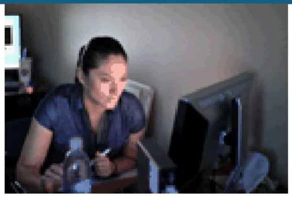
