling Material Interactions Using Multiphase Material Point Method

Duan Z. Zhang*, Xia Ma, Paul T. Giguere, Balaji Jayraman

*Corresponding Author, dzhang@lanl.gov
Fluid Dynamics and Solid Mechanics Group, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Interaction of materials is ubiquitous in real life scenarios and has attracted vast interest from the computational modeling community. The challenge of numerically simulating such problems, in spite of advances in computing resources and numerical methods, arises from the limitations in the algorithmic framework that can handle a whole range of problems such as moving boundary and large deformation. Many of the existing approaches seem to break down under large material deformation scenarios while performing adequately for more benign situations.

Most numerical simulation methods are either Eulerian or Lagrangian. Eulerian descriptions of problems involving large deformations require advection of the various state variables, causing significant numerical diffusion error. When using a Lagrangian treatment, one encounters significant mesh entanglement and distortion issues that result in significant errors and even failure of the calculation in some cases. Fifteen years ago, Anderson et al. [1] modeled the interaction of a tungsten projectile with a steel target using an Eulerian code and compared the results with experimental data. To avoid numerical diffusion, more recent approaches to solve such problems are often based on the finite element method with rezoning to mitigate the effects of grid distortion [2]. These methods limit the amount of rezoning to reduce the numerical diffusion associated with this process. For numerical stability, these methods also remove highly distort elements resulting in the loss of mass and momentum in the calculation. This practice is a significant source of error in impact phenomena, where the effects of momentum and inertia are important. To avoid such errors, Huang et al. [3] and Grujicic et al. [4] recently employed a method that converts the highly distort or failed elements into particles and then use smooth particle hydrodynamics (SPH) to handle them. This type of approach combines the advantages of the individual techniques and has gained some popularity in recent years. However, switching between methods is often computationally inefficient and introduces numerical errors.

In an effort to avoid the difficulties mentioned above, the modeling community has realized the need for a hybrid Eulerian-Lagrangian method that allows particles and mesh nodes to communicate information in every time step without causing numerical diffusion errors. The particle-in-cell (PIC) method first developed by the Fluid Dynamics Group at the Los Alamos national laboratory (Harlow [5]) is one such technique. In the PIC method the Eulerian mesh stays fixed while Lagrangian particles move through the mesh during material deformation. This method combines mesh and particle capabilities while eliminating the difficulty related to mesh deformation in a Lagrangian method and the numerical diffusion issues plaguing an Eulerian calculation. Since its inception in the 1960s, many improvements have been made to the PIC method, with the material point method (MPM) being the most recent variant. The work of Sulsky et al. [6] provides a mathematical basis for this approach. The MPM lends itself naturally to modeling large material deformations. The amount of computation per cell for the MPM is much greater than that for a pure Eulerian or Lagrangian method. However, in many finite volume or finite element based calculations, the amount of elements or cells needed for a dynamic problem is determined by the need to avoid mesh distortion or to limit numerical diffusion. Such difficulties are not present in the MPM. For a given problem, much fewer cells are needed in the MPM than in a pure Eulerian or Lagrangian method, thus making the overall efficiency of the MPM greater.

Direct application of the MPM to multimaterial interactions requires tracking material interfaces and developing an appropriate contact algorithm. Furthermore, material interactions often result in mixing of the materials and blurring their boundaries. To avoid dealing with these difficulties, we employ an approach used in the study of multiphase flows. Specifically, we treat the interacting materials as inter-penetrating continua. Their actual locations or interfaces are represented by volume fractions or the change in the volume fraction. In this way we avoid the need to deal with the contact region or interface directly. The interaction between the materials is represented by the exchange force in the mixed cells or control volumes in the calculation. This multiphase flow approach is often more convenient in dealing with problems of material impact or fluid-structure interactions. For example, many solid materials always contain some porosity. This porosity has little effect for slow deformation. However, for high strain rate motions, such as shock wave impact on solid structures, the porosity has a significant effect on wave speed. In projectile-armor and other material impact problems, the melting of the materials could cause a mixed layer near the contact surface. For modeling such situations, the multiphase approach seems to be the only choice. In this study we employ a set of equations developed based on the ensemble phase averaging method for multiphase flows or multimaterial interactions (Zhang et al. [7]).

In solving the model equations, we extend the MPM for solids to multiphase flows or multimaterial interactions. This combination of multiphase flow theory and the MPM is attractive for multimaterial simulations. Using this approach, one can not only model interacting solids, but also fully coupled fluid-structure interactions. The main objective of this paper is to assess the performance of this approach of combining the multimaterial interaction theory and the MPM in the context of fluid-structure interactions. In this study we first validate the model implementation in CartaBlanca with the experimental data of Anderson et al. [1]. We then study the numerical behavior of various modeling options such as single phase and multiphase approaches. Following this we extend the capability to include an anisotropic elastic stress model for handling composites. To illustrate this, we model the interaction of a tungsten projectile with a steel-composite sandwich target.

References

[1] C.E.Anderson Jr., V.Hohler, J.D.Walker and A.J.Stilp, Time-resolved penetration of long rods into steel targets, *Int. J. Impact Engg.* 16(1) (1995) 1.

[2] AUTODYN-2D and 3D, Version 5.0, User Documentation, Century Dynamics Inc., 2004.

[3] H. Huang, C. T. Dyka and S. Saigal, Hybrid particle methods in frictionless impact-contact problems, *Int. J. Numer. Meth. Engng* 61 (2004) 2250.

[4] M.Grujicic, B.Pandurangan, K.L.Koudela and B.A.Cheeseman, A Computational analysis of the ballistic performance of light-weight hybrid composite armors, *Appl. Surf. Sci.* 253 (2006) 730.

[5] F.H.Harlow, The particle-in-cell computing method for fluid dynamics, *Methods Comput. Phys* 3 (1963) 219.

[6] D. Sulsky, Z. Chen, and H.L. Schreyer, A Particle Method for History-Dependent Materials, *Computer Methods in Applied Mechanics and Engineering*, 118, (1994) 179.

[7] D.Z. Zhang, W. B. VanderHeyden, Q. Zou and Nely T. Padial-Collins, Pressure calculations in disperse and continuous multiphase flows, *Int. J. Multiphase Flow.* 33 (2007) 86.

Modeling Material Interactions Using Multiphase Material Point Method

Duan Z. Zhang, Xia Ma, Paul T. Giguere
and
Balaji Jayaraman

Fluid Dynamics and Solid Mechanics Group
Theoretical Division, T-3, B216,
Los Alamos National Laboratory,
Los Alamos, NM 87545, USA

