Mesh-Free Computational Shock and Fracture

In Memory of Larry Libersky.

Andrew Brydon
Los Alamos National Laboratory

Second SPHERIC Workshop

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LA-UR-07-3937

Overview

- How we ended up using particles for fracture.
- What principles guide our particle methods?
- Linear completeness, Dual Particles and time stepping.
- Why aren't we there yet ?
- We to from here.

Larry Libersky

- Interested in shock, fracture and fragmentation with particle methods;
  - Strength in SPH.
  - Corrected kernels and MLS.
  - Dual space particles.
- Larry like to tell jokes during talks !

Large, Lumbering, Grid-based

Fast, Beautiful, Flexible, Mesh-Free

Collaborators

Al Petschek

Collaborators

Phil Randles

Carl Dyka

Collaborators

Steve Beissel

Gordon Johnson

Collaborators

Vignjevic

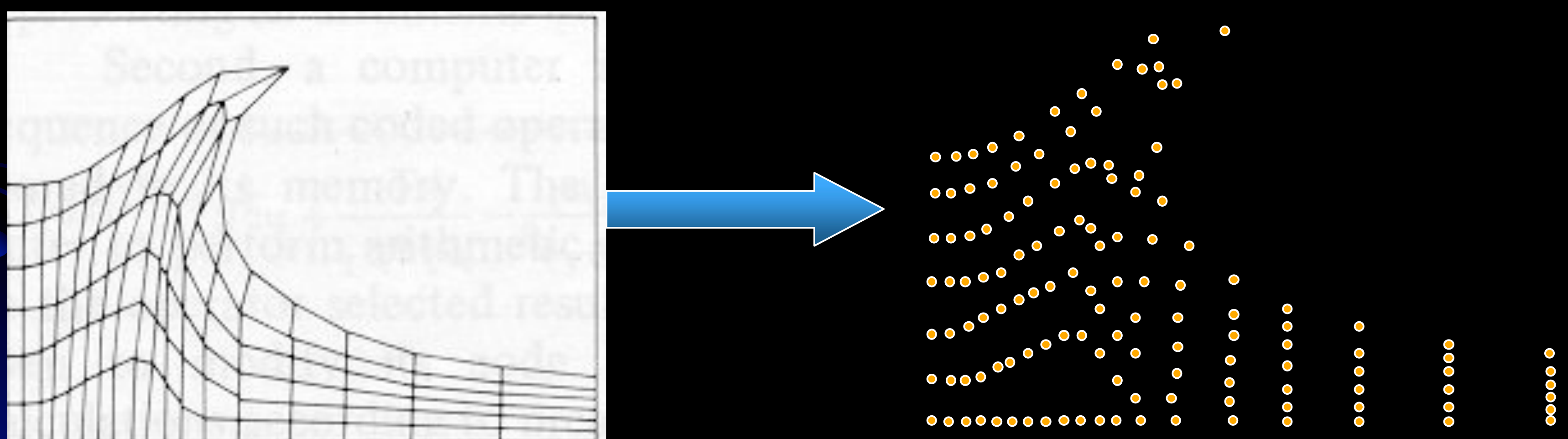
Campbell

Collaborators

- Many others that I failed to mention.
  - Sorry !

Why Particles

We believe there is opportunity to extend Lagrangian computing to larger deformations of materials, fracture and fragmentation.



Stability !

In the beginning ….

Mon. Not. R. astr. Soc. (1977) **181**, 375–389

Smoothed particle hydrodynamics: theory and application to non-spherical stars

R. A. Gingold and J. J. Monaghan* *Institute of Astronomy, Madingley Road, Cambridge, CB3 0HA*

Received 1977 May 5, in original form February 2

Summary. A new hydrodynamic code applicable to a space of an arbitrary number of dimensions is discussed and applied to a variety of polytropic stellar models. The principal feature of the method is the use of statistical techniques to recover analytical expressions for the physical variables from a known distribution of fluid elements. The equations of motion take the form of Newtonian equations for particles. Starting with a non-axisymmetric distribution of approximately 80 particles in three dimensions, the method is found to reproduce the structure of uniformly rotating and magnetic polytropes to within a few per cent. The method may be easily extended to deal with more complicated physical models.

1 Introduction

Many of the most interesting problems in astrophysics involve systems with large departures from spherical symmetry. This may occur either because the initial state lacks spherical symmetry, as in the case of a protostar forming from a dense interstellar cloud, or because non-spherical forces arising from rotation or magnetic fields, as in the case of the fission of a rotating star, play an important part in the dynamics. Frequently these sources of non-spherical symmetry will be found combined.

Because of the complexity of these systems numerical methods are required to follow their evolution. However, the standard finite difference representations of the continuum equations are of limited use, because of the very large number of grid points required to treat each coordinate on an equal footing. If, for example, 20 points along the radial direction give adequate accuracy for a spherical polytrope, we may require $(20)^3$ such points to give the same accuracy for a highly distorted polytrope. This difficulty is mirrored in the evaluation of multiple integrals.

For the astrophysical problems a numerical method which allows reasonable accuracy for a small number of points is required. Ideally it should also be simple to program and robust. An early attempt to provide such an alternative to the standard finite difference method was made by Pasta & Ulam (1959). They replaced the continuous fluid by a fictitious set of

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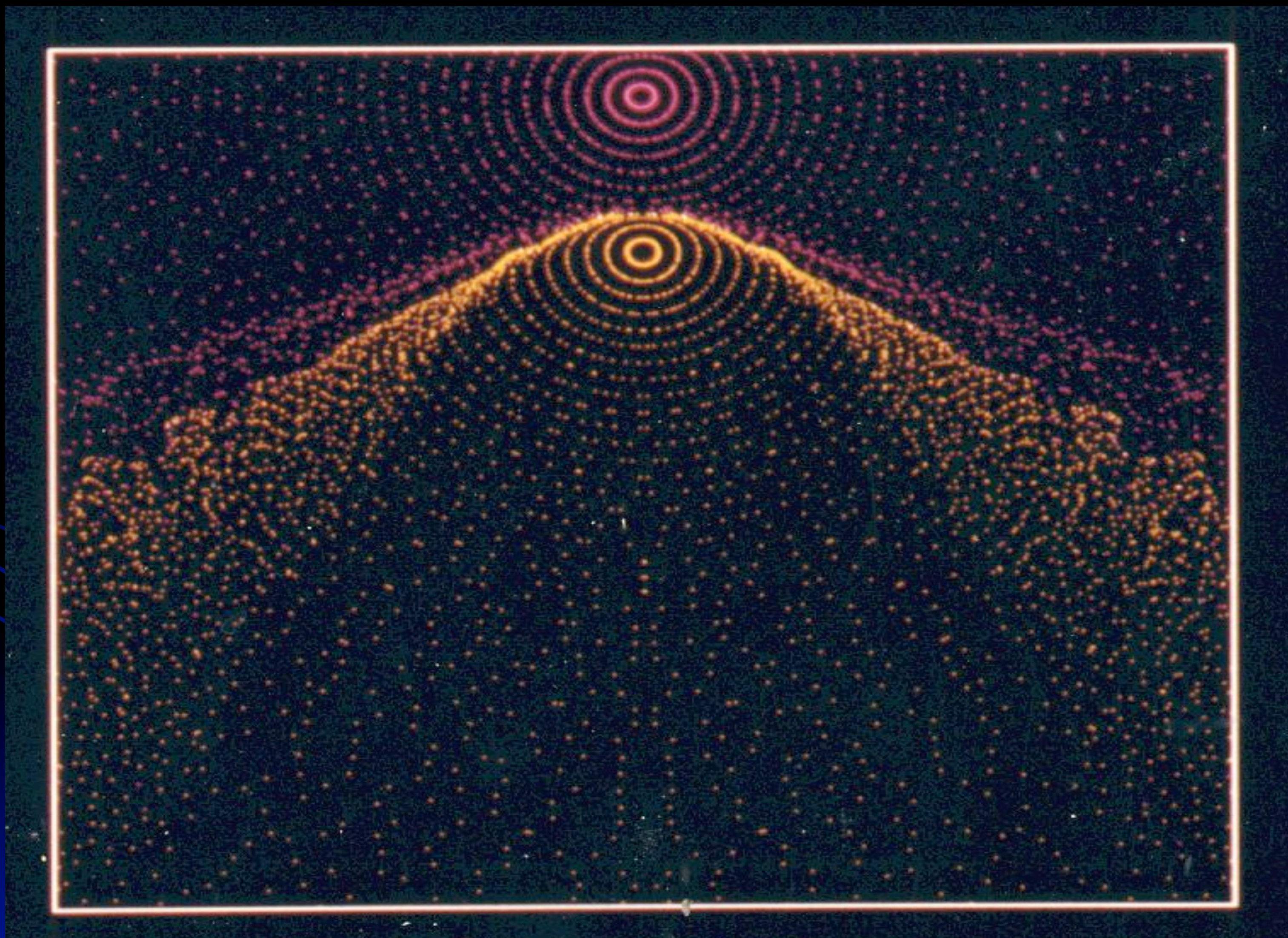
The Binary System C444 Cygni



Using SPH for mechanical response.

- Magi
  - Libersky and Carney

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High Strain Lagrangian Hydrodynamics

A Three-Dimensional SPH Code for Dynamic Material Response

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Received December 11, 1991; revised March 11, 1993

MAGI, a three-dimensional shock and material response code which is based on smoothed particle hydrodynamics (SPH) is described. Calculations are presented and compared with experimental results. The SPH method is unique in that it employs no spatial mesh. The absence of a grid leads to some nice features such as the ability to handle large distortions in a pure Lagrangian frame and a natural treatment of voids. Both of these features are important in the tracking of debris clouds produced by hypervelocity impact—a difficult problem for which SPH seems ideally suited. We believe this is the first application of SPH to the dynamics of elastic-plastic solids. © 1993 Academic Press, Inc.

INTRODUCTION

Traditionally, Lagrangian codes have been used to simulate material response when the amount of deformation is small. When the deformation is large, Eulerian calculations have been employed. The Lagrangian calculation is more accurate—the Eulerian calculation has greater applicability. These strengths and weaknesses are due to the convective derivative which is absent in the equations written in the moving Lagrangian frame. Numerical treatment of this advection term is difficult and introduces inaccuracies into the calculation. However, if the errors can be made small, the Eulerian calculation can be used to treat a variety of high strain phenomena.

Various methods have been devised in order to achieve the best features of both approaches. Such "hybrid" techniques normally use two grids, one Lagrangian—the other Eulerian, with information exchanged between them. These mappings add a good deal of complexity to the calculation and can also introduce inaccuracies. Nevertheless, many hybrid techniques have been successful and are widely used today.

Unique in computational fluid dynamics is smoothed particle hydrodynamics (SPH). The SPH technique uses no underlying grid—it is a pure Lagrangian particle method developed by Lucy [1], Gingold [2, 3], Monaghan [4–6], and Benz [7]. The absence of a mesh and the calculation of interactions among particles based on their separation alone means that large deformations can be computed without difficulty. It is for this reason that SPH has the potential to be a valuable computational tool. Although SPH has been proven excellent for astrophysical applications, it has not been applied to problems requiring the entire stress tensor. This paper addresses the extension of SPH to such problems.

0021-9991/93 $5.00

Our History

1990: SPH With Strength of Materials

1995: Tension Instability Identified

1996: Accuracy Issues Addressed

1996: Stress Points

1997: Corrected Derivative = MLS

1997: Neighbors From "Interior Hull"

2000: Stability……Again

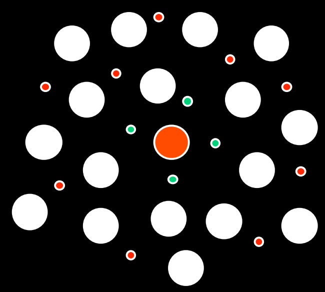
2000: Artificial Viscosity

2002: Boundary Conditions

Swegle

Johnson-Bissel
Randles
Liu
Vignjevic
Dilts
Bonet

Dyka



Bonet
Belytschko
Randles

Tension Instability
- Historical Record -

Swegle (1995): "Unstable"

SPH: No Order of Completeness

Belytschko (2000): "Unstable"

Linear Completeness in 2D for 2 particle arrangements with stress points. Weak form. RHS only. Uniform spacing.

Bonet (2001): "May be unstable"

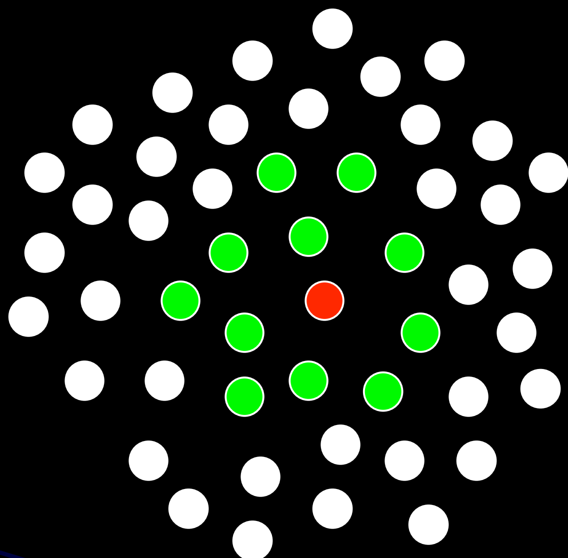
Linear Completeness in 1D
Strong form. RHS only.
Uniform particle spacing.

Randles (2001): "Stable"

Linear Completeness in 2D, 3D
Predictor-Corrector Schemes.
Arbitrary neighborhoods. MLS.

"The Stability of DPD and SPH", Springer Lecture Series, Meshfree Methods for solution of PDE's, Bonn Germany, Sept, 2001.

SPH



$$\frac{dU_i^\alpha}{dt} = \sum_j m_j \left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} \right) \frac{\partial W_{ij}}{\partial x^\beta}$$

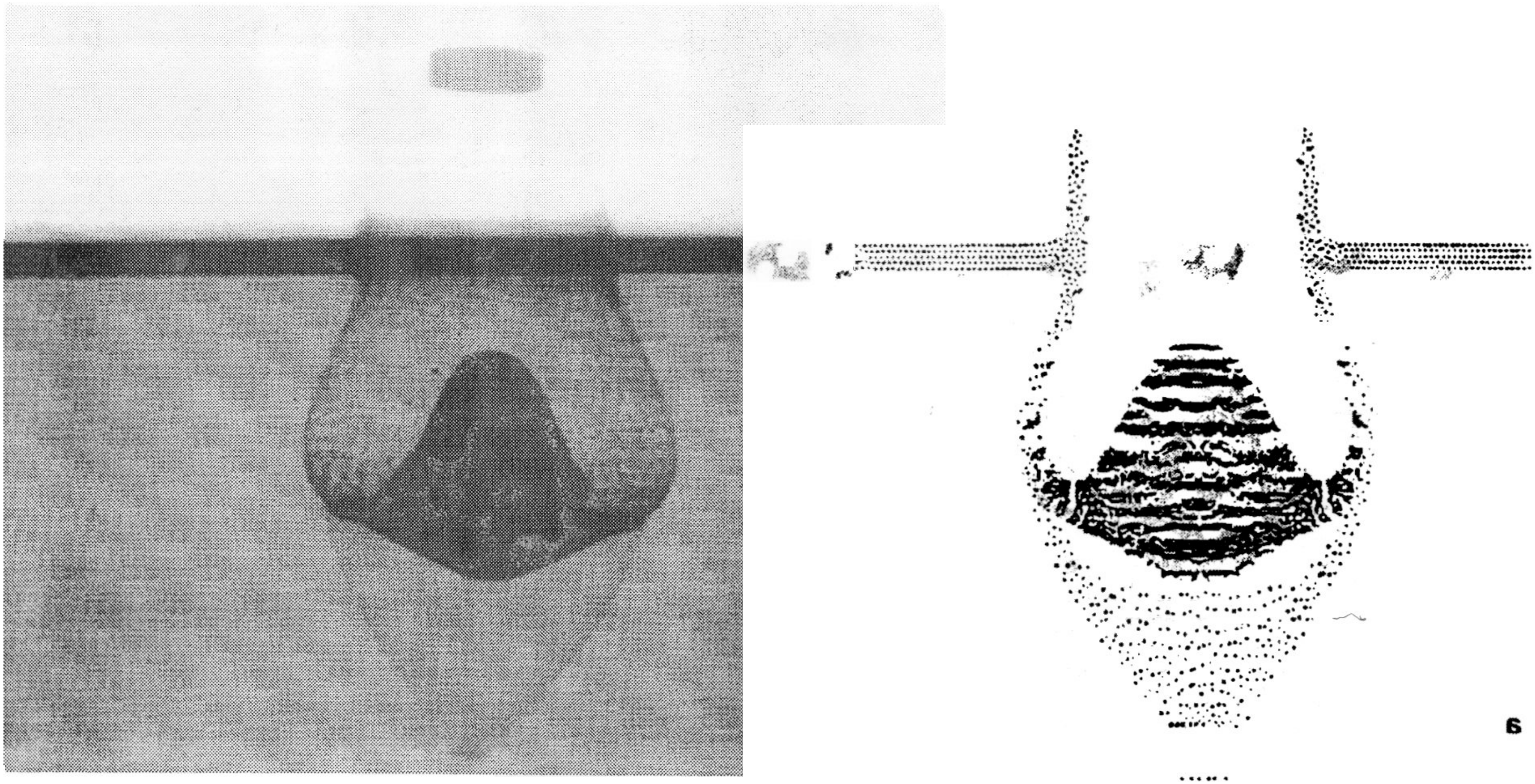
+

- **Conceptual Simplicity**
- **Extraordinary Robustness**
- **Ease of Going to 3D**
- **Arbitrary Deformation in Lagrange Frame**
- **Ideally Suited for Fracture**
- **Exact Local Conservation of Momentum**