LA-UR 11-04744

Disperse and continuous multiphase problems

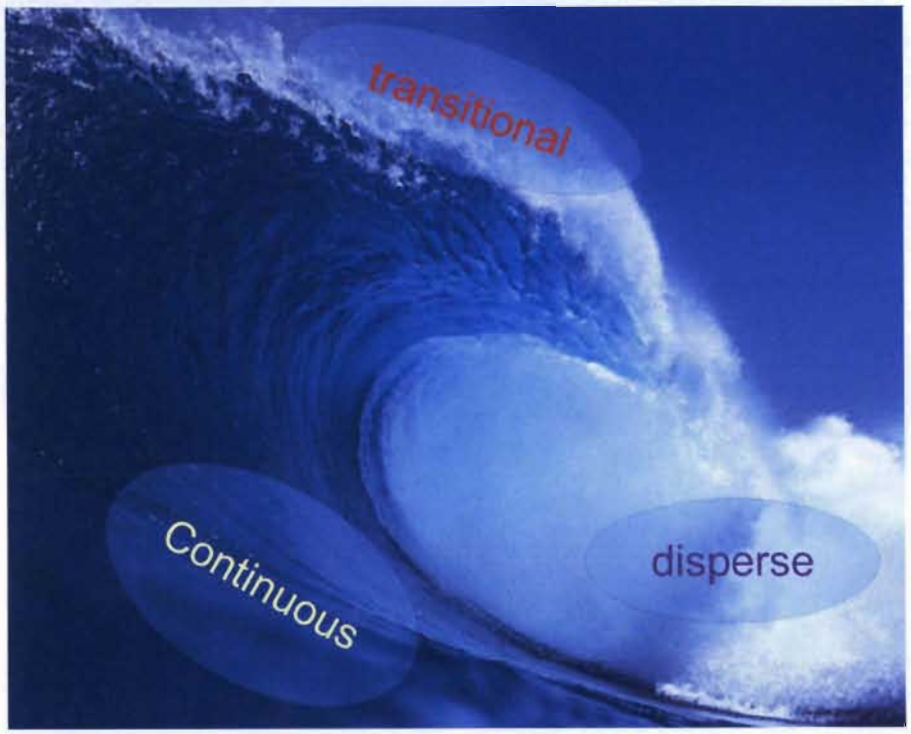
Disperse multiphase flow: Only one continuous phase. All other phases are in forms of particles, droplets, bubbles, with sizes small compared to the length scale of the problem.

Continuous multiphase flow: two or more phases occupying domains with length scales comparable to that of the problem.

The theories for disperse multiphase flows are reasonably well developed, but not so for continuous multiphase flows.

For continuous multiphase flows, material motion of each phase is often described by the equation set for the phase. Phase interactions are considered as boundary conditions. Numerically, various contact algorithms, such as level set, volume of fluid, and immersed boundary, are used.

Even less theories for transitional flows: Current theories: jet breakup, fragmentation model.

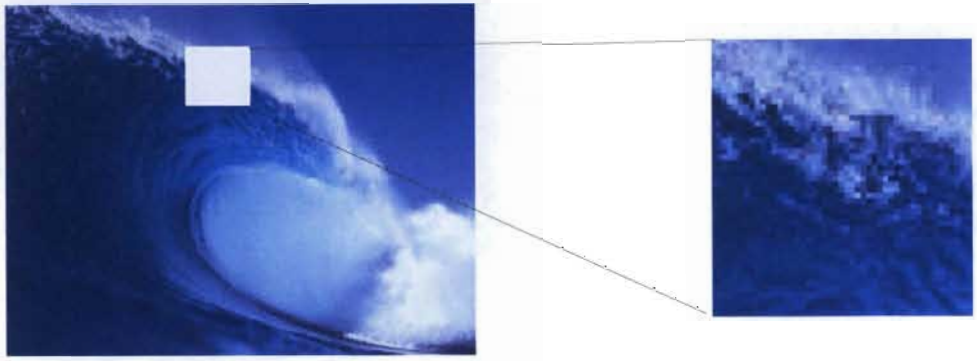


How to derive a unified theoretical framework to deal with the transitional flows?

How to solve the equations numerically?

Probabilistic Description

- Exact positions of interfaces or phase boundaries are difficult, but not very interesting to track.
- Phase interactions on the interfaces can have very small length and time scale. Often, it is random.
- A probabilistic description is necessary.
  - A philosophical question: If we are able to make great effort to trace every interaction in all details (to know all hidden variables), do we still need a probabilistic description? The answer: Yes!
  - This is related to Einstein-Podolsky-Rosen paradox (1935) in quantum mechanics. A series of experiments in early 1980's disproved Bell's inequality, and the hidden variable theory.
  - The need for probabilistic descriptions is not because we don't know enough. It is part of the nature.



Let P(M) be the probability of motions (flows, physical systems) and

$$C^{(i)}(\boldsymbol{x}, M) = \begin{cases} 1, & if\ \boldsymbol{x} \in phase\ i \\ 0, & otherwise \end{cases}.$$

The volume fraction of phase i is defined as

$$\theta^{(i)} = \int C^{(i)}(\boldsymbol{x}, t, M) P(M)\, dM.$$

For a quantity $q^{(i)}$ of phase i we define its average as

$$\langle q^{(i)} \rangle = \frac{1}{\theta^{(i)}} \int C^{(i)}(\boldsymbol{x}, t, M) q_i(\boldsymbol{x}, t, M) P(M)\, dM.$$

In ensemble phase average, we only average over those motions in which the point x is occupied by the phase at that time t.

Different from time or volume averaging technique, in ensemble average, there is no need to pre-specify length or time scale.

Ensemble Phase Averaging Method

In ensemble phase average (Zhang et al. *Int. J. Multiphase flow,* 2007):

$$\nabla\langle q^{(i)}\rangle=\langle\nabla q^{(i)}\rangle+\frac{1}{\theta^{(i)}}\int[q^{(i)}-\langle q^{(i)}\rangle]\nabla C^{(i)}P(M)\,dM.$$

$$\frac{\partial}{\partial t}\langle q^{(i)}\rangle=\langle\frac{\partial}{\partial t}q^{(i)}\rangle+\frac{1}{\theta^{(i)}}\int[q^{(i)}-\langle q^{(i)}\rangle]\frac{\partial}{\partial t}C^{(i)}P(M)\,dM.$$

$$\frac{\partial}{\partial t}(\theta_i\langle q^{(i)}\rangle)+\nabla\cdot(\theta^{(i)}\langle\boldsymbol{v}^{(i)}q^{(i)}\rangle)$$

Phase change

$$=\theta^{(i)}\left\langle\frac{\partial q^{(i)}}{\partial t}+\nabla\cdot(\boldsymbol{v}^{(i)}q^{(i)})\right\rangle+\int\dot{C}^{(i)}q^{(i)}P(M)\,dM$$

Let $q^{(i)}=\rho^{(i)}$, and noting $\frac{\partial q^{(i)}}{\partial t}+\nabla\cdot(\boldsymbol{v}^{(i)}q^{(i)})=0$, without phase change, we have the averaged mass conservation equation:

$$\frac{\partial}{\partial t}(\theta^{(i)}\langle\rho^{(i)}\rangle)+\nabla\cdot(\theta^{(i)}\langle\boldsymbol{v}^{(i)}\rho^{(i)}\rangle)=0$$

Let $q^{(i)}=\rho^{(i)}\boldsymbol{v}^{(i)}$ we have the momentum equation:

$$\frac{\partial}{\partial t}(\theta^{(i)}\langle\rho^{(i)}\rangle\tilde{\boldsymbol{v}}^{(i)})+\nabla\cdot(\theta^{(i)}\langle\rho^{(i)}\rangle\tilde{\boldsymbol{v}}^{(i)}\tilde{\boldsymbol{v}}^{(i)})$$

$$=\theta^{(i)}\left\langle\frac{\partial\rho^{(i)}\boldsymbol{v}^{(i)}}{\partial t}+\nabla\cdot(\rho^{(i)}\boldsymbol{v}^{(i)}\boldsymbol{v}^{(i)})\right\rangle$$

$$=-\theta^{(i)}\nabla p+\nabla\cdot[\theta(\langle\boldsymbol{\sigma}^{(i)}\rangle+\boldsymbol{\sigma}_{Re}^{(i)}+p\boldsymbol{I})]+\boldsymbol{f}^{(i)}$$

Other than extremely non-linear constitutive relations, we assume

$$\langle\boldsymbol{\sigma}^{(i)}\rangle=\sigma^{(i)}(\langle\nabla\boldsymbol{v}^{(i)}\rangle,\int\langle\nabla\boldsymbol{v}^{(i)}\rangle(\tau)K^{(i)}(t-\tau)\,d\tau,\cdots)$$

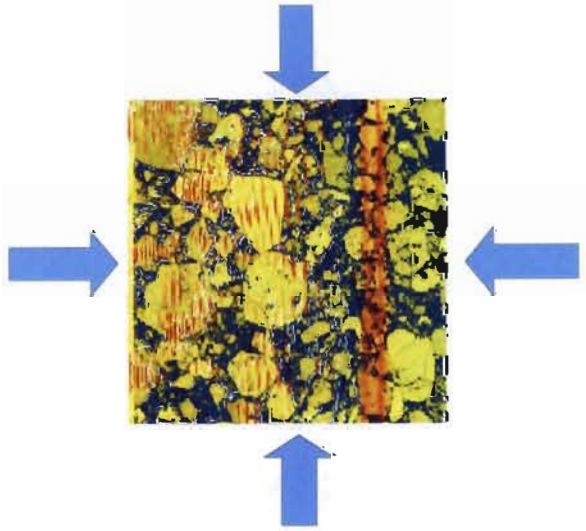
In an ensemble phase average

$$\langle\nabla\cdot\boldsymbol{v}^{(i)}\rangle\neq\nabla\cdot\langle\boldsymbol{v}^{(i)}\rangle.$$

We use

$$\langle\nabla\cdot\boldsymbol{v}^{(i)}\rangle=\alpha^{(i)}\nabla\cdot\langle\boldsymbol{v}^{(i)}\rangle+B^{(i)}$$

where $B^{(i)}$ is related to compressibilities, thermal expansion, species change, etc, inside phase i.



Multi-velocity Formulation

Multi-velocity formulation is obtained from the ensemble phase averaging technique.

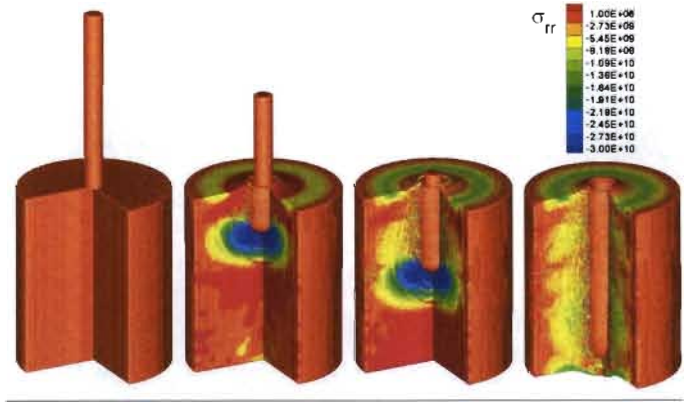
Advantages:

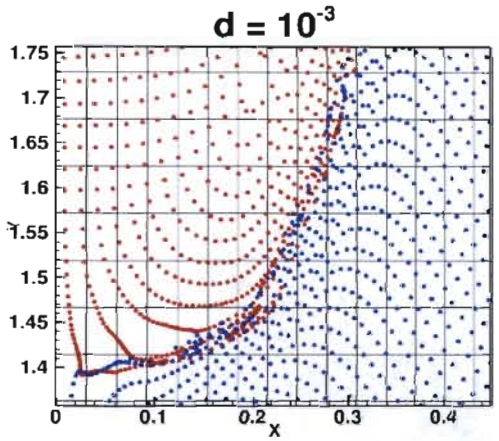
- Unified framework of equations for impact, fragmentation, and debris flows.
- No need to switch equations and numerical codes in different stage of material interactions.
- Applicable to all fluid-structure interactions.
- Can be used to consider material interactions happening inside material, such as porous solid in a fluid.

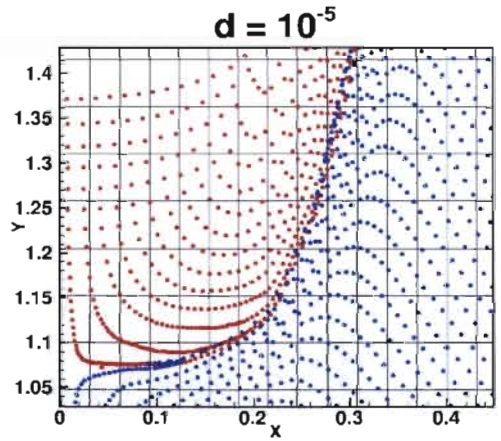
New issues:

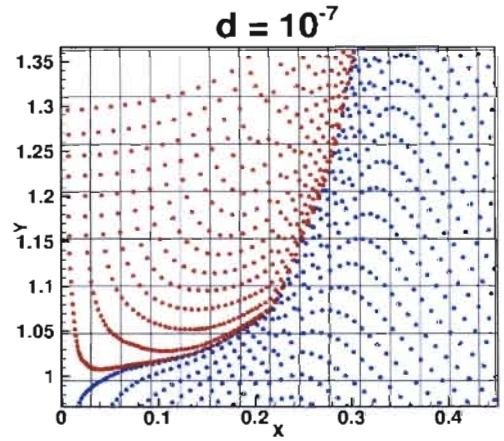
- Material interactions models.
- Velocity and traction continuity across material interfaces.
- Enforcing continuity: $\sum \theta^{(i)} = 1.$
- Comparison with traditional method.

For interface interaction: $\boldsymbol{F}^{ij} = -\dfrac{\theta^{(i)}\theta^{(j)}}{d}\rho_f |\boldsymbol{v}^{(i)} - \boldsymbol{v}^{(j)}| (\boldsymbol{v}^{(i)} - \boldsymbol{v}^{(j)})$