–

- **Unstable in tension**
- **No order of completeness**

Debris Cloud

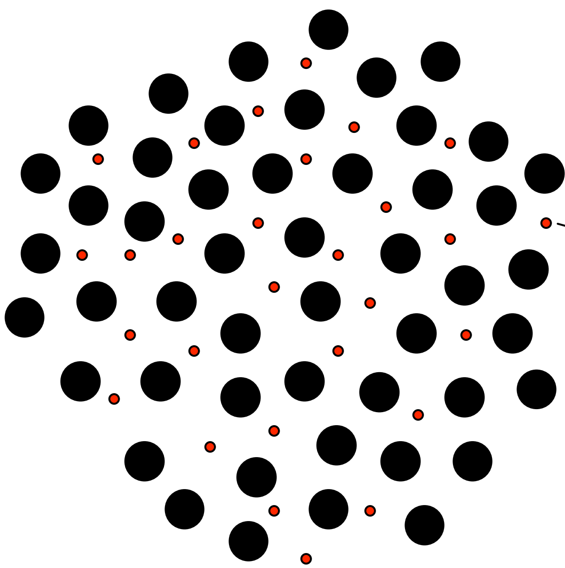


Dual Particle Dynamics

- Dual space of particles
  - Reduces null-space modes.
  - Analogy with staggered grid or finite elements.
- Use Moving Least Squares fits for particle interpolation
  - Linear completeness.
- Uses convex hull to find neighbors.
  - Deals well with anisotropic particle arrangements.
  - Reduced support for derivative operators.
- Predictor-Corrector.
  - Care required for stability of arbitrary particle arrangements.
- VVN velocity update.
  - Smooth velocity estimator reduces hourglass modes.

Dual Particle Dynamics (DPD)

$$\left\langle \frac{dU^{\alpha}}{dt} \right\rangle_i = \frac{1}{\langle \rho_i \rangle} \left\langle \frac{\partial \sigma^{\alpha\beta}}{\partial x^{\beta}} \right\rangle_i$$

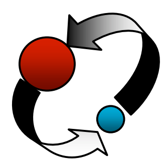


Motion Points U^{α}

Matter

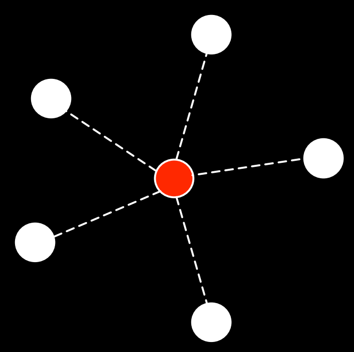
Stress Points $\sigma^{\alpha\beta}$

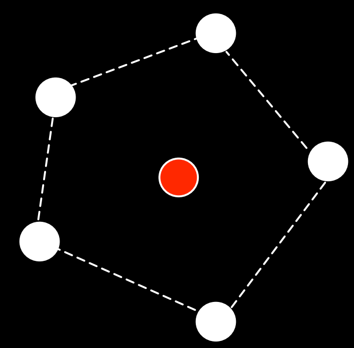
Field



$$\left\langle \sigma^{\alpha\beta} \right\rangle_i = F\left(\left\langle \frac{\partial U^{\alpha}}{\partial x^{\beta}} \right\rangle_i, \rho, E, \ldots \right)$$

The use of MLS fits.





SPH

$$\frac{dU_i^\alpha}{dt} = \sum_j m_j \left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} \right) \frac{\partial W}{\partial x^\beta}$$

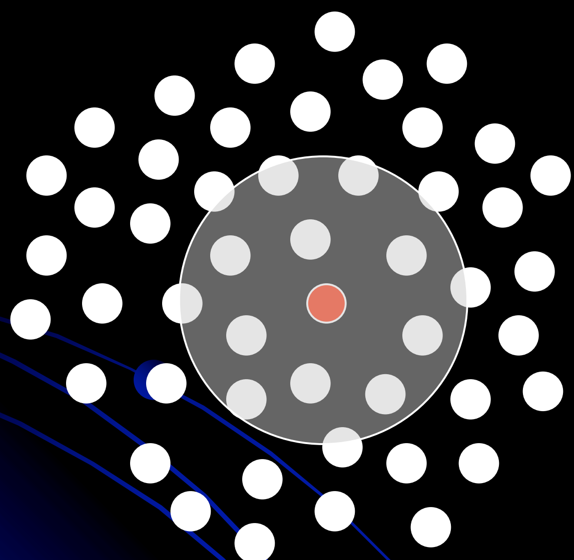
Normalized SPH or MLS

$$\frac{dU_i^\alpha}{dt} = \sum_j m_j \left(\frac{\sigma_i^{\alpha\gamma}}{\rho_i^2} - \frac{\sigma_j^{\alpha\gamma}}{\rho_j^2} \right) \frac{\partial W}{\partial x^\beta} B_{\beta\gamma}^{-1}$$

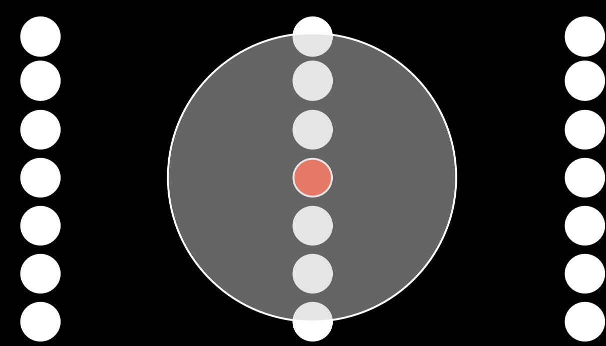
Inversion is local (3x3). Cost is minimal and fixed order.

Finding Neighbors

Discarding of a background computational mesh means that neighbors must be determined as the calculation proceeds. A more sophisticated approach than taking all points within a sphere is required because of anisotropy in the particle distribution. The case shown below would introduce undesirable effects.

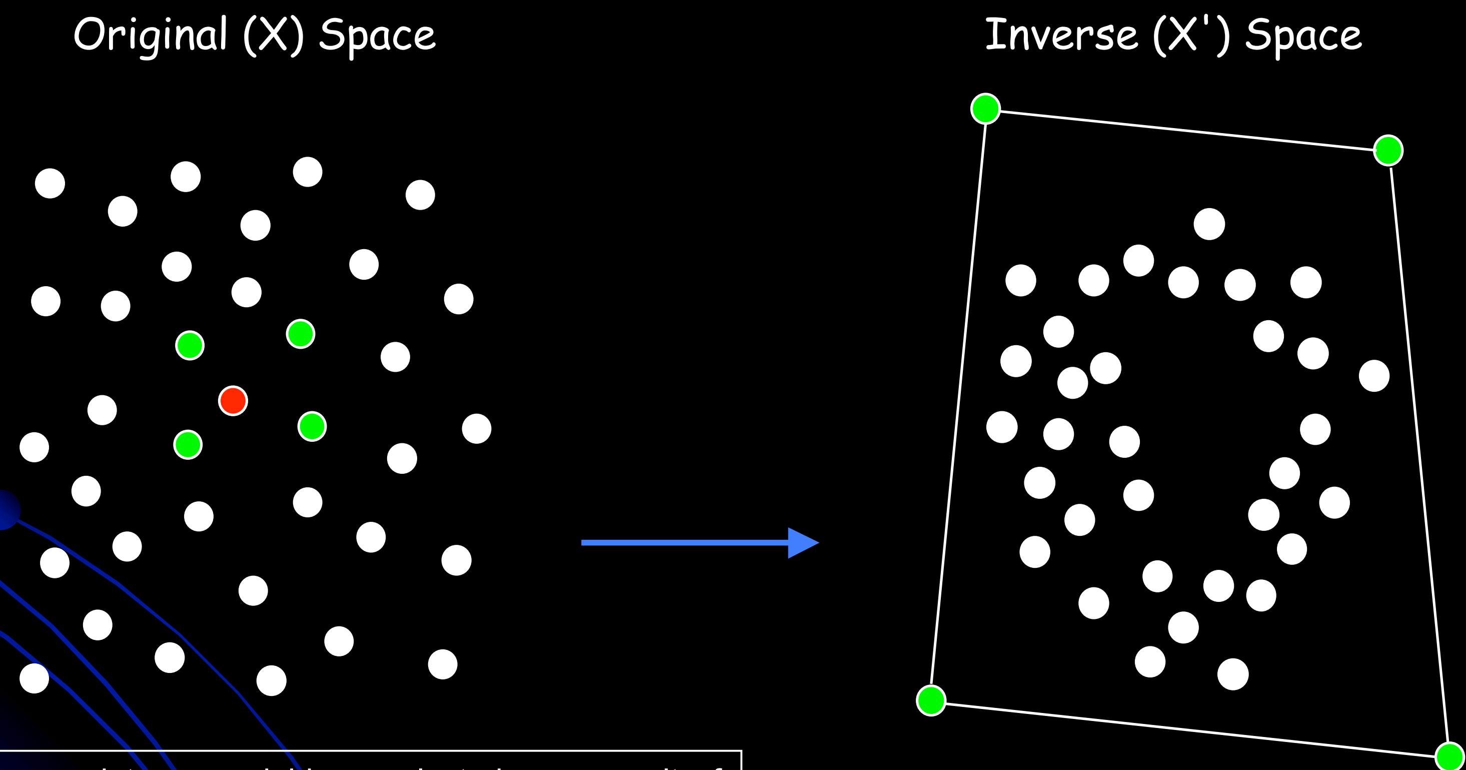


~Isotropy



~Anisotropy

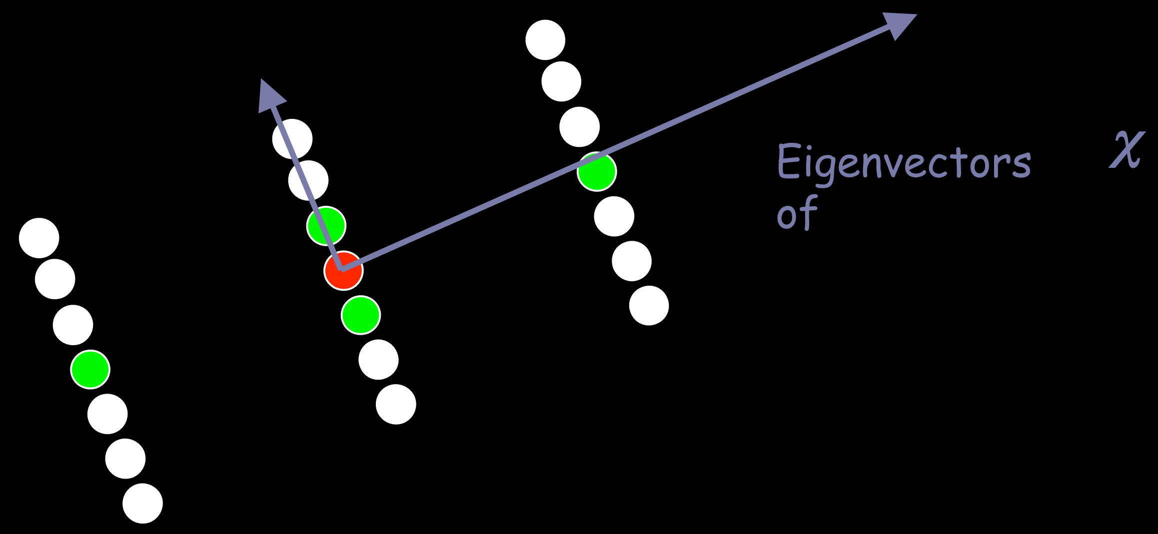
Finding Neighbors; Inverse Hull



The green points are neighbors selected as a result of applying (1) a simple inverse mapping and (2) fast running convex hull algorithm. The result is an “inner skin” of surrounding points, regardless of the anisotropy.

(Find convex hull in the inverse space)

Local Anisotropy in Particle Spacing



$$\chi_i^{\alpha\beta} = \sum_j \left(X_i^{\alpha} - X_j^{\alpha}\right)\left(X_i^{\beta} - X_j^{\beta}\right)$$

Artificial Viscosity

von Neumann - Richtmyer

$$Q = \rho h U^{\alpha,\alpha}\left(a_1 c + a_2 h U^{\alpha,\alpha}\right)$$

Monaghan - Gingold

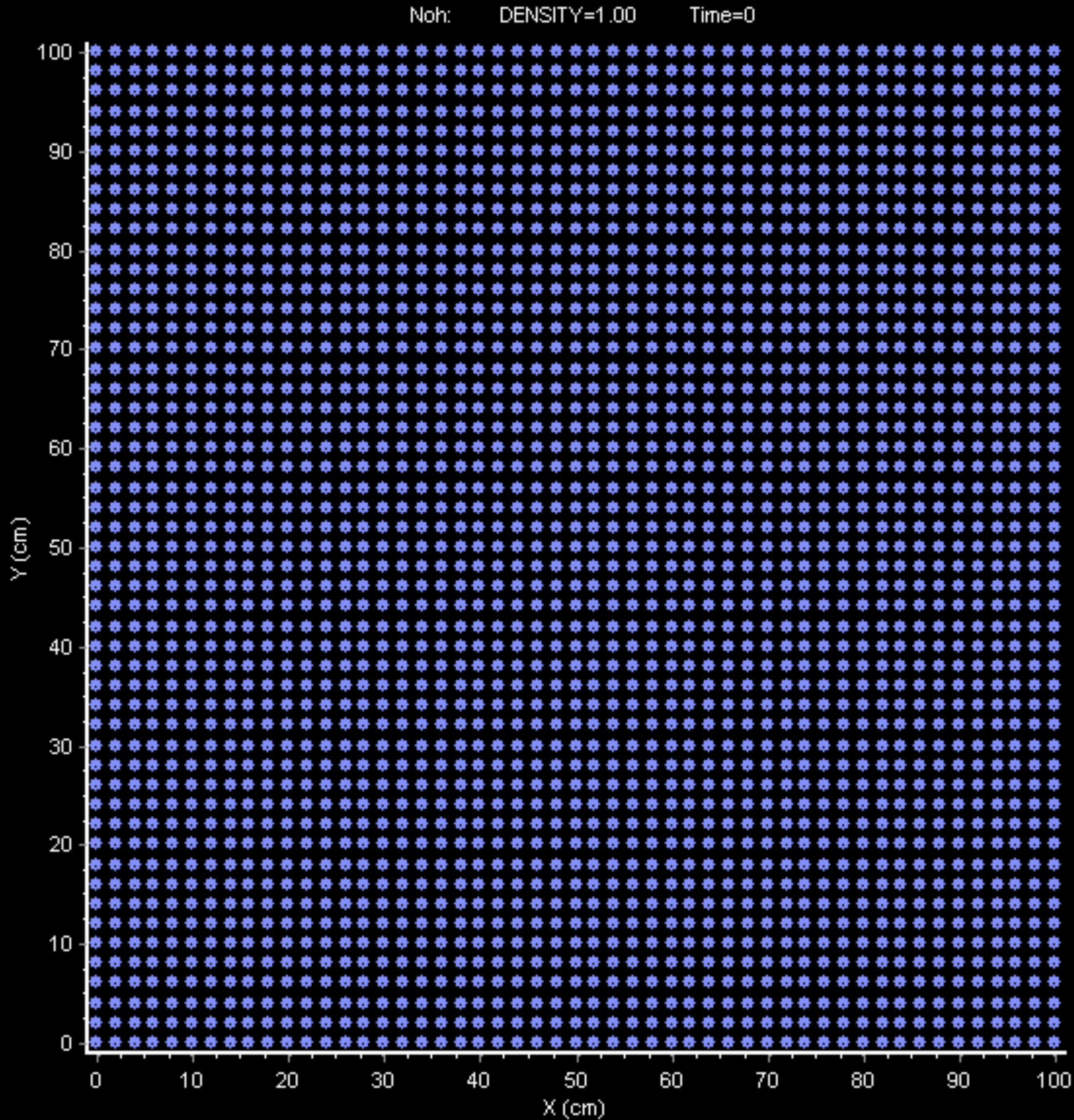
$$Q_{ij} = \frac{-a_1 \bar{c}_{ij}\mu_{ij} + a_2 \mu_{ij}^2}{\bar{\rho}_{ij}} \qquad \mu_{ij} = \frac{h U_{ij}^{\alpha} X_{ij}^{\alpha}}{r^2 + \varepsilon h^2}$$