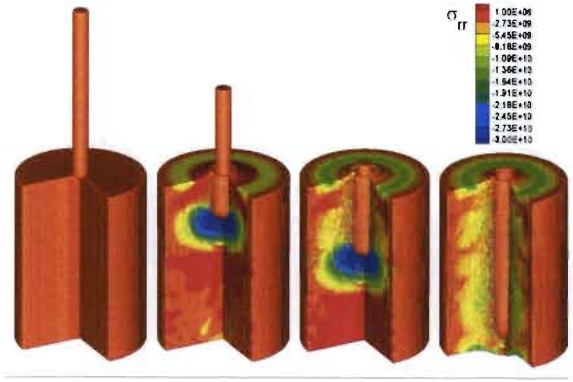


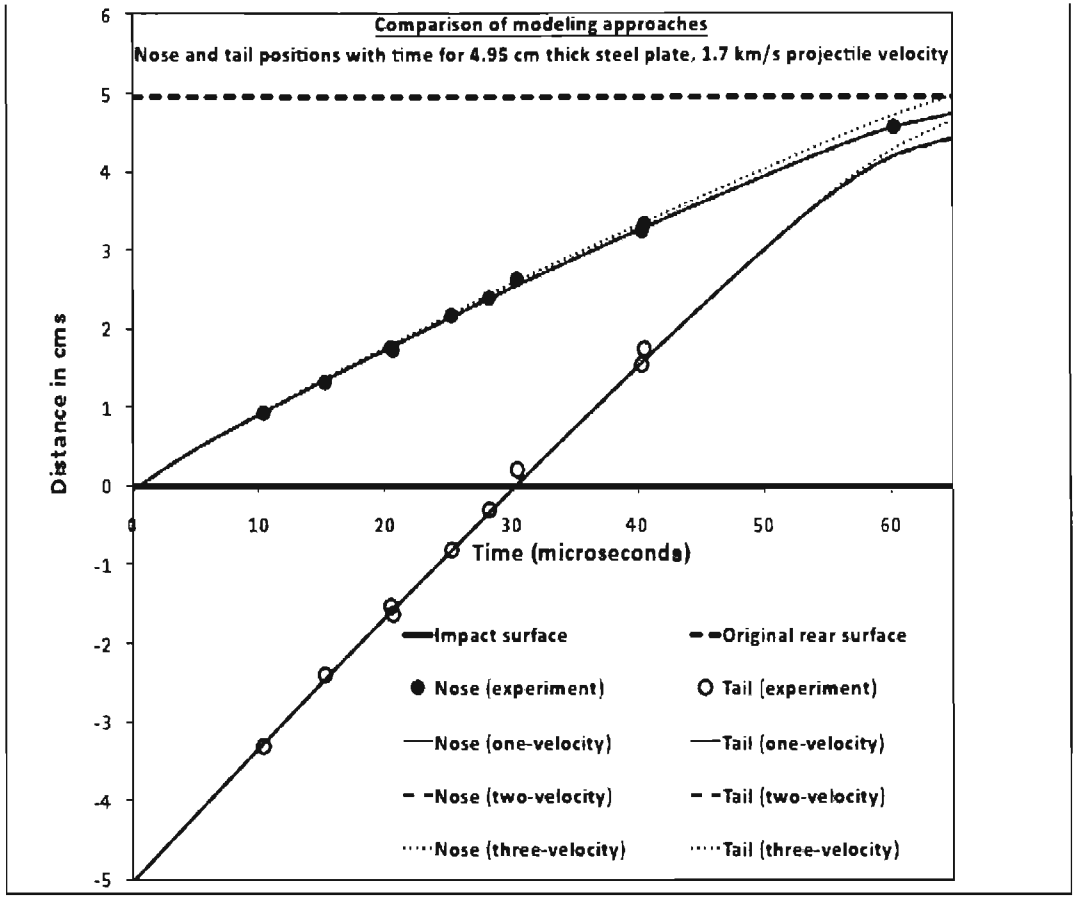






Comparison of single and multi-velocity results

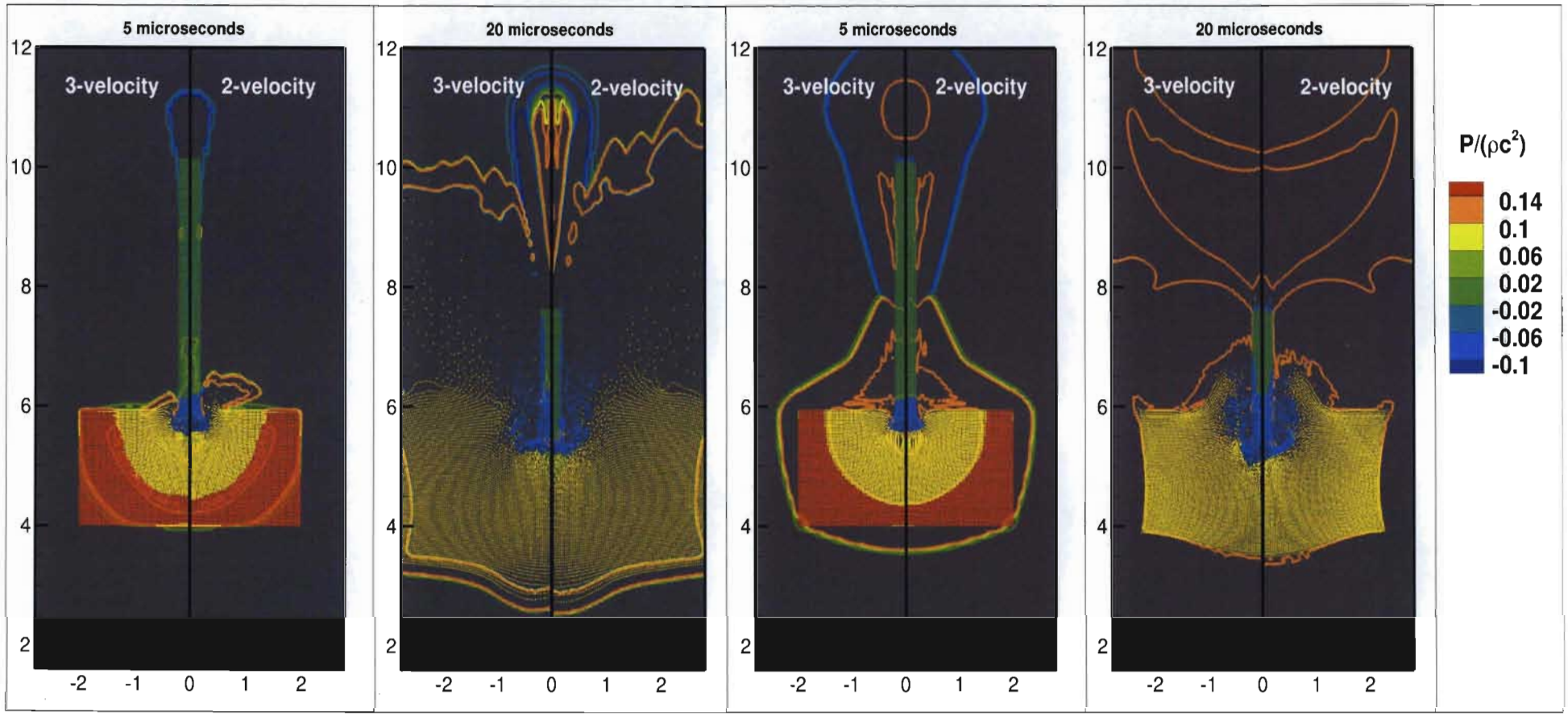




- One-velocity: projectile and target are modeled in velocity field. Air is not considered.
- Two-velocity: projectile and target are modeled in one velocity field. Air is modeled as the other velocity field.
- Three-Velocity: projectile, target and air are modeled by separate velocity fields.

$$\frac{\partial \rho^{(i)} \boldsymbol{v}^{(i)}}{\partial t} + \nabla \cdot (\rho^{(i)} \boldsymbol{v}^{(i)} \boldsymbol{v}^{(i)})$$
$$= -\theta^{(i)} \nabla \cdot p + \nabla \cdot [\theta^{(i)} (\boldsymbol{\sigma}^{(i)} + p \boldsymbol{I})] - \boldsymbol{F}^{(ij)}.$$

Comparison of single and multi-velocity results



Projectile-concrete interaction in air

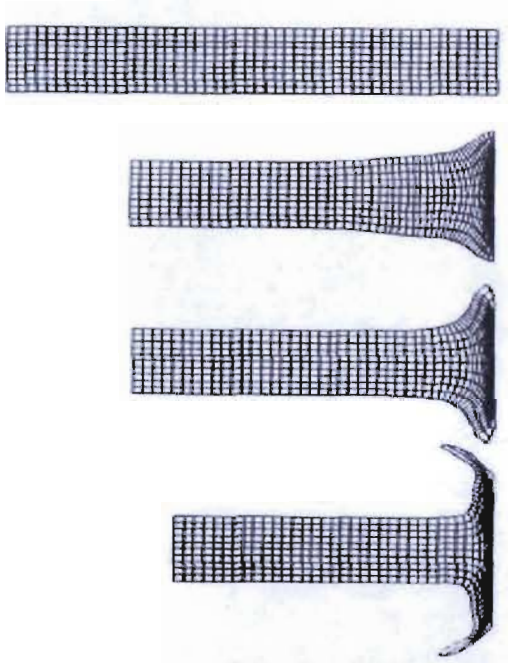
Projectile-concrete interaction in water

This results are obtained using dual domain material point (DDMP) method that eliminated the noise associated with cell crossing of material points (Zhang et al. 2011, JCP).

Numerical Methods for the Averaged Equations

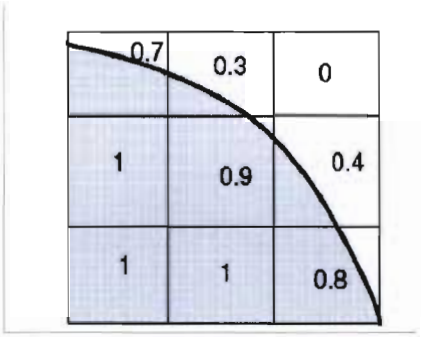
- Traditionally used finite element methods suffer mesh distortion difficulties because of fragmentation and debris flow.

- Eulerian method, such as finite difference, finite volume, cannot be efficiently used because of failure flags need to follow the motion of the material and cannot be averaged.
  - For brittle materials, at a point the material is either failed (failure = 1) or not failed (failure = 0).



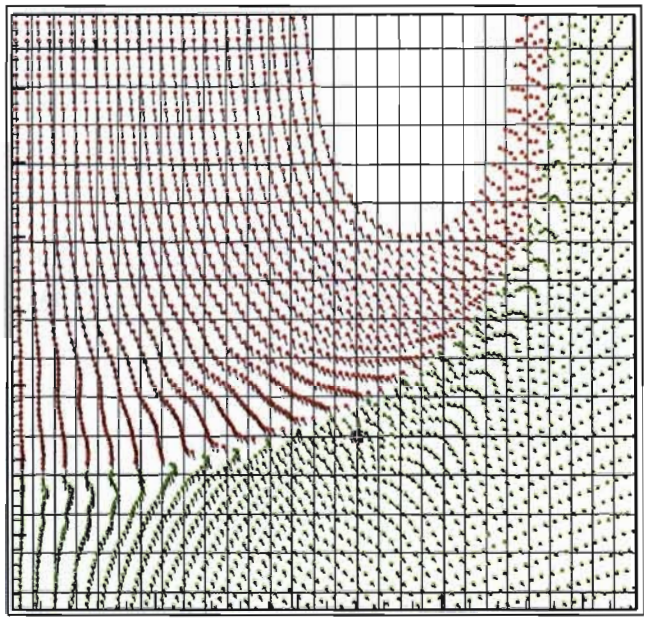
FEM, (Lagrangian Method)

Cline and Reaugh, J. De. Physique IV, 1991



failure = 0.9 ?!

Eulerian method



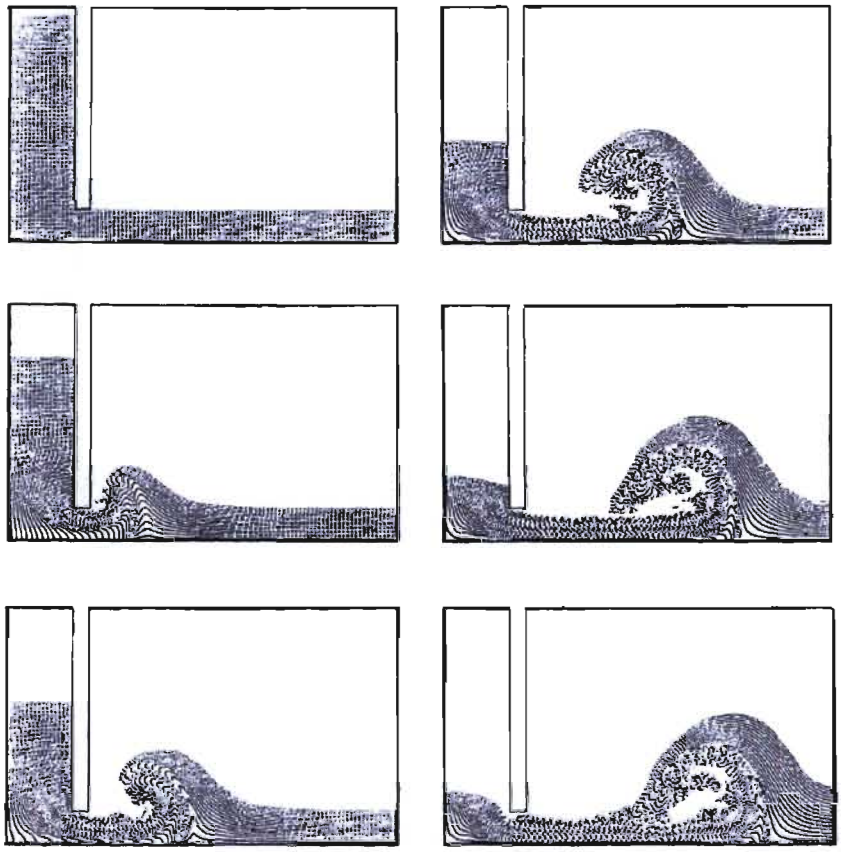
Material point method

The Material Point Method (MPM)

For problems involving large deformation and history of the materials. To avoid difficulties of numerical diffusion associated with Eulerian methods, and mesh distortion associated with Lagrangian method, we choose material point method (MPM) .

The material point method (MPM), uses both Eulerian mesh and Lagrangian points. The Lagrangian points are also called material points, or particles.

- Particle-in-cell (PIC) method was invented by Frank Harlow in the 1960's. Nearest grid point interpolation was used.
- In the late 1980's, shape functions were introduced. The method is then called FLuid Implicit Particle (FLIP) method.
- In the 1990's 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 material point method (MPM).



F. H. Harlow and A. A. Amsden, LA-4700, 1971

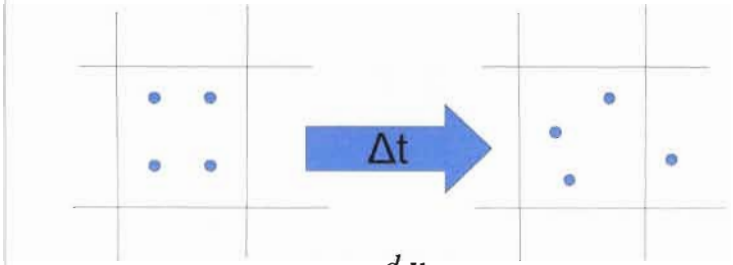
Material point method (MPM) vs. finite element method (FEM)

$$m_{ij}\frac{d\boldsymbol{u}_j}{dt}=-\int \sigma\cdot\nabla S_i(\boldsymbol{x})\,dv+\int \rho\boldsymbol{g}\,S_i(\boldsymbol{x})\,dv+\int_{\partial v} S_i(\boldsymbol{x})\,\boldsymbol{t}\cdot\boldsymbol{n}\,dS\,,$$ (the virtual work principle).