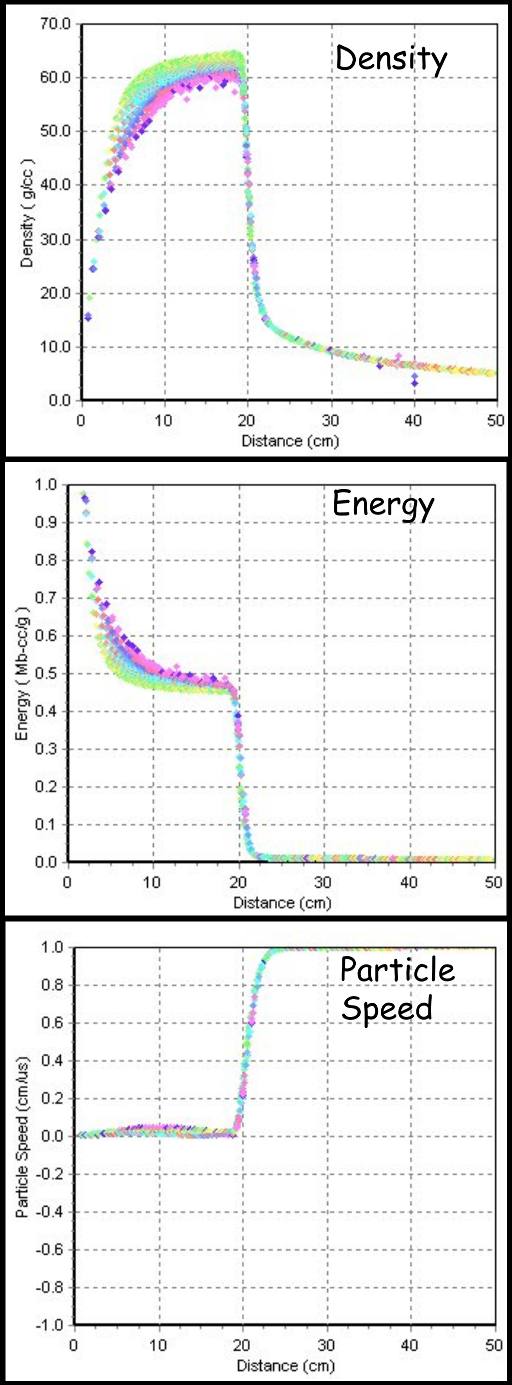
Petschek – Randles - Libersky

$$Q^{\alpha\beta} = \rho\left(a_1 c\sqrt{\hat{\dot{\varepsilon}}^{\alpha\gamma}}\sqrt{\chi^{\gamma\lambda}}\sqrt{\hat{\dot{\varepsilon}}^{\lambda\beta}} + a_2 \hat{\dot{\varepsilon}}^{\alpha\gamma}\chi^{\gamma\lambda}\hat{\dot{\varepsilon}}^{\lambda\beta}\right)$$

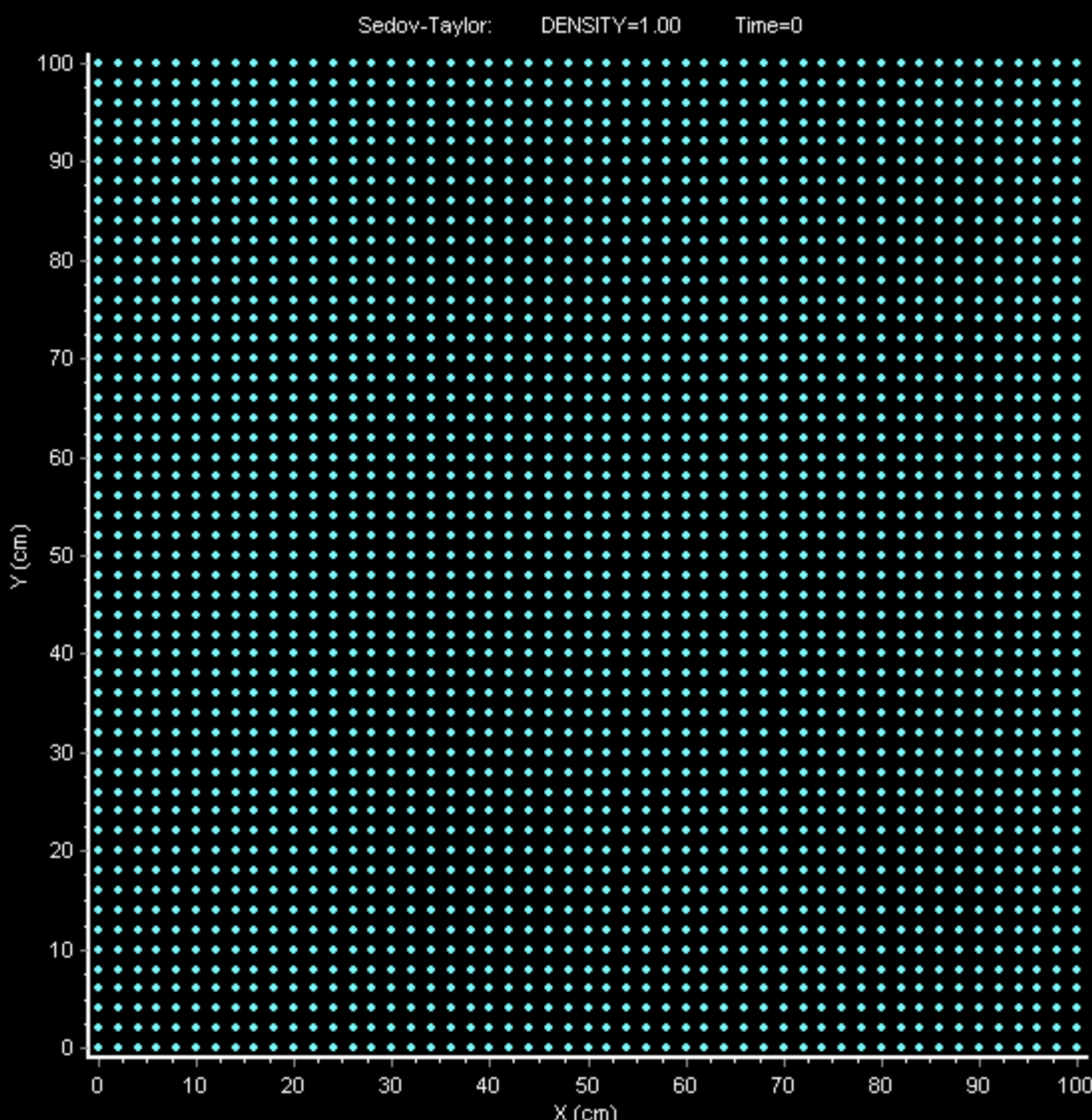
χ_i tensor is good measure of length for viscosity

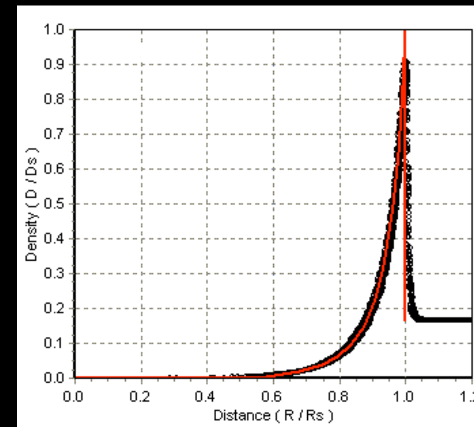
The Noh Problem

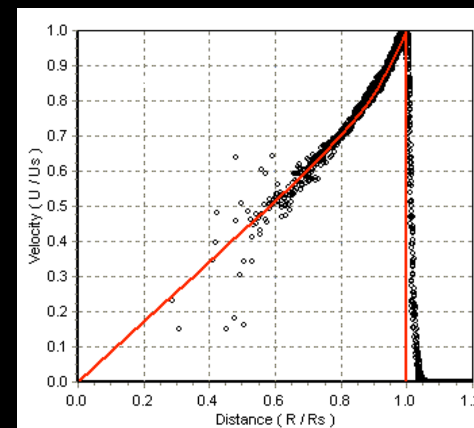


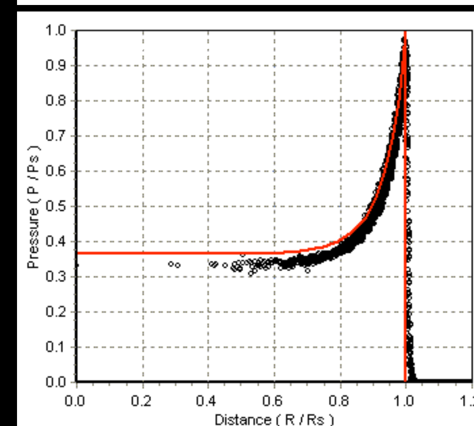


DPD: Sedov-Taylor









Stability

"You cannot rob Peter to pay Paul. If you do that you're dead in the water – you're going nowhere!"

Ed Caramana

$$\left\langle \frac{dU^{\alpha}}{dt} \right\rangle_i = \frac{1}{\langle \rho_i \rangle} \left\langle \frac{\partial \sigma^{\alpha\beta}}{\partial x^{\beta}} \right\rangle_i$$

Paul Peter

Stability of DPD (Randles)

System: Linear, forward Euler

$$u_m^{n+1} = u_m^n + \frac{\delta t}{\rho_m^{n+\frac{1}{2}}}(\nabla \bullet \sigma)_m^{n+\frac{1}{2}}$$

$$\sigma_m^{n+1} = \sigma_m^n + \delta t C : (\nabla u)_s^{n+1}$$

Spatial derivatives: MLS

$$(\nabla \bullet \sigma)_m^{n+\frac{1}{2}} = \sum_{s \in N(m)} \sigma \bullet \chi\, w$$

$$(\nabla u)_s^{n+1} = \sum_{m \in N(s)} u \bullet \chi\, w$$

Assume: Plane harmonic wave solution

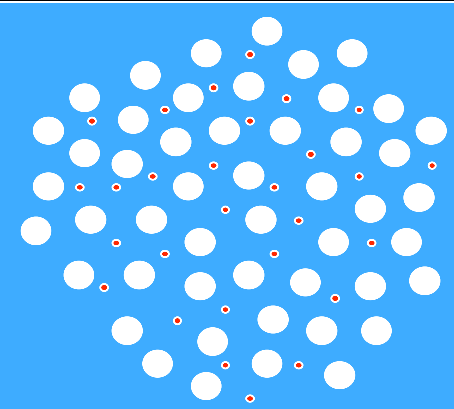
$$u_m^n = u_o \xi^n e^{ik \bullet x_m}$$

$$\sigma_s^n = \sigma_o \xi^n e^{ik \bullet x_s}$$

On substitution:

$$(1-\xi)u_o + \frac{\delta t}{\rho_o}\xi^{\frac{1}{2}}\sigma_o A_m = 0$$

$$(1-\xi)\sigma_o + \delta t\, \xi^{\frac{1}{2}}\, C : u_o B_s = 0$$



Eliminate to put in terms of u0

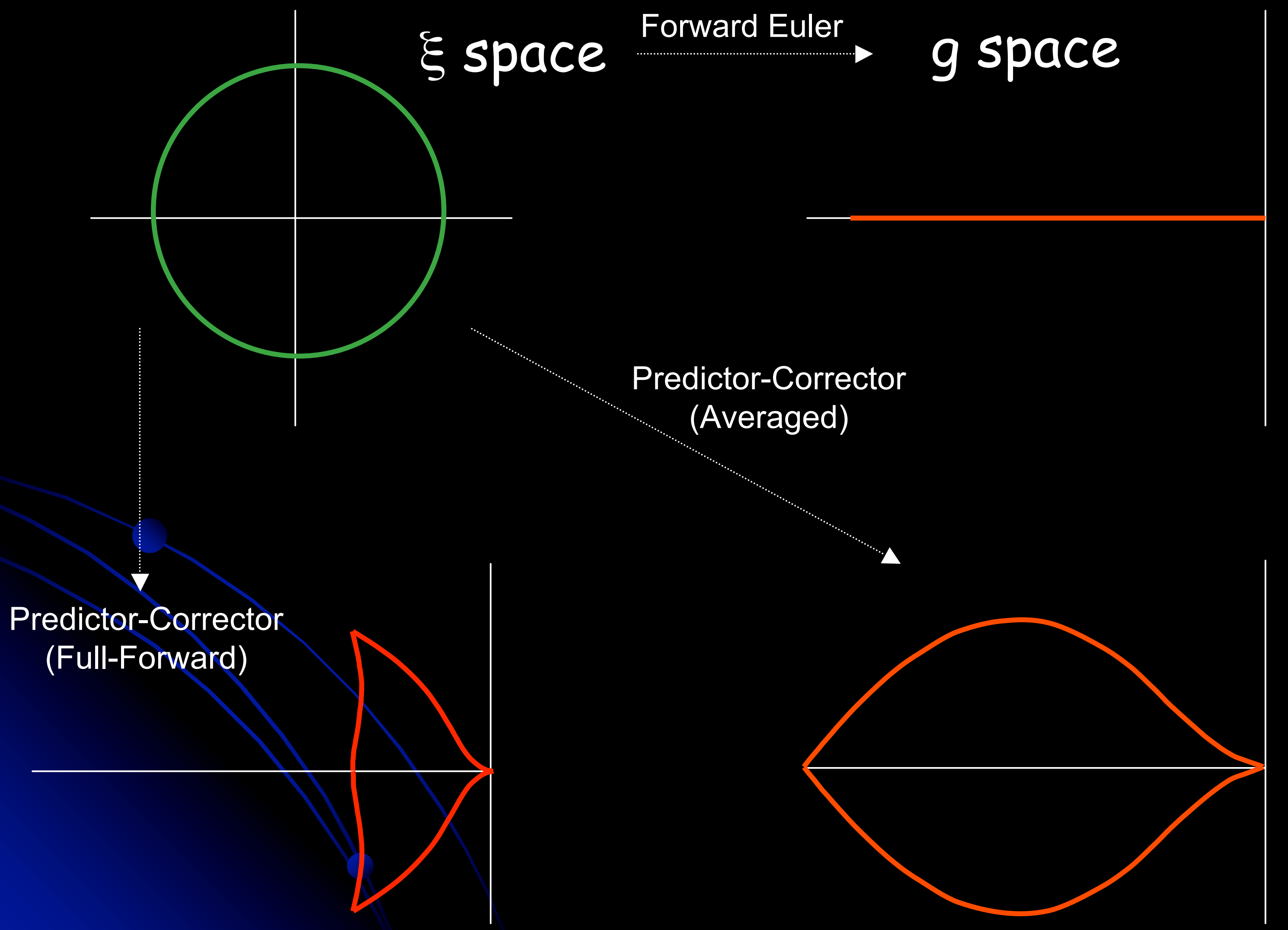
$$\left[G - f(\xi) I\right] \bullet u_o = 0$$

$$g_\alpha = f(\xi)$$

f is function of time stepping method
G is a function of local geometry

$$\mathbf{A} = \left(\left\langle \nabla\left(e^{\iota \kappa \bullet x}\right)\right\rangle / e^{\iota \kappa \bullet x}\right)_\alpha \ \textbf{\textit{and}}\ \mathbf{B} = \left(\left\langle \nabla\left(e^{\iota \kappa \bullet x}\right)\right\rangle / e^{\iota \kappa \bullet x}\right)_\beta$$