MPM

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

where subscript p denotes material points that move across the Eulerian mesh.



$$\boldsymbol{u}_p^{n+1}=\boldsymbol{u}_p^n+\Delta t\sum_i\frac{d\boldsymbol{u}_i}{dt}S_i(\boldsymbol{x}_p)$$

$$\boldsymbol{x}_p^{n+1}=\boldsymbol{x}_p^n+\Delta t\sum_i(\boldsymbol{u}_i+0.5\frac{d\boldsymbol{u}_i}{dt}\Delta t)S_i(\boldsymbol{x}_p)$$

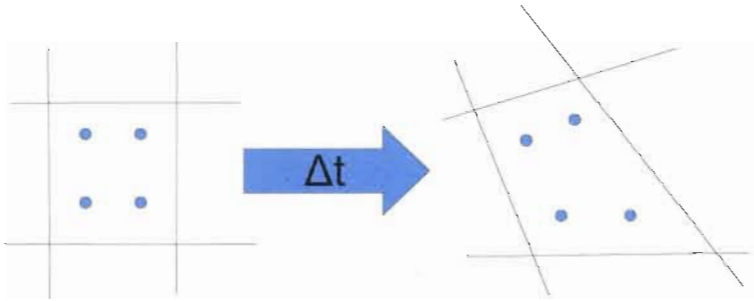
$$m_i\boldsymbol{u}_i^{n+1}=\sum_p m_p\boldsymbol{u}_p^{n+1}S_n(\boldsymbol{x}_p^{n+1})$$

Mesh cells or elements are Eulerian. They are fixed.

FEM

$$\int \sigma\cdot\nabla S_i(\boldsymbol{x})\,dv=\sum_g w_g J_g\ \ {}_g\cdot\nabla S(\boldsymbol{x}_g),$$

where subscript g denotes Gauss integration points.



Gauss points are fixed on elements.

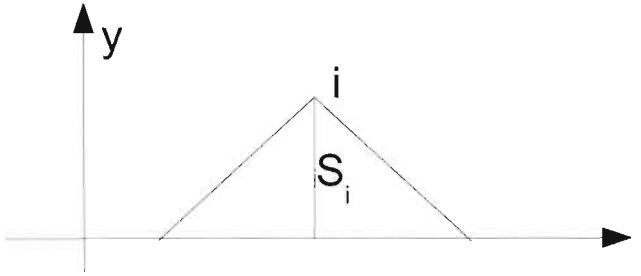
Elements are Lagrangian. They can become distorted for large material deformation.

Both the material points and Gauss points are Lagrangian points and can be used to track deformation history of the material. However, FEM has the difficulty of mesh distortion. The original MPM has also its own difficulties, but has been overcome by the dual domain material point (DDMP) method.

Dual domain material point (DDMP) method

$$m_i \frac{d\boldsymbol{u}_i}{dt} = -\sum_p v_p \boldsymbol{\sigma}_p \cdot \nabla S_i(\boldsymbol{x}_p) + \int \rho \boldsymbol{g} S_i(\boldsymbol{x}) dv + \int_{\partial v} S_i(\boldsymbol{x}) \boldsymbol{\sigma} \cdot \boldsymbol{n} dS,$$

The discontinuity of the shape function gradient causes an instability (Bardenhagen and Kober, 2004).

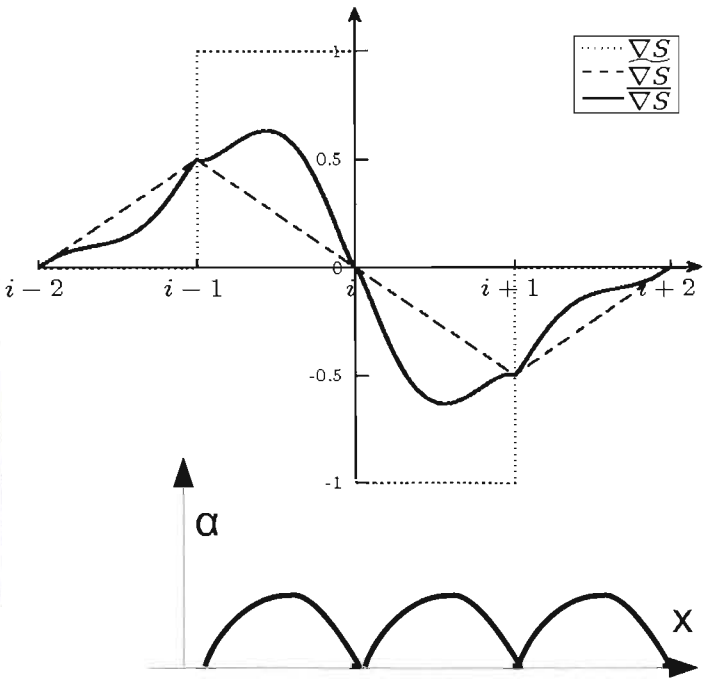


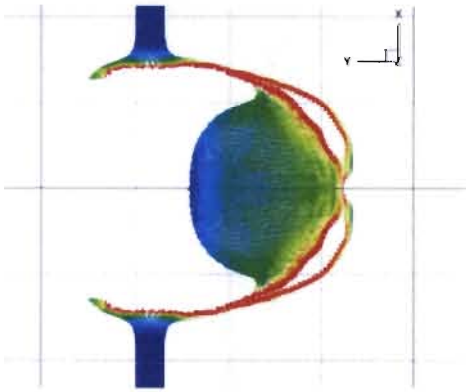
Solution: Replace ∇S_i by

$$\overline{\nabla S_i}(\boldsymbol{x}) = \alpha(\boldsymbol{x}) \nabla S_i(\boldsymbol{x}) + [1 - \alpha(\boldsymbol{x})] \widetilde{\nabla S_i}(\boldsymbol{x}),$$

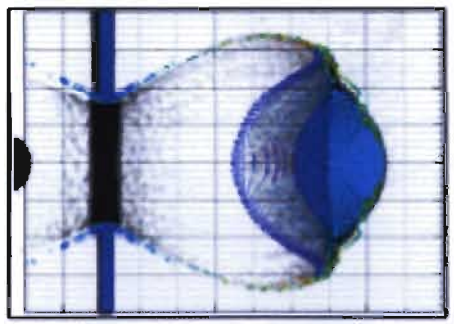
$$\widetilde{\nabla S_i}(\boldsymbol{x}) = \sum_{j=1}^{N} \frac{1}{V_j} (S_j, \nabla S_i) S_j(\boldsymbol{x}),$$

where α(x) = 0 on cell boundary.





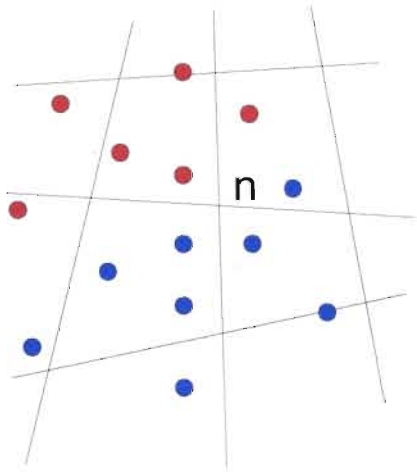
Original MPM



Dual domain material point (DDMP) method

Continuity: $\sum_i \theta^{(i)} = 1.$

- To ensure no unphysical void, crack, or over-lap of the materials, in the multi-velocity formulation, the volume fractions of all phases sum to one.