Stability Analysis



Stability Boundaries for DPD

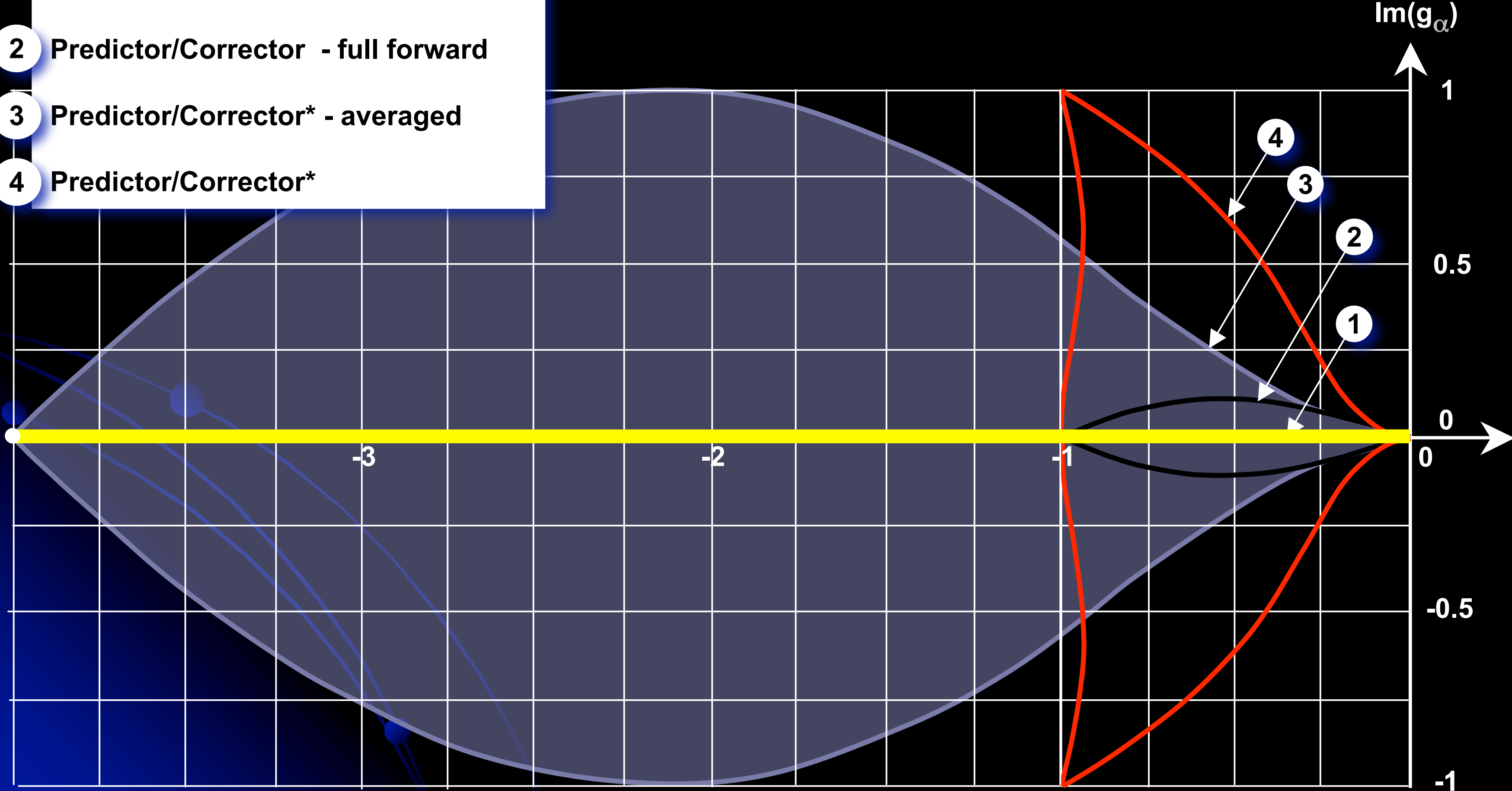
LEGEND

1. Euler update using current velocities* to calculate stress.
2. Predictor/Corrector - full forward
3. Predictor/Corrector* - averaged
4. Predictor/Corrector*

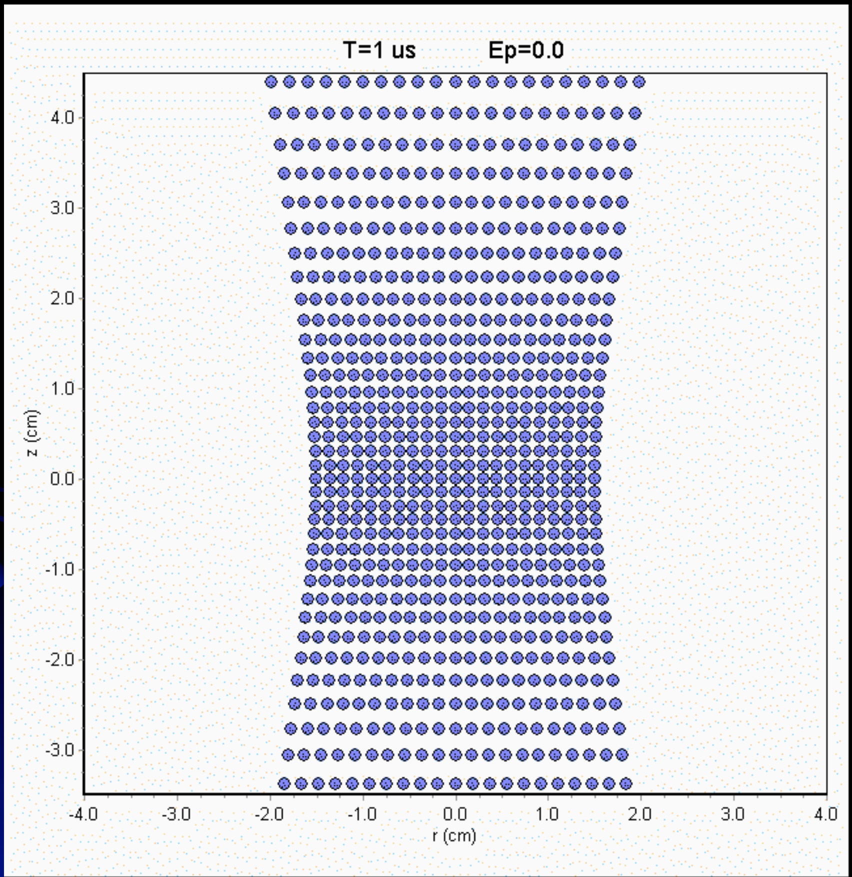
Complex g_α space:

Eigenvalues of

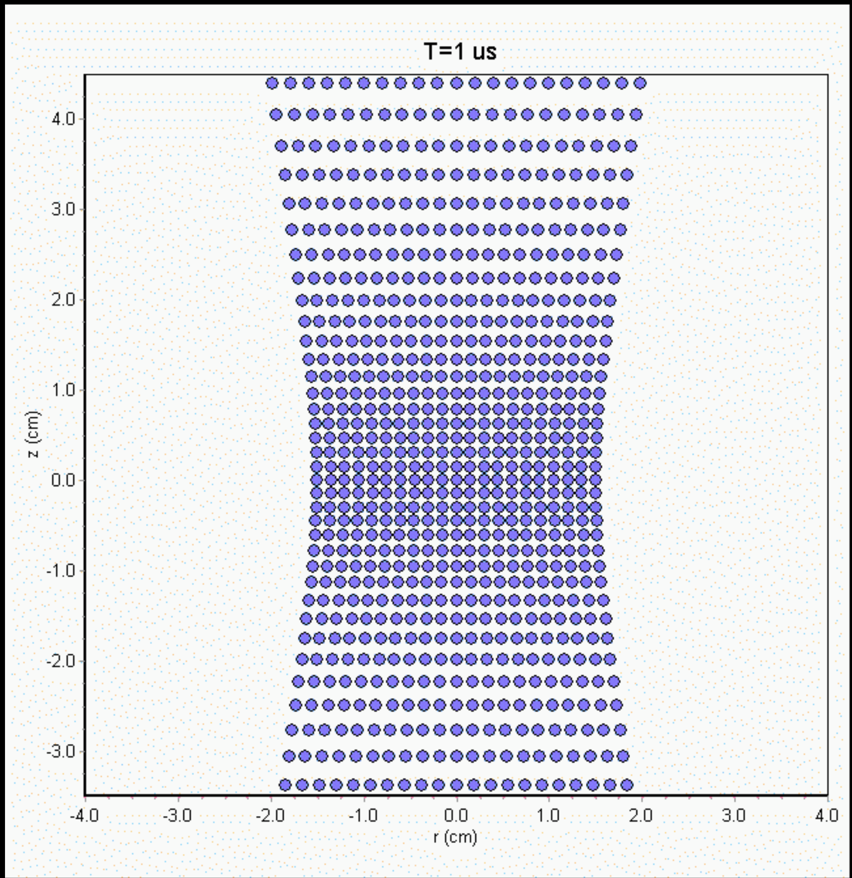
$$G = (\delta t^2/\rho_o)\{\lambda AB + \mu[(A \bullet B)I + BA]\}$$



DPD Simulation of Tensile Test



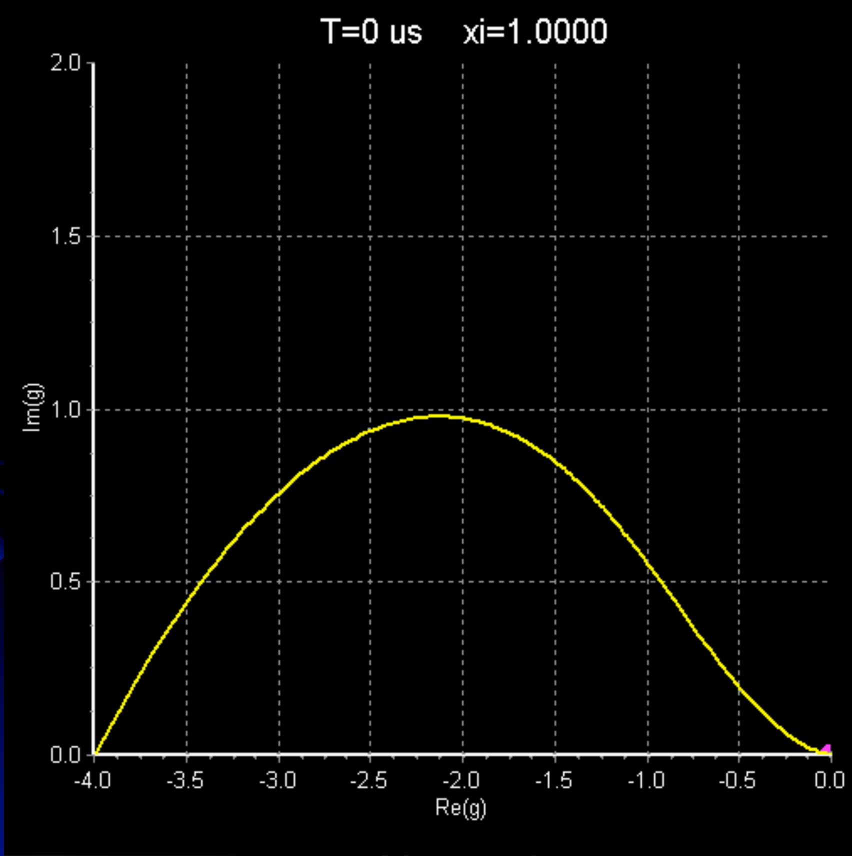
Plastic Strain

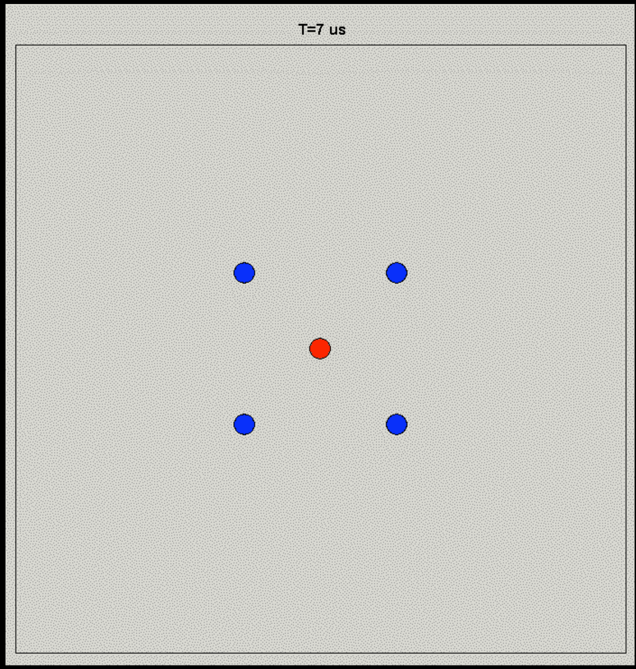


Vertical Velocity

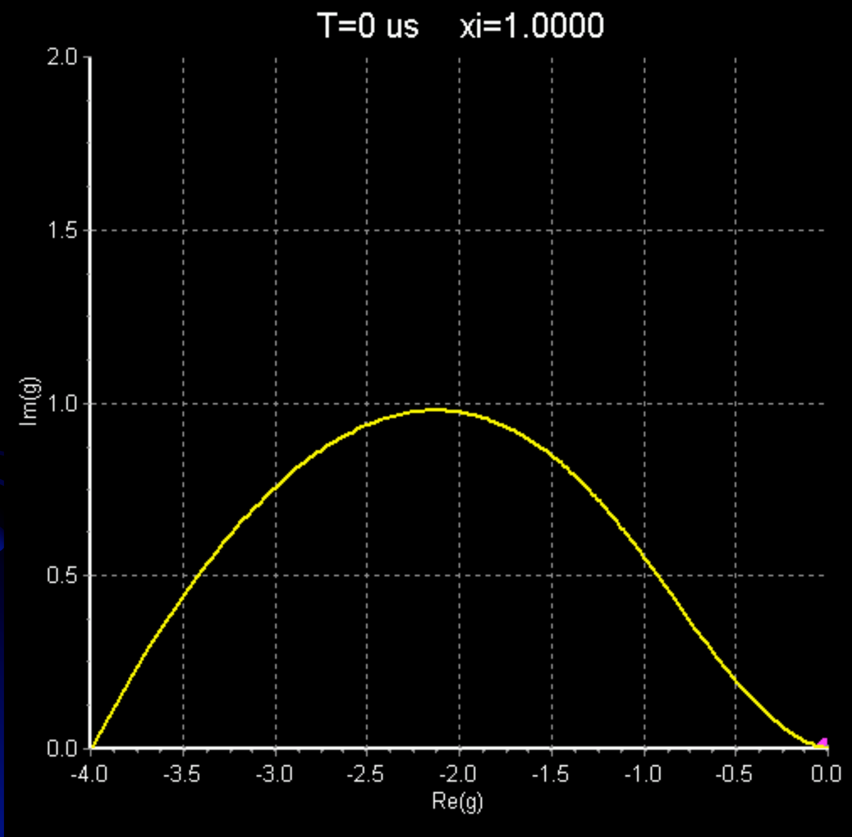
Q=0!

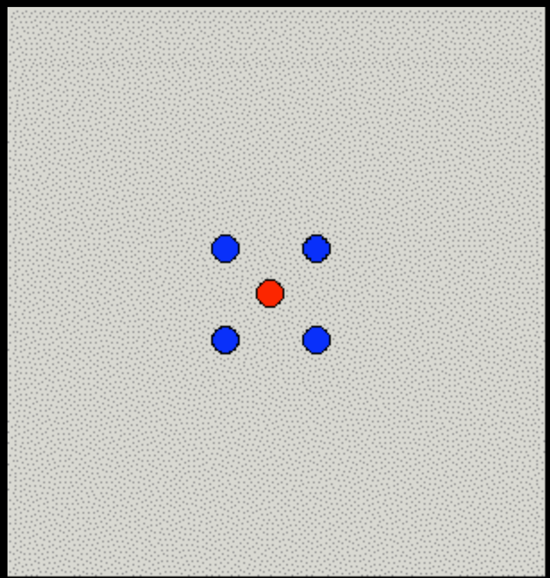
Stability Eigenstate for Particle in Neck of Pulled Bar – Fixed Neighbors





Stability Eigenstate for Particle in Neck of Pulled Bar – Variable Neighbors





How do we relate neighbors to stability?

- The stability Eigenstate for a particle tells us when a new neighborhood is necessary.
- We need search for new neighbors only when $g_\alpha > g_c$, with search criteria tied to the stability analysis. i.e. when we cant find a stable time step for this configuration.

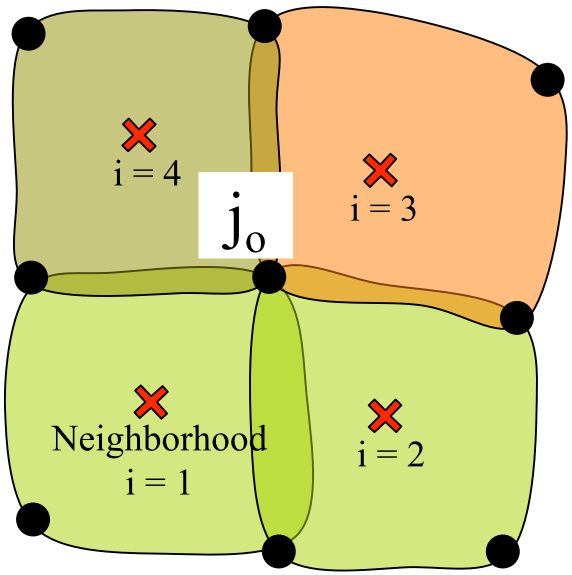
Stability Conclusions

- Time stepping method affects stability.
- Local geometry affects stability.
  - Cannot rob one to pay the other.
- A simple CFL conditions is often not good enough.
- Forward Euler is only stable with regular particles (i.e. an Eulerian grid).
- Viscosity affects the results, but not enough.

Updating Positions

- It seems like having a particle velocity should tell you how to move it.
  - Seen in SPH; causes problems with hourglass modes.
  - Can allow inter-penetration when we know it shouldn’t.
- Can use XSPH with DPD.
- VVN is DPD’s equivalent of XSPH.
  - Looking for consistent way to get ‘smooth’ update velocity.

Outline of VVN



- **Motion point j_o has stress point neighbors i=1,2,3,4 (red crosses)**
- **Associated with each neighbor is a neighborhood also denoted by i and bounded by j_o and other motion points that are neighbors of neighbors of j_o (black dots)**

- **<u>Step 1:</u> Linear MLS approximation of velocity field in neighborhood of i (same as MLS velocity to move i)**

$$\bar{u}_i \cong \bar{a}_i + \bar{b}_i \bullet (\bar{x} - \bar{x}_i)$$

$$\bar{a}_i = (\overline{uw}_i - \bar{b}_i \bullet \overline{xw}_i)/sw_i \ , \quad \bar{b}_i = \overline{sux}_i \bullet (\overline{sxx}_i)^{-1}$$

$$sw_i = \sum_{j \in N_i} w_{ij} \ , \quad \overline{uw}_i = \sum_{j \in N_i} \bar{u}_j w_{ij} \ , \quad \overline{xw}_i = \sum_{j \in N_i} \bar{x}_{ij} w_{ij} \qquad (\bar{x}_{ij} = \bar{x}_j - \bar{x}_i)$$

$$\overline{sux}_i = \overline{uxw}_i sw_i - \overline{uw}_i \overline{xw}_i \ , \quad \overline{sxx}_i = \overline{xxw}_i sw_i - \overline{xw}_i \overline{xw}_i$$

$$\overline{uxw}_i = \sum_{j \in N_i} \bar{u}_j \bar{x}_{ij} w_{ij} \ , \quad \overline{xxw}_i = \sum_{j \in N_i} \bar{x}_{ij} \bar{x}_{ij} w_{ij}$$

- **<u>Step 2:</u> Average residual velocity at j_o**

$$\overline{ru}_{j_o} = \sum_{i \in N_{j_o}} (\bar{u}_{j_o} - \bar{a}_i - \bar{b}_i \bullet \bar{x}_{ij_o}) w_{ij_o} \Big/ \sum_{i \in N_{j_o}} w_{ij_o}$$

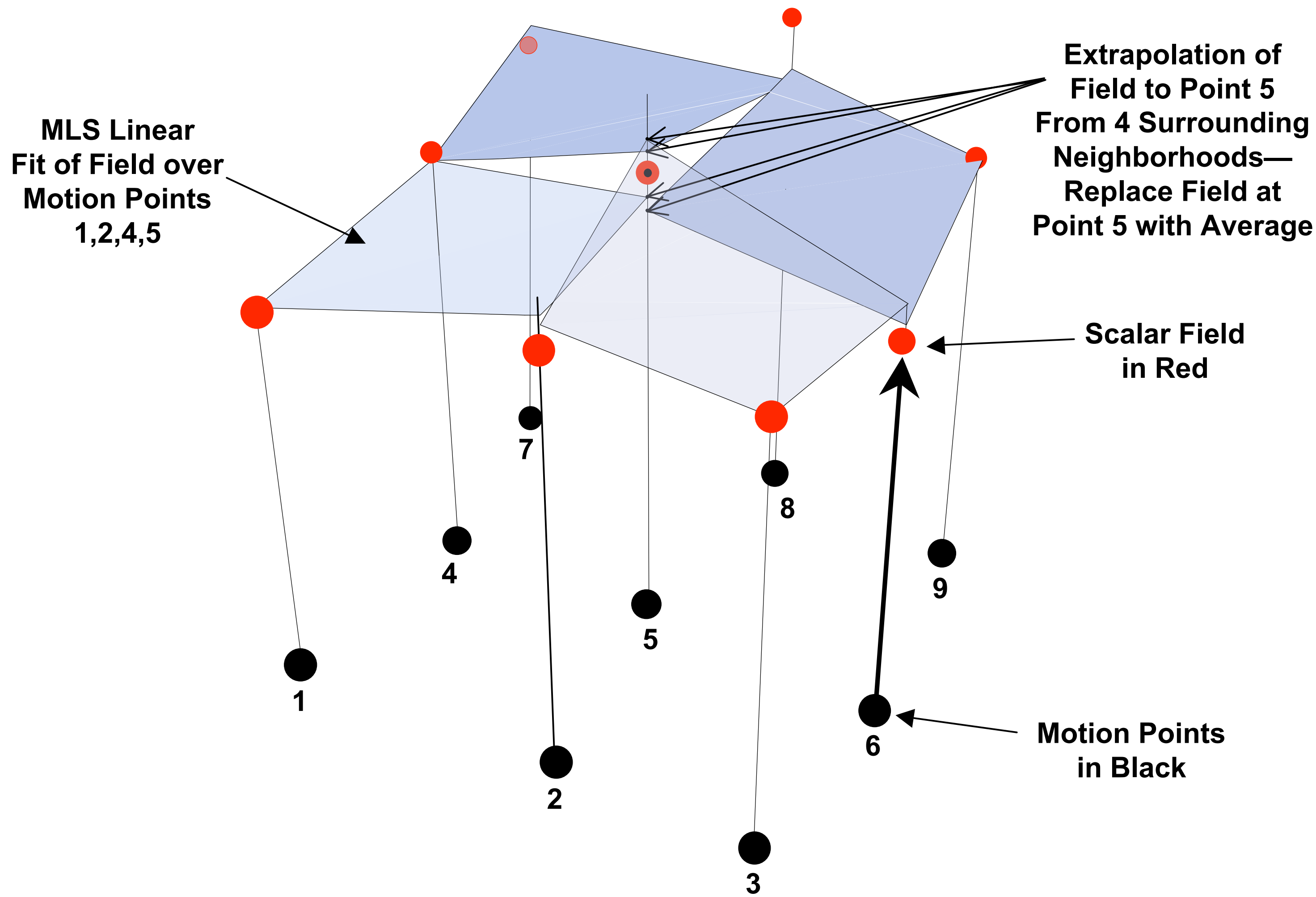
- **<u>Step 3:</u> Impose boundary constraints on residual (symmetry and contact boundary conditions)**

$$\overline{ru}_{j_o} \bullet \bar{N} = 0$$

- **<u>Step 4:</u> Adjust velocity at j_o to remove average variations from a piecewise linear field**

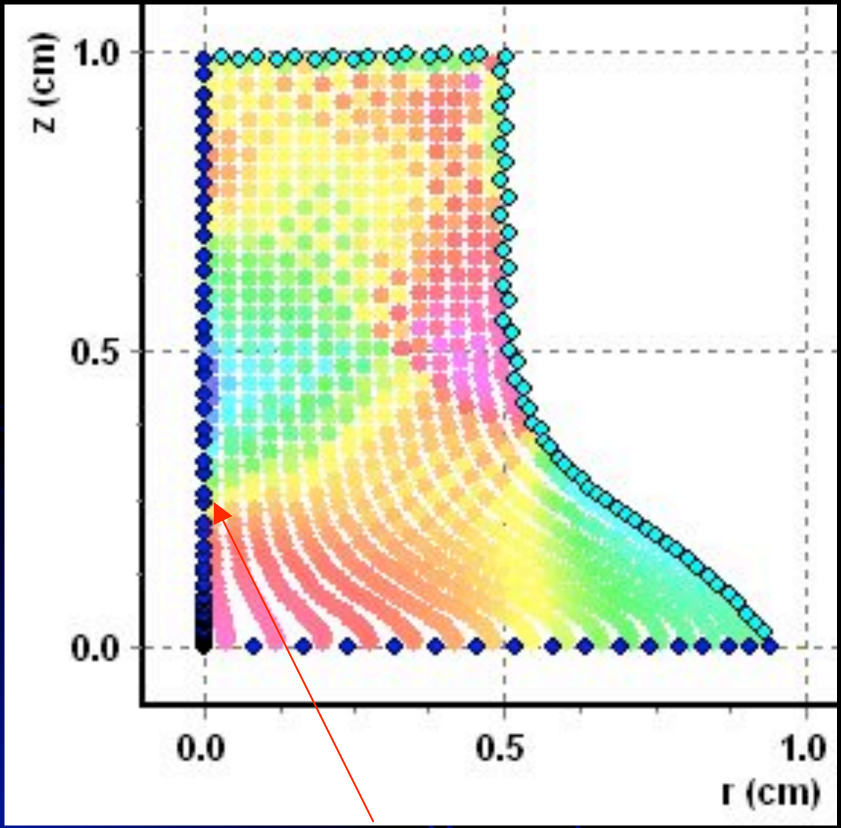
$$\bar{u}_{j_o} \to \bar{u}_{j_o} - \overline{ru}_{j_o}$$

Schematic of Velocity Update

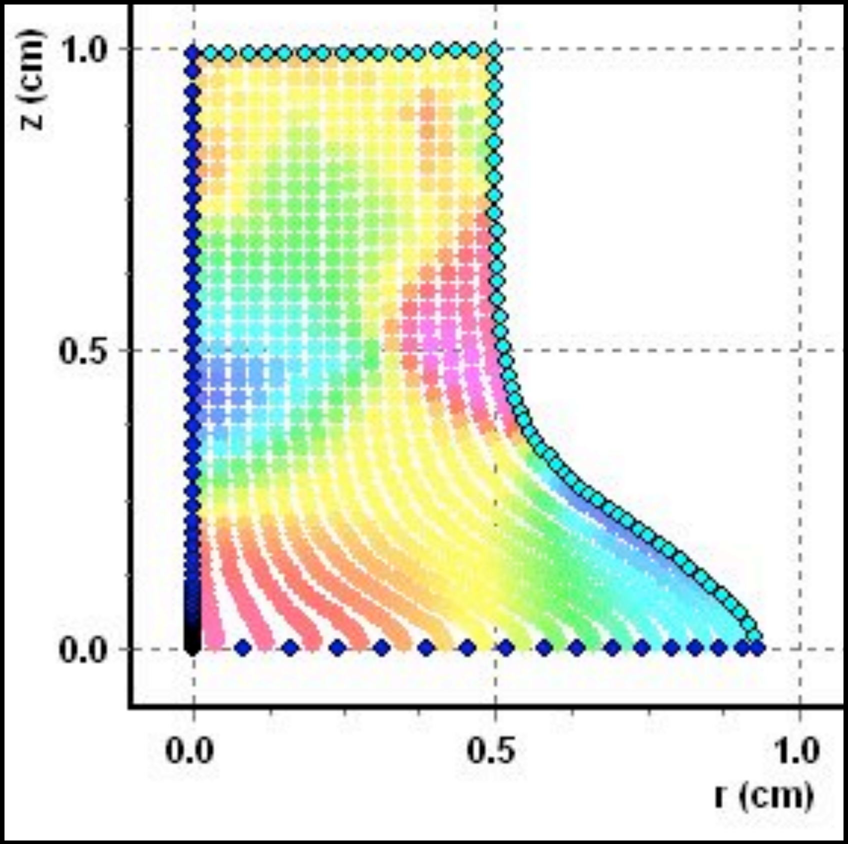


Controlling free modes with VVN

Move with own velocity.



Move with normalized (VVN) velocity.



Pairing

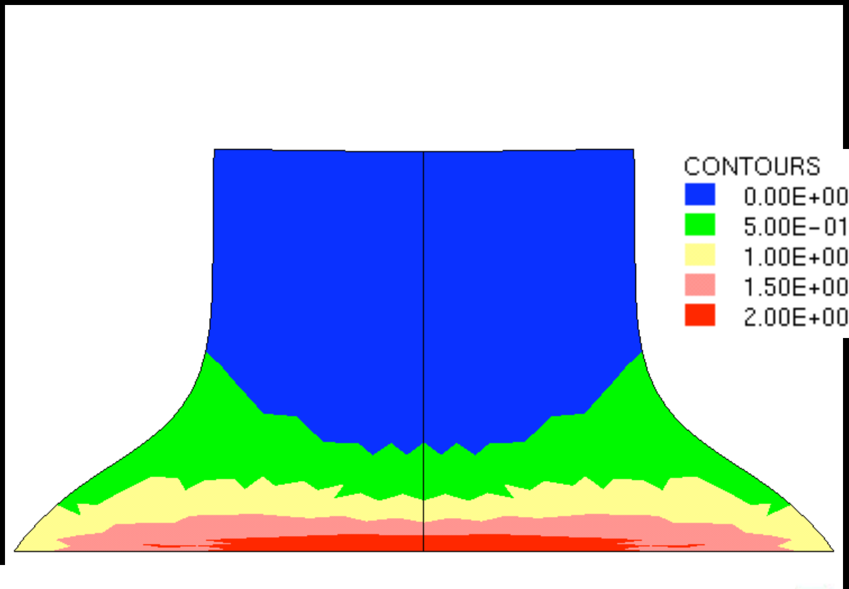
DPD for 3D Solids

- Smoothness of field hard to match with competing methods
  - No sign of tensile instabilities or checker-boarding.
  - Extreme deformations compared to competing Lagrangian solid schemes.
  - No advection of sensitive material properties.

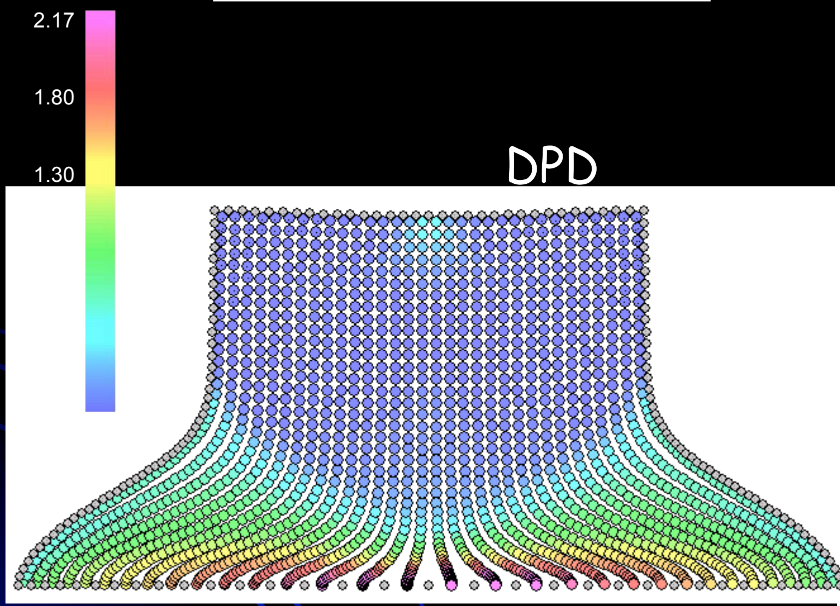
Taylor Anvil: Code Comparisons

Steel at 300 m/s, Elastic - perfectly plastic, 2D Axi-symmetric coordinates. Color contours on plastic strain.