- However, in the material point method:

$$\theta_n^{(i)} = \frac{\sum_p v_p^{(i)} S_n(\boldsymbol{x}_p)}{V_n}$$

and there is no way to ensure $\sum_i \theta_n^{(i)} = 1$

numerically. If this constraint is used directly in MPM, significant error will occur (Zhang, et al. 2008, *J. of Comp. Phys.* **227**, pp. 3159-3173) .

- To ensure the continuity constraint, we use

$$\frac{\partial}{\partial t}\left(\sum \theta_n^{(i)}\right) + \boldsymbol{u}^{(m)} \cdot \nabla \sum \theta_n^{(i)} = 0.$$

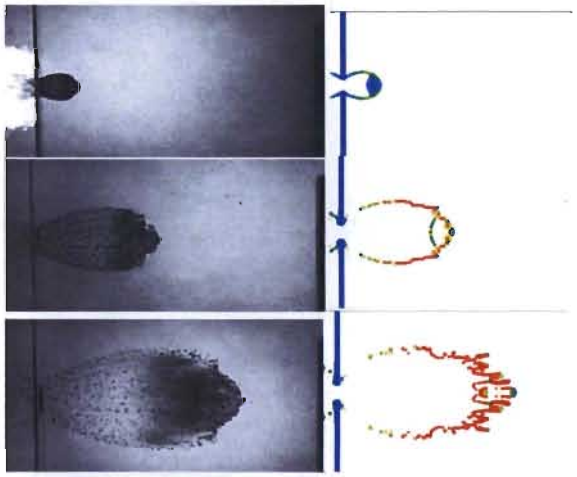
In the sense of weak solution, this constraint is equivalent to $\sum_i \theta_n^{(i)} = 1.$

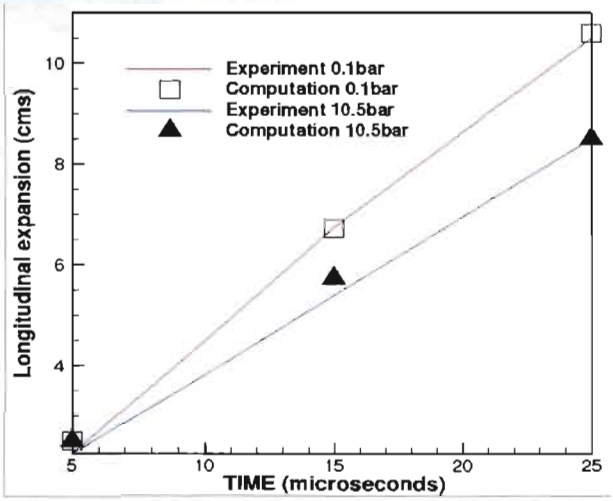
Transition from continuous to disperse flows

Chamber pressure 0.1Bar

Experiment of Piekutowskii (1996)

DDMP calculation



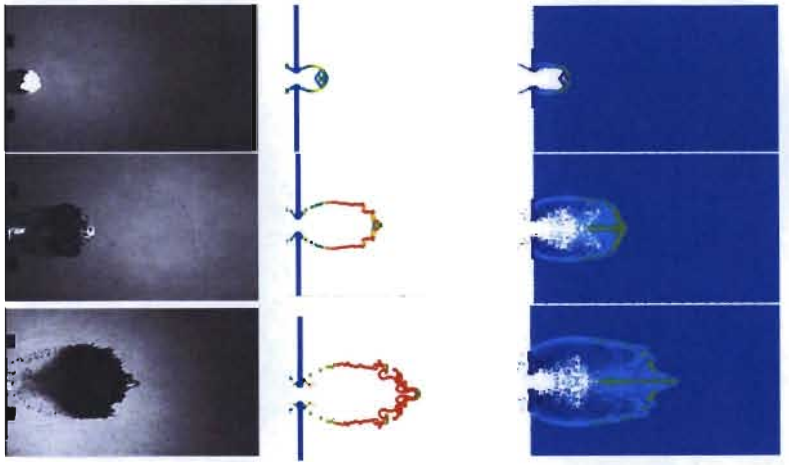


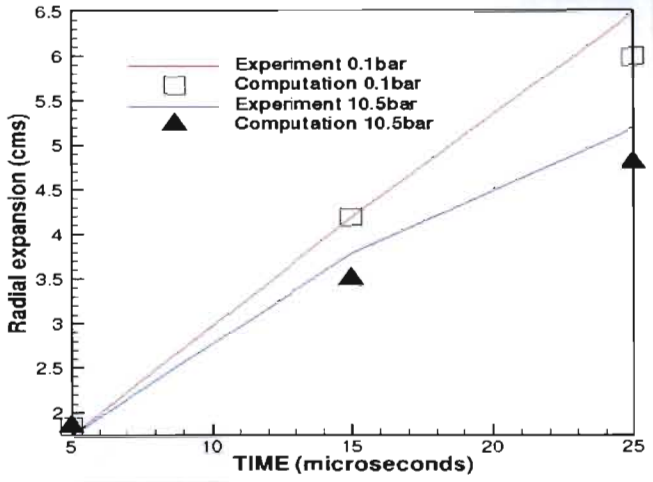
Chamber pressure 10.5 Bar

Experiment of Piekutowskii (1996)

DDMP calculation

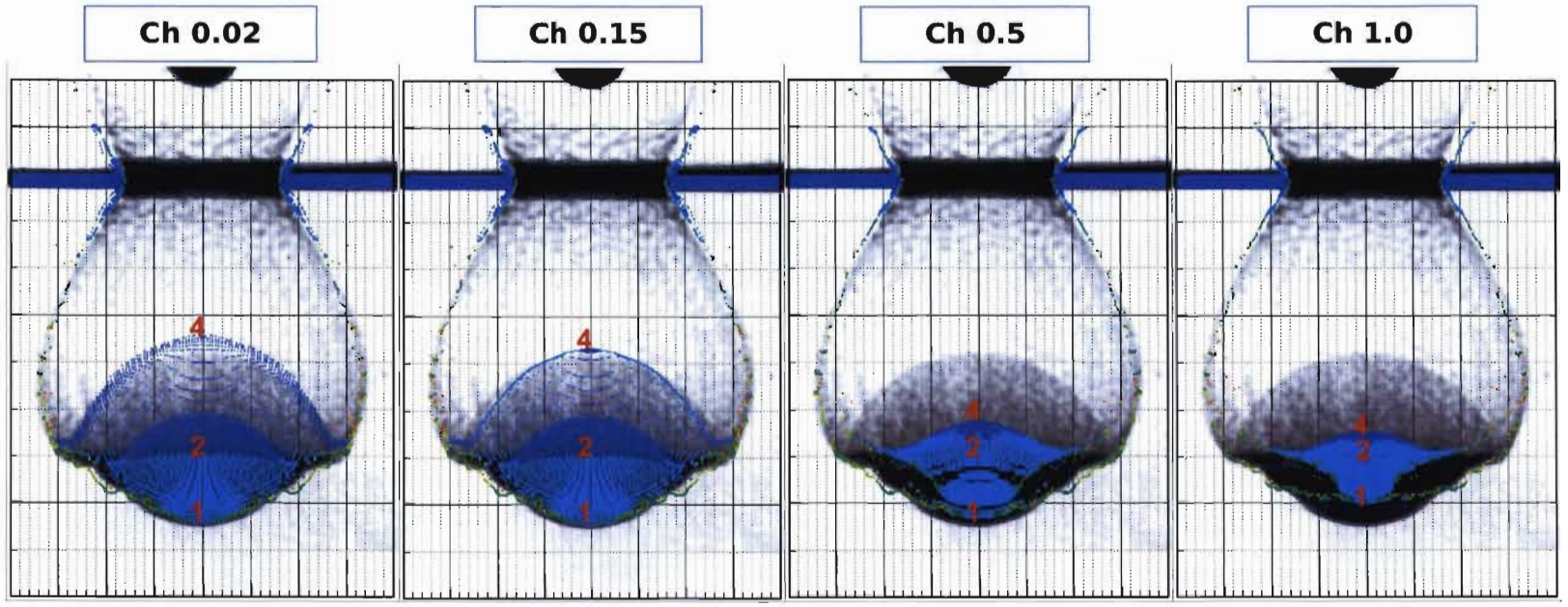
SPH calculation of Hiermaier et al. (1999)