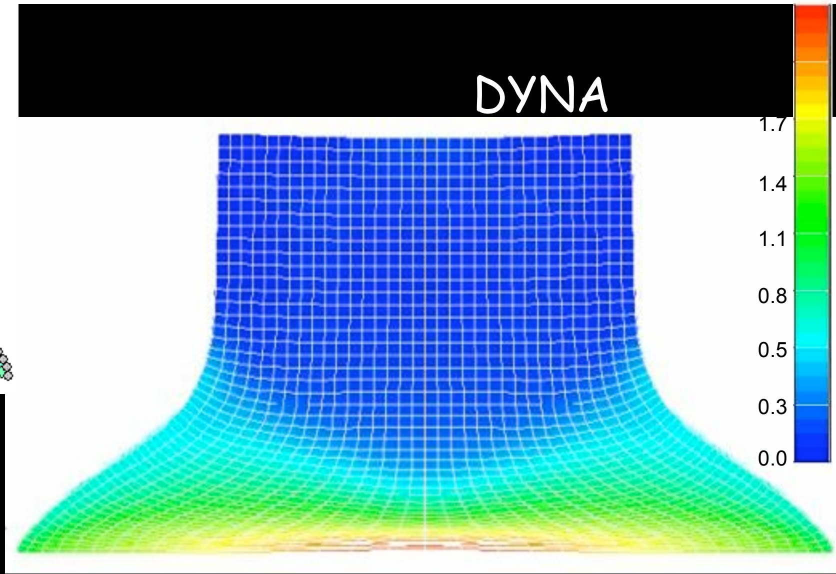
EPIC



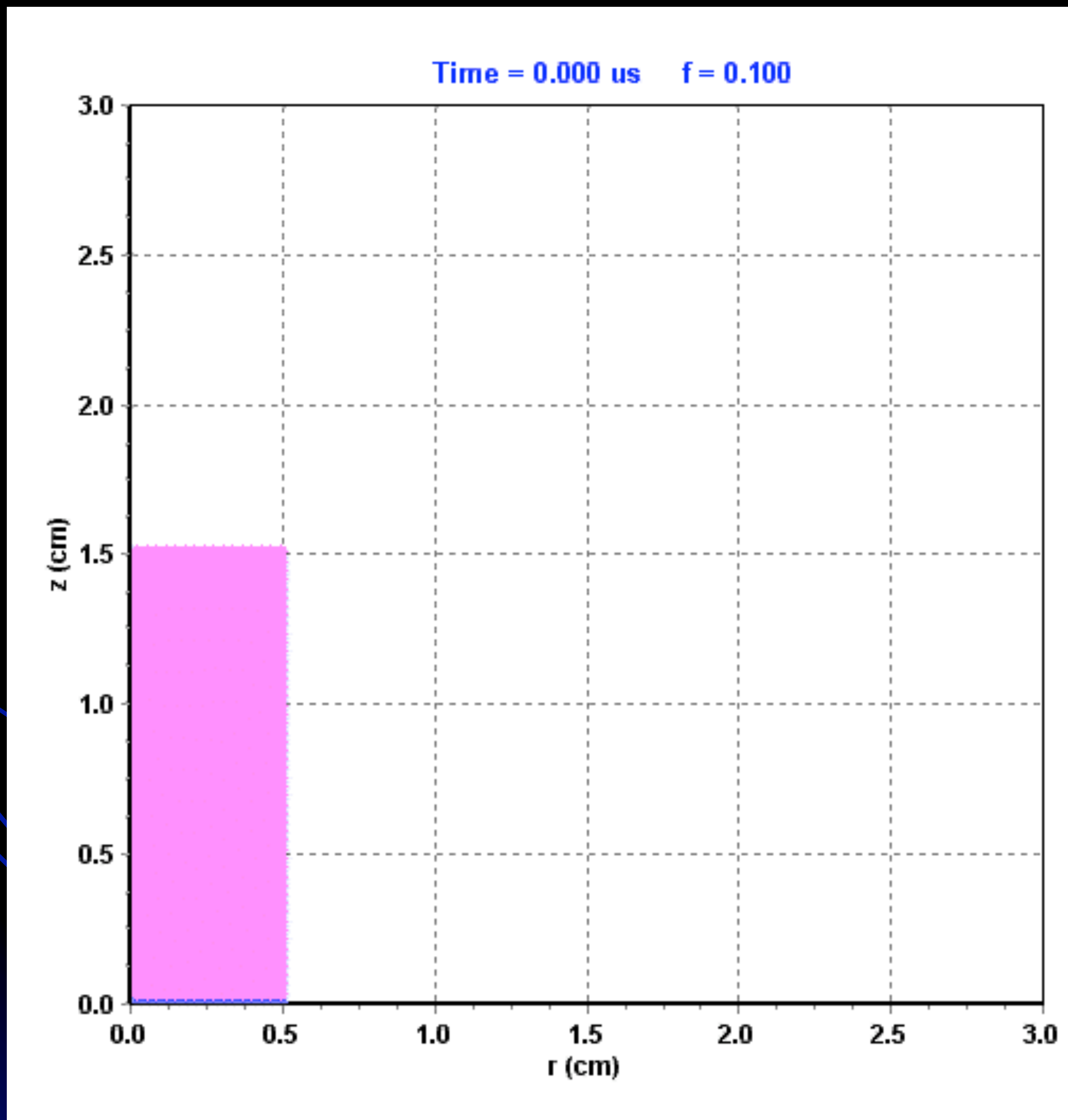
DPD



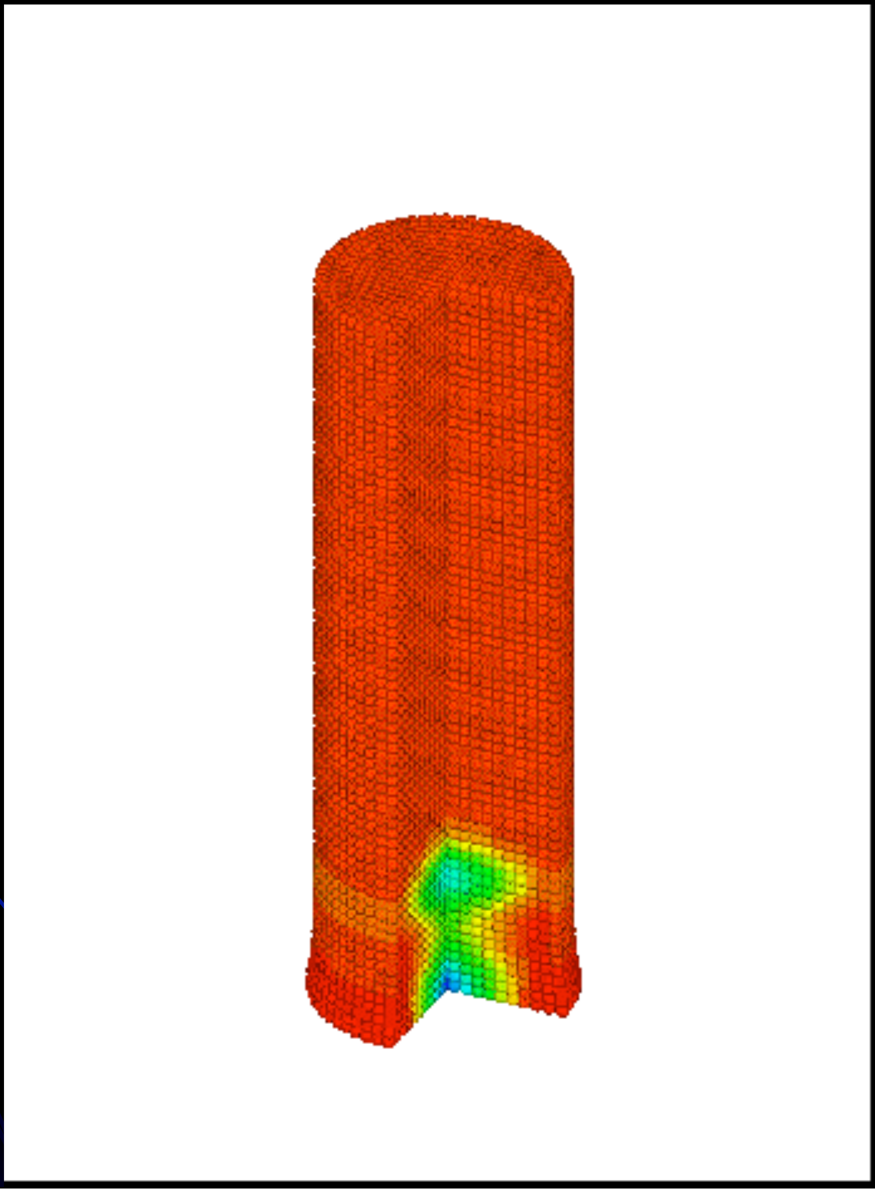
DYNA



Very Fast Anvil (1km/s)

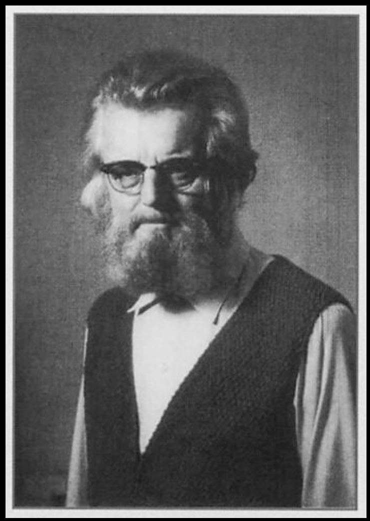


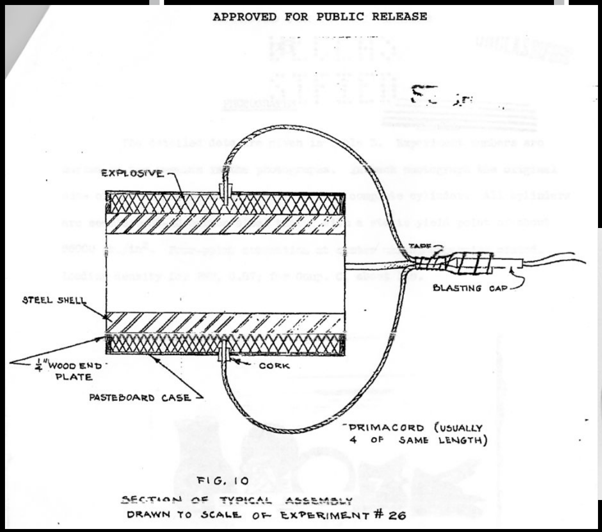
Taylor Anvil



An implosion problem

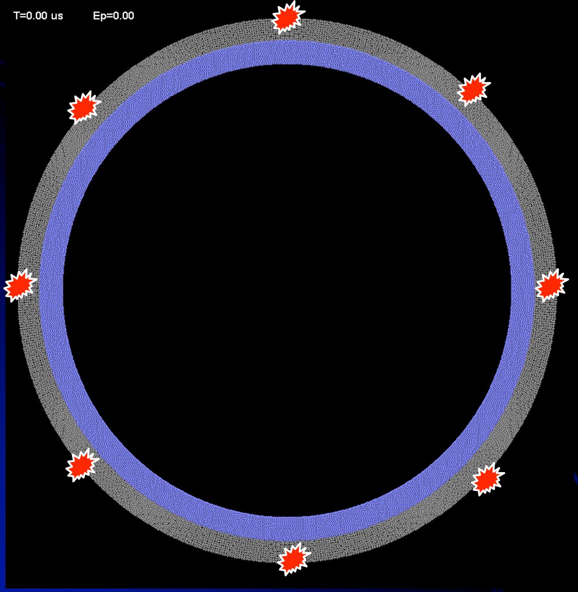
Seth Neddermeyer



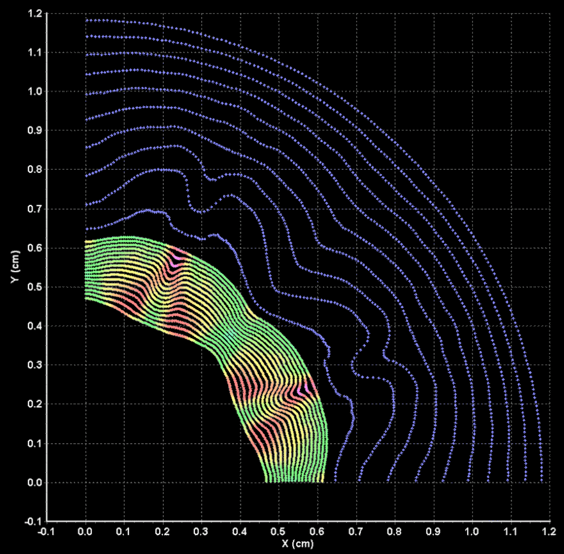


Result of implosion test

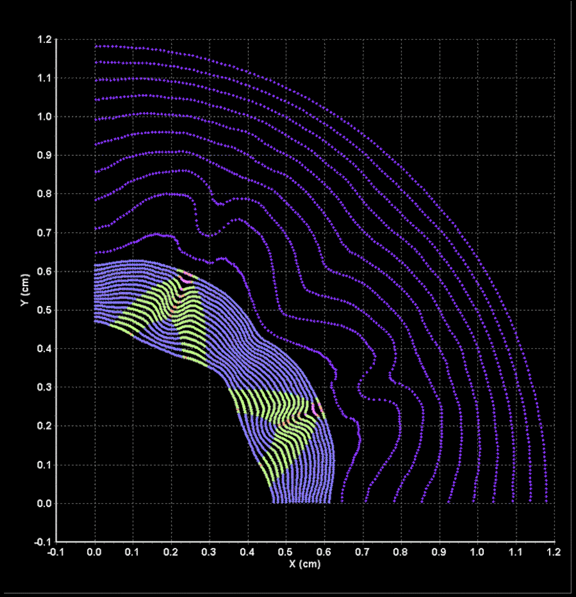
Setup (8 det pts). Gray is HE, Blue is steel.

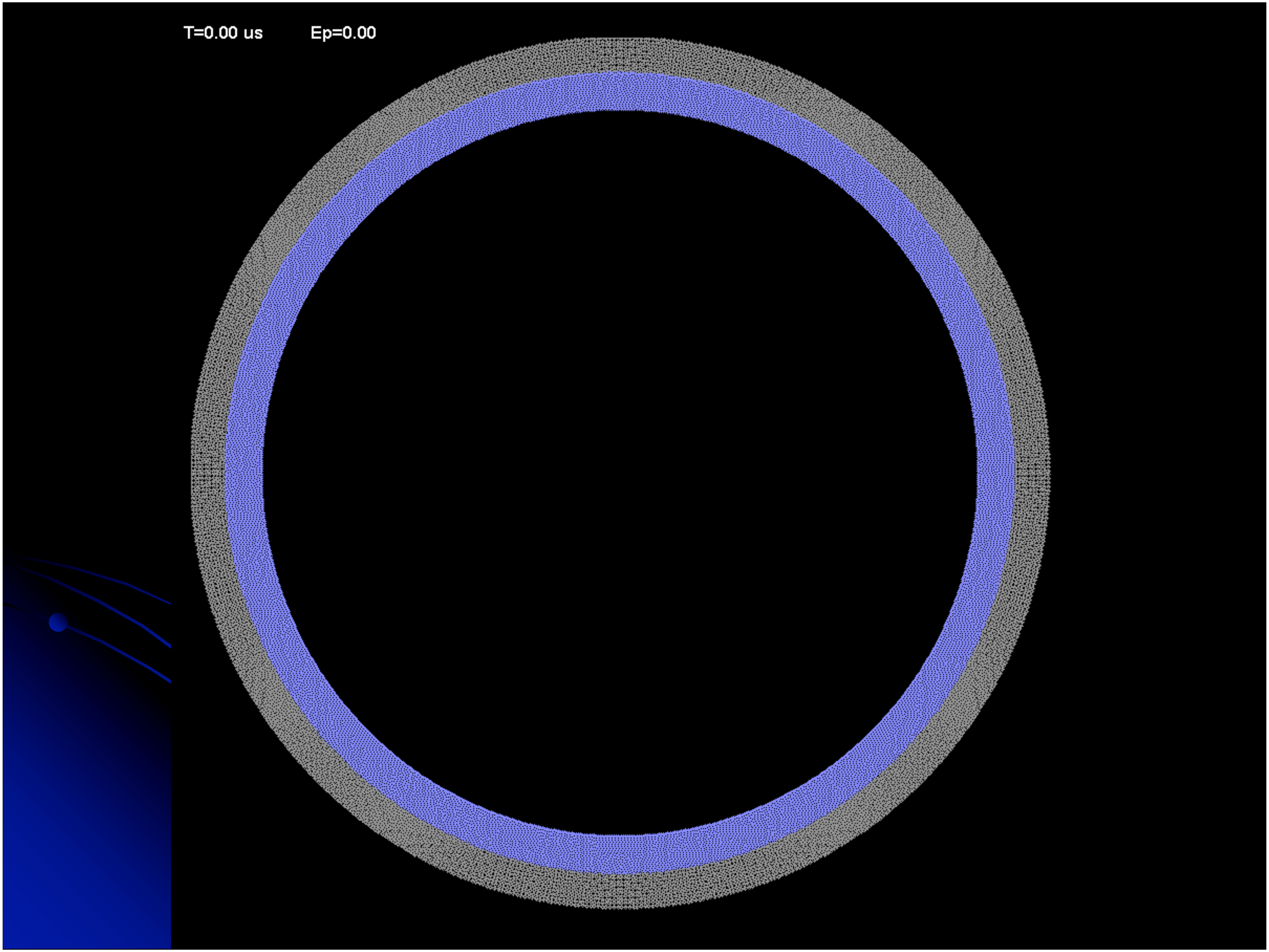


Plastic Strain

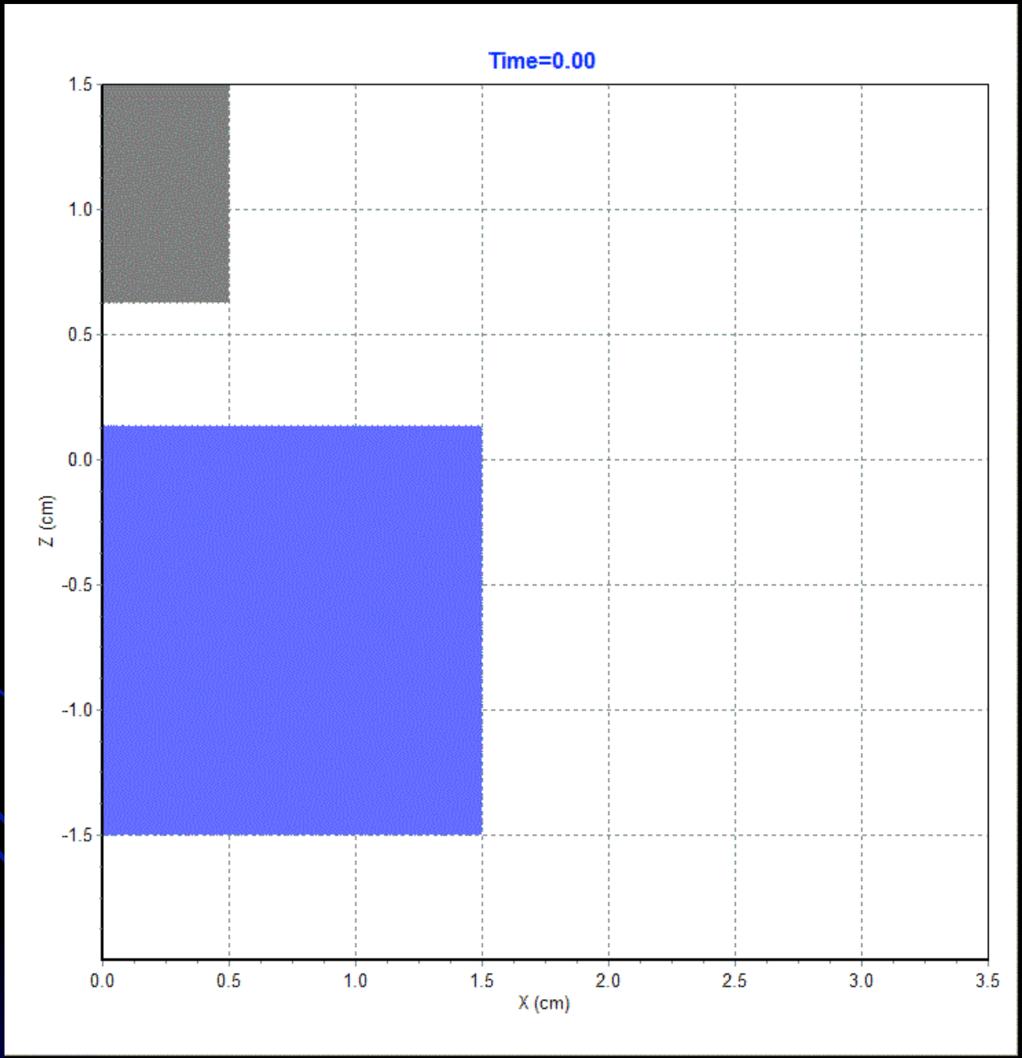


Numbers of neighbors automatically increase in region of plastic strain localization for stability.

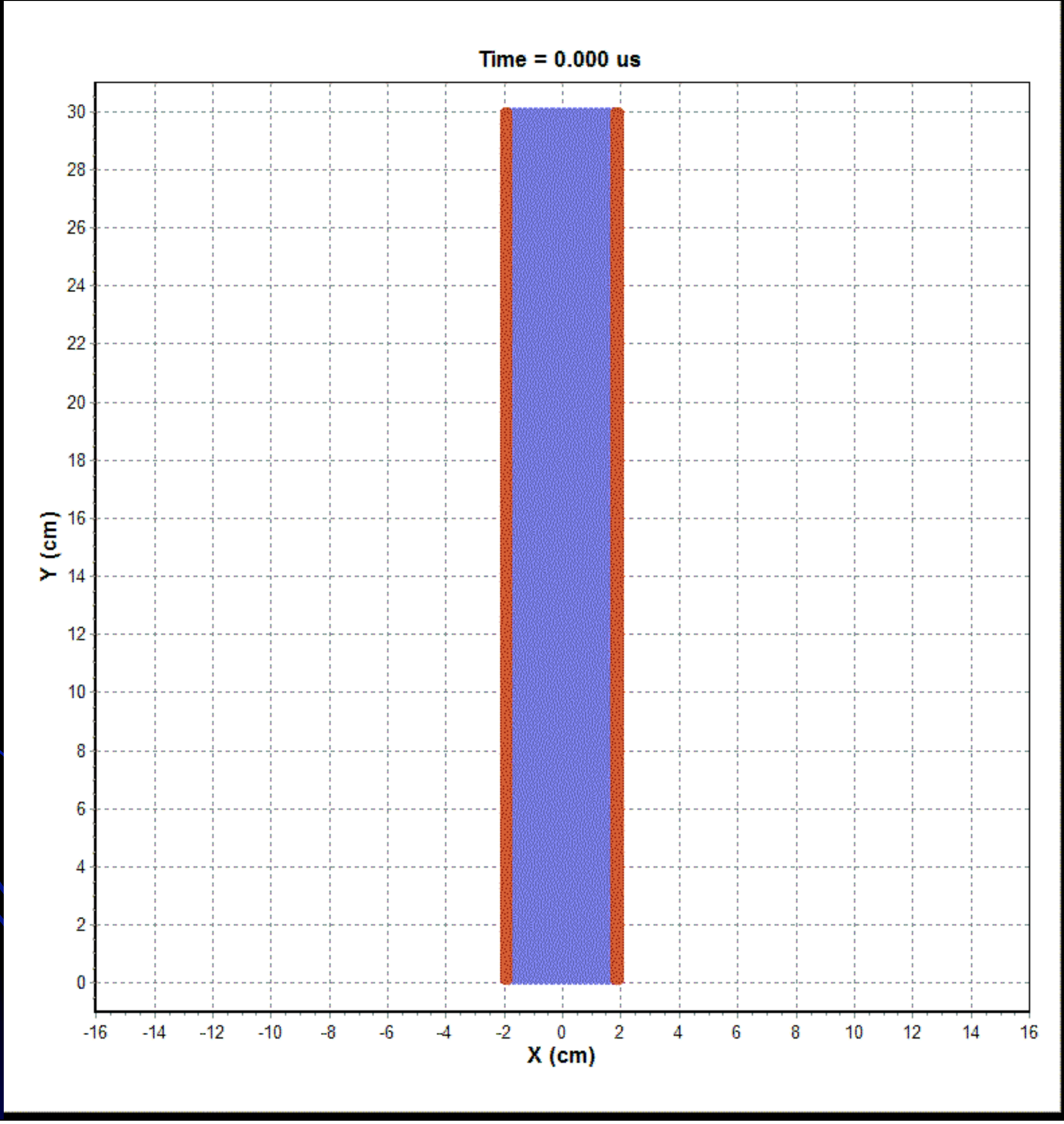



T=0.00 us
Ep=0.00

DPD with contact



DPD: Cylinder test

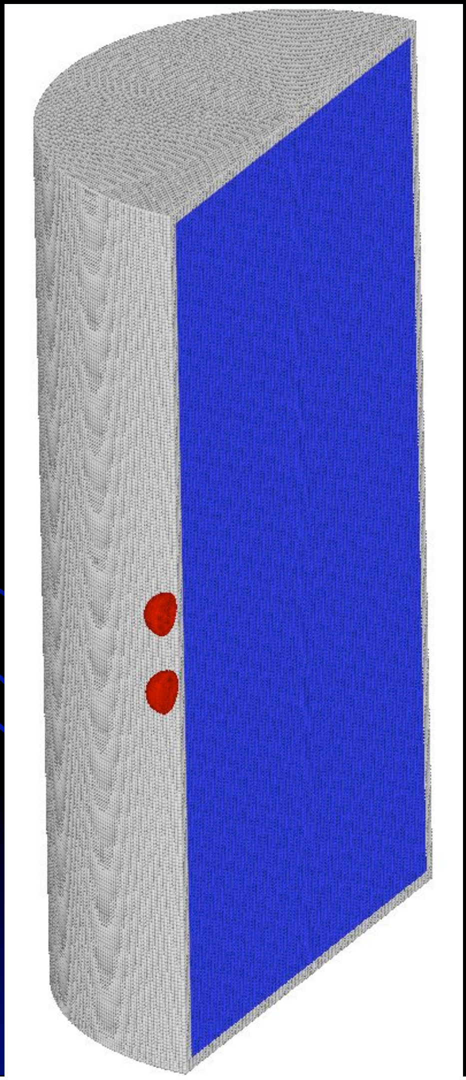


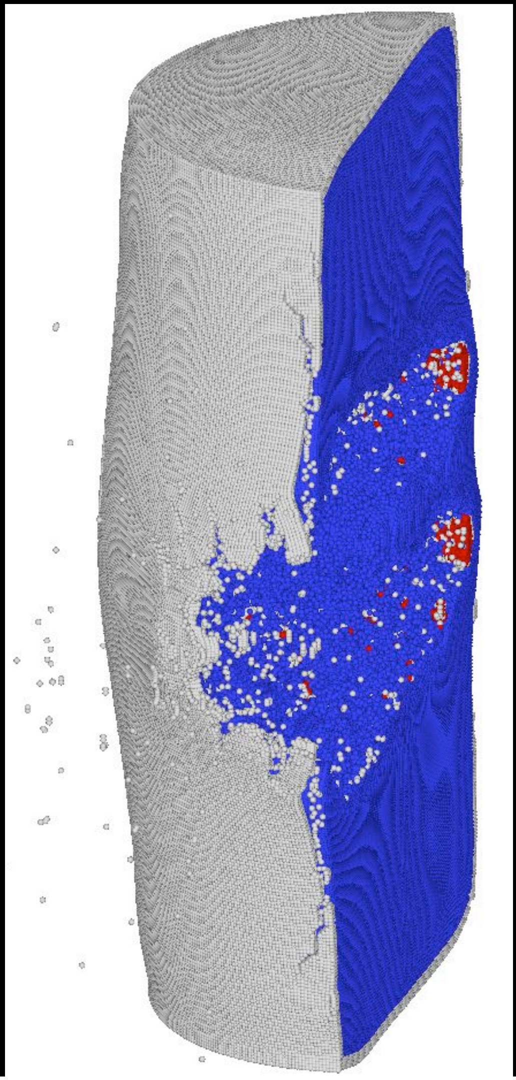
SPH Simulations

- Traditional SPH more suited to large scale fragmentation.
- Easy to generate new surfaces.
- Care must be taken in tension.