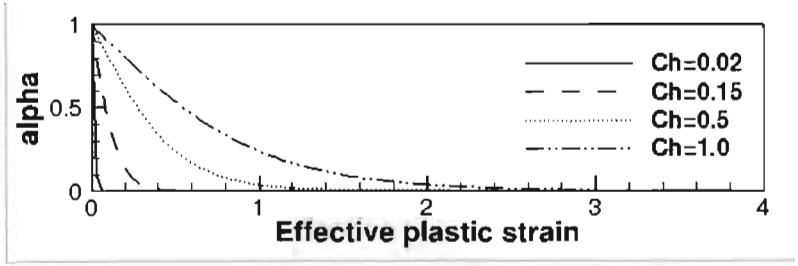
Continuous to disperse flow transition

Debris cloud from an Impact:
Velocity: 6.71km/s. Materials: Al-2024

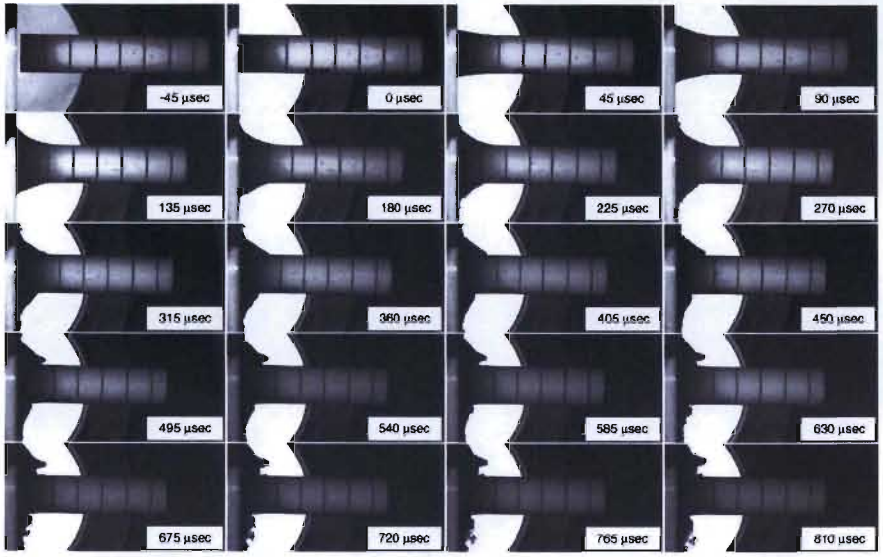


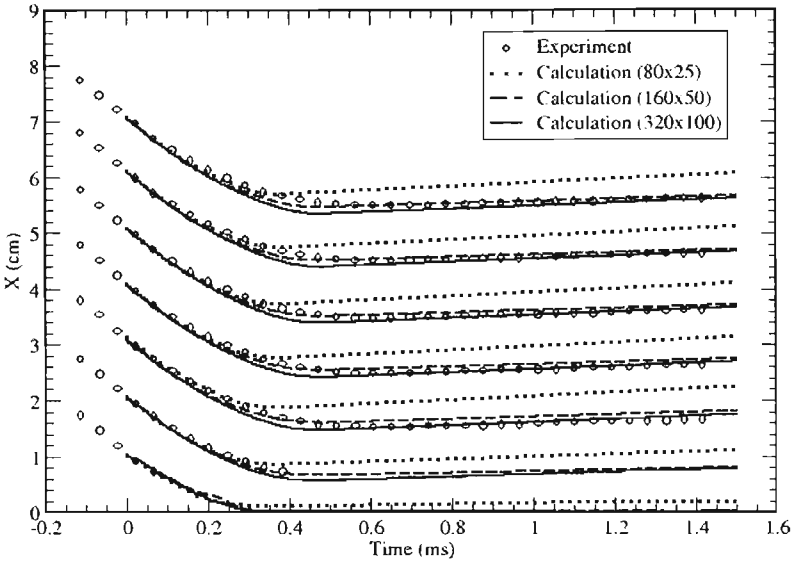
Axial velocities (km/s)	Experiment (Piekutowskii, 1993)	Ch= 0.02	Ch= 0.15	Ch= 0.5	Ch= 1.0
Point 1	6.3	6.29	6.25	5.9	5.77
Point 2	6.1	5.97	5.94	5.8	6.02
Point 4	3.9	3.92	4.09	6.1	6.11

$$\langle \nabla \cdot \boldsymbol{v}^{(i)} \rangle = \alpha^{(i)} \nabla \cdot \langle \boldsymbol{v}^{(i)} \rangle + B^{(i)}, \quad \alpha^{(i)} = 1 - \tanh\left(\frac{\epsilon_{ps}^{(i)}}{C_h}\right)$$

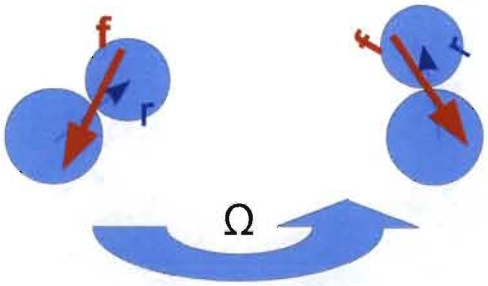


Taylor impact of brittle material





$$\sigma = \frac{1}{V}\sum \boldsymbol{f} \otimes \boldsymbol{r}$$



$$\frac{d\,\sigma}{dt} - \boldsymbol{\Omega}\cdot\boldsymbol{\sigma} + \boldsymbol{\sigma}\cdot\boldsymbol{\Omega} = -\frac{\sigma}{\tau} + \lambda\, tr(\dot{\varepsilon})\,\boldsymbol{I} + 2\mathrm{G}\,\dot{\varepsilon}\,,$$

$$\lambda = \frac{E\,\nu}{(1+\nu)(1-2\nu)},$$

$$G = \frac{E}{2(1+\nu)}$$

Conclusions

- Ensemble phase averaging method and multi-velocity formulation is applicable to both continuous and disperse flows.
- The derived equations can be solved using the improved material point method (DDMP) to simulation material failure, breakup, fragmentation and transition from continuous to disperse flows.
- This combination of mathematical formulation and numerical method avoids many conceptual and numerical difficulties associated with conventional methods, such as code or formulation switching for different flow regimes.
- To recover conventional results only a very simple material interaction model is needed.
- Currently not many material interaction models are available, because of lack of numerical tool.
- I hope that this combination of the formulation and the numerical method will encourage the model development.