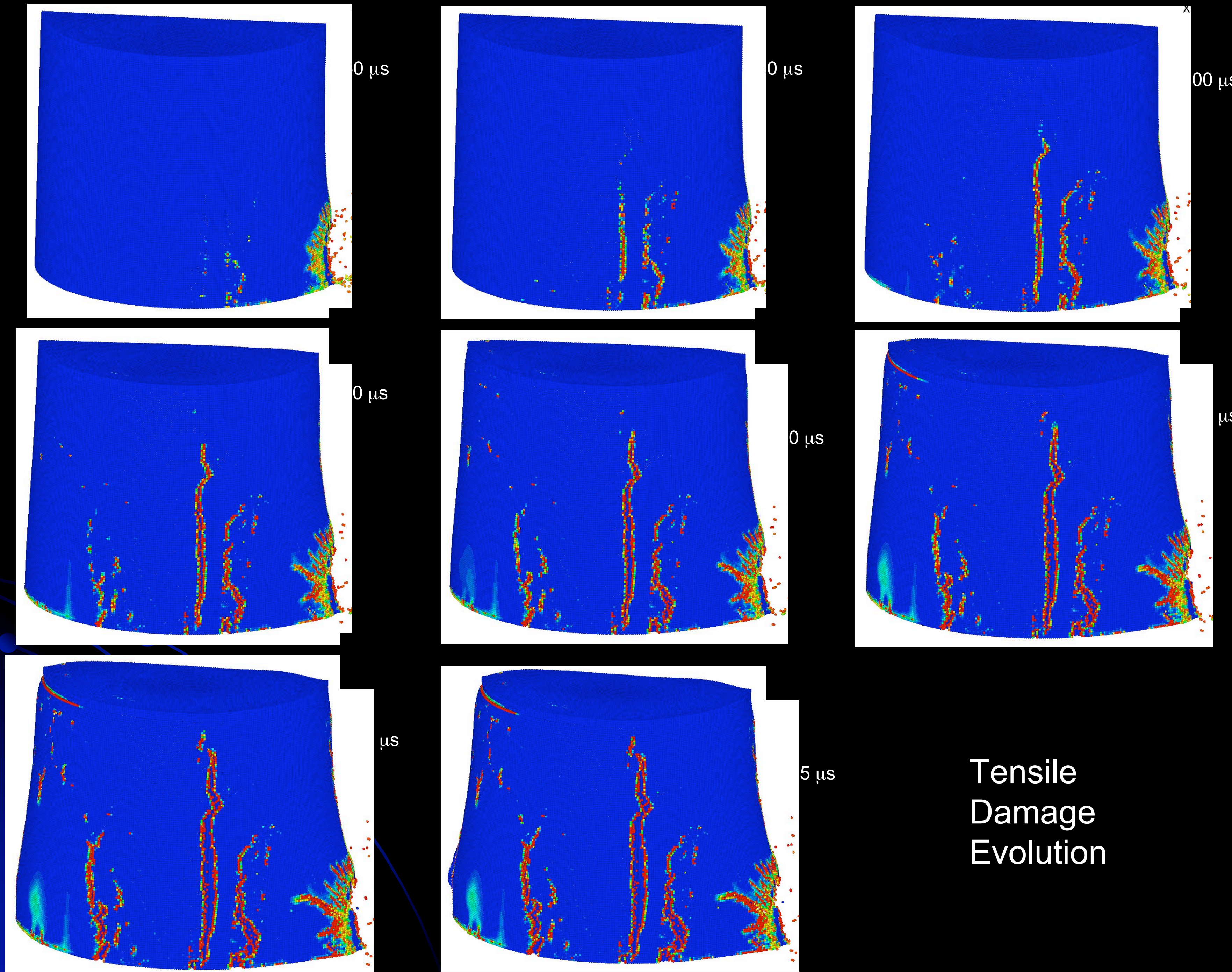
SPH HRam

Time=0





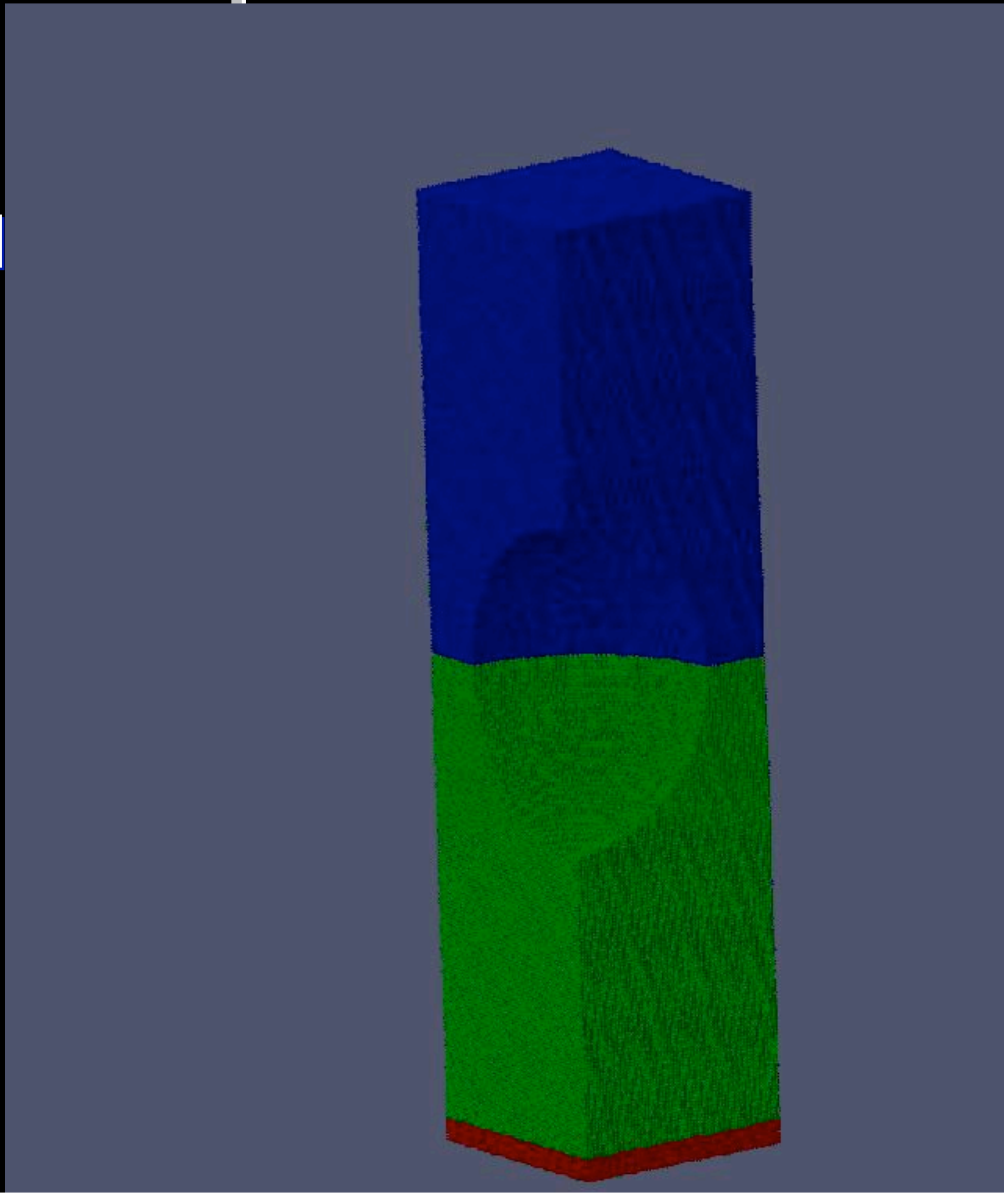
Time=200 μs



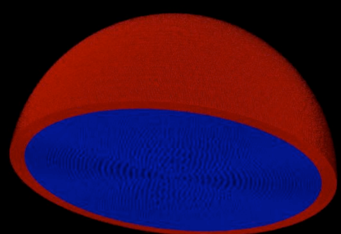
Tensile
Damage
Evolution

Void Collapse

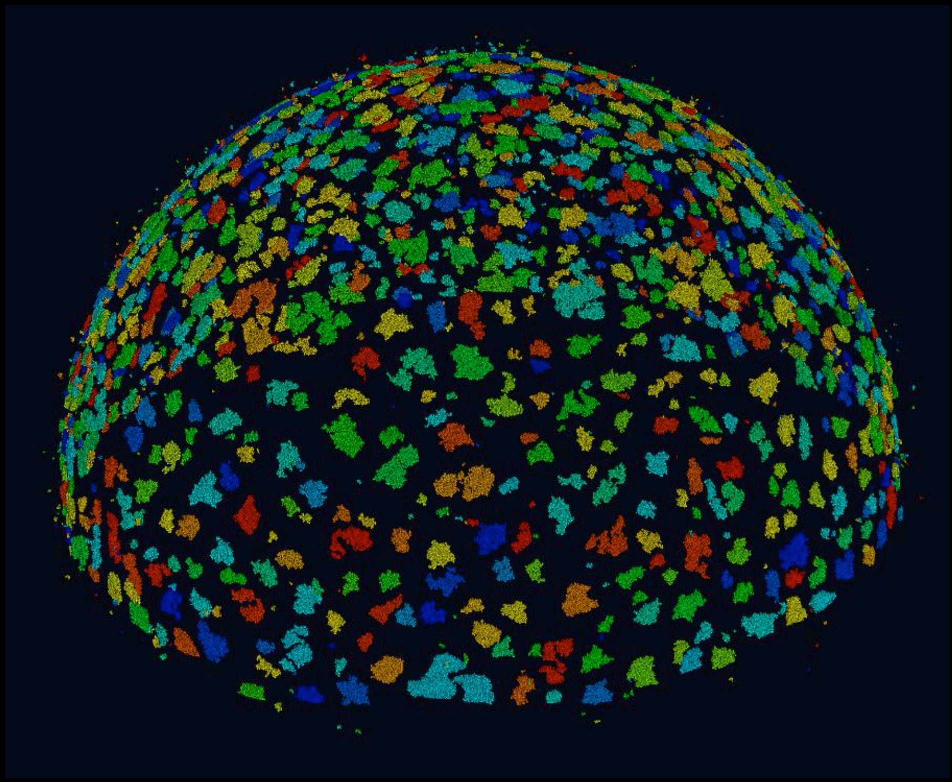
- Represents class of high energy solid-fluid transition problems.
- Large deformations, large gradients.



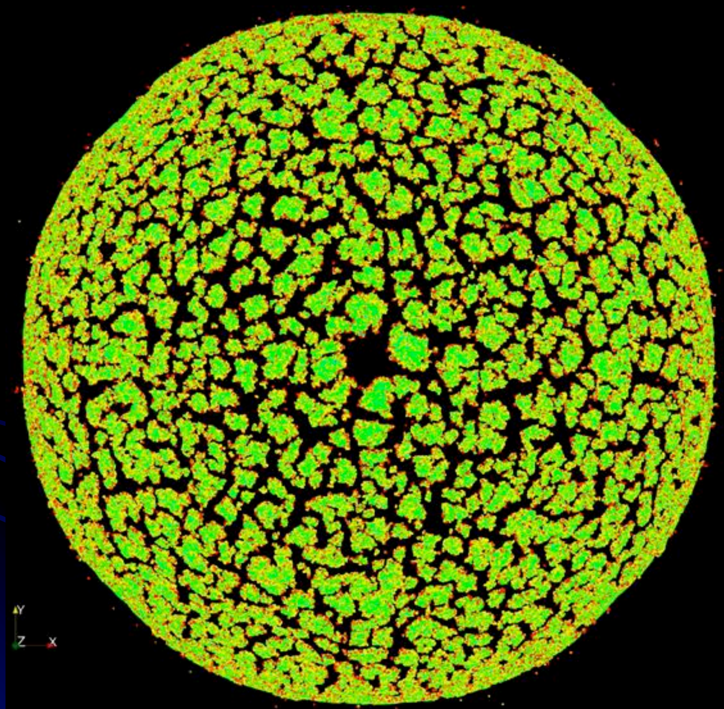
Explosively Driven Fragmentation



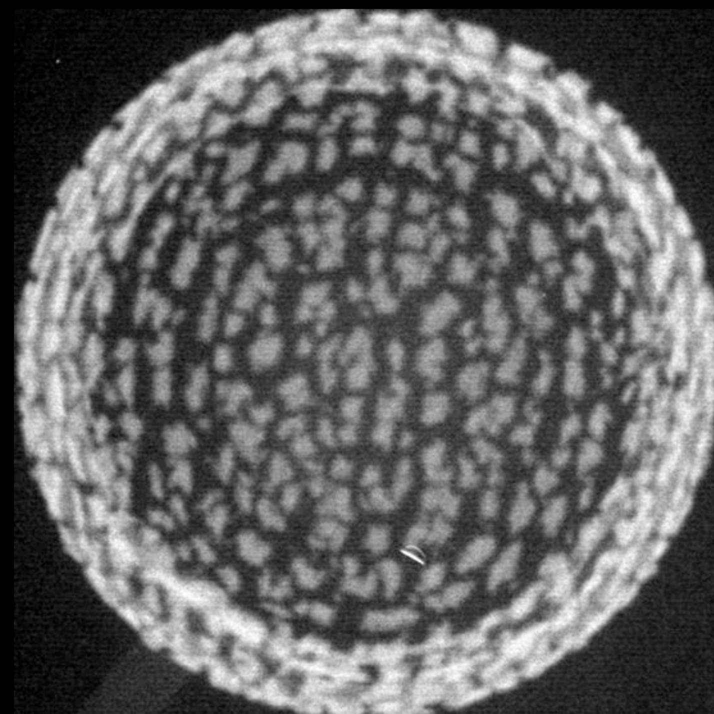
SPH simulated 40 mm x 2 mm 4340 Steel Hemi with PBX-9501 fill at 30 μs.



LANL 40mm x 2mm 4340 steel

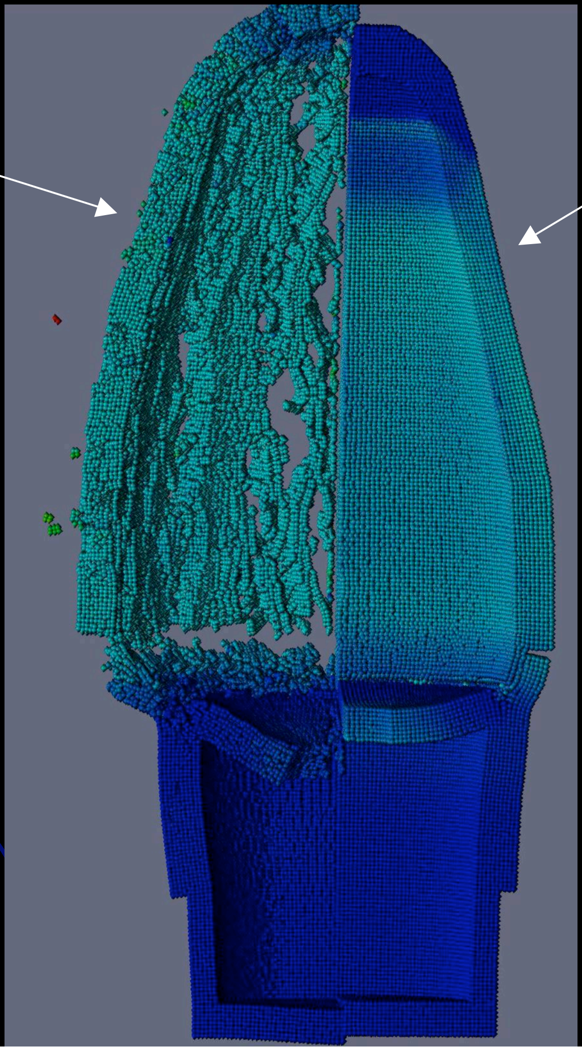


SPH simulated Hemi at t=20 μs.

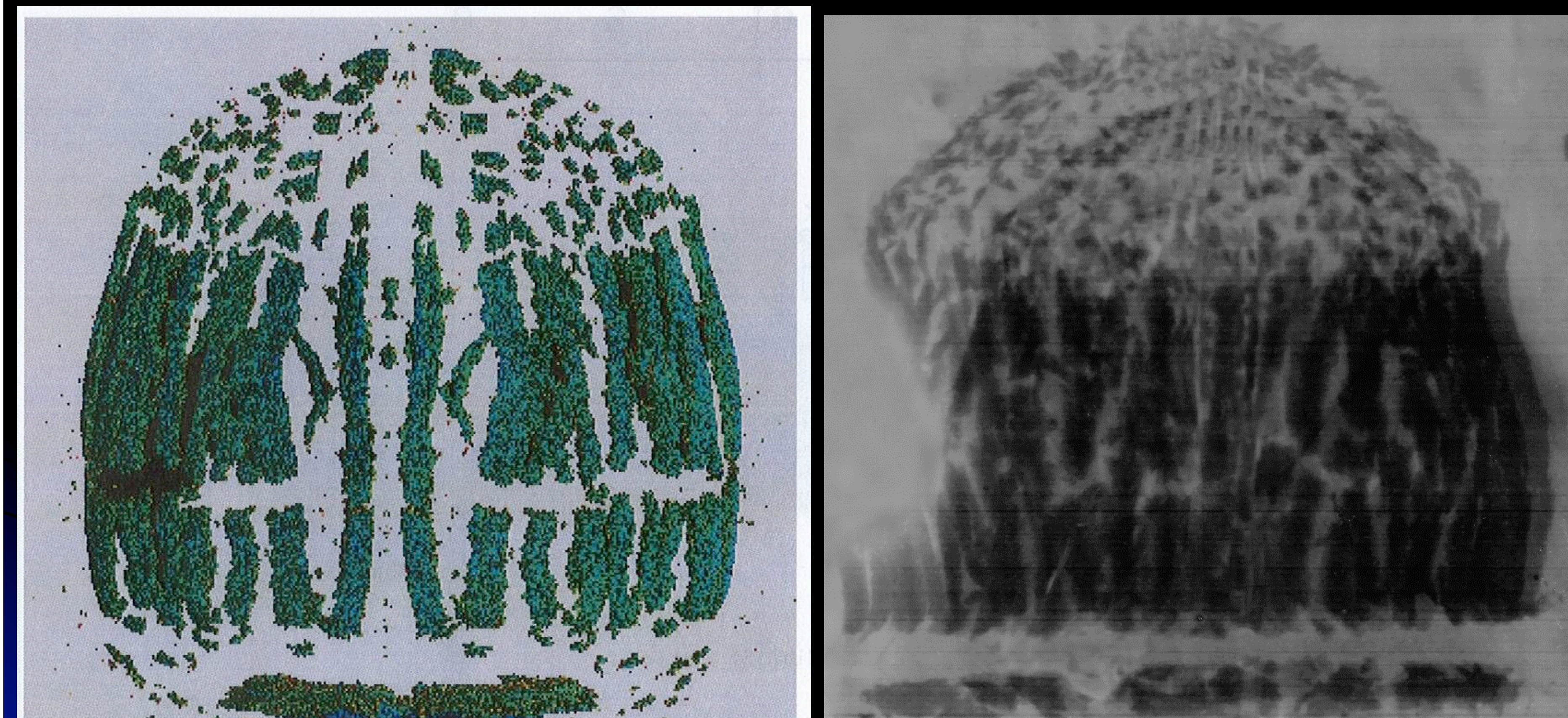


Radiograph (H3187, DX-2) at t=20 μs.

With numerical techniques there are no magic bullets



But with care



MAGI: Smoothed Particle Hydrodynamics

RDEC 40 mm Bullet at 45.5 μs

Trends towards Meshfree

- Smoke free
- Sugar free
- Duty free
- Fat free
- Lead free
- Mesh free

Summary

- Mesh-free particle methods can be used effectively to treat extreme loading (large deformation) of material in a Lagrange frame.
- These methods come in a wide variety of formulations (discretization), each having its own desirable and undesirable characteristics.
- SPH has the most extremes of character…good and bad. (e.g., exact local conservation, tensile instabilties.) If one has intimate knowledge of its behavior, it can be used to gain insight into problems other methods are not suitable to address.
- DPD has good stability and accuracy properties, but contact and fragmentation remain to be worked out. Often faster than SPH because a minimal neighbor set is used. Initial 3D results encouraging.

Ongoing work

- Traditional SPH with strength is a robust workhorse – looking at hybrid methods
- For large scale simulations, converting FE to Dual Particles. When surface behaviour dominates (fragmentation), convert Dual Particles to SPH.

Space – What is it?

Space is not a conception which has been derived from outward experiences. For, in order that certain sensations may relate to something without me (that is, to something which occupies a different part of space from that in which I am); in like manner, in order that I may represent them not merely as without, of, and near to each other, but also in separate places, the representation of space must already exist as a foundation. Consequently, the representation of space cannot be borrowed from the relations of external phenomena through experience; but, on the contrary, this external experience is itself only possible through the said antecedent representation.

Immanuel Kant

Space is blue and birds fly through it.

Werner Heisenberg

"You know, Sid, I really like bananas . . . I mean, I know that's not profound or nothin' . . . Heck! We ALL do . . . But for me, I think it goes much more beyond that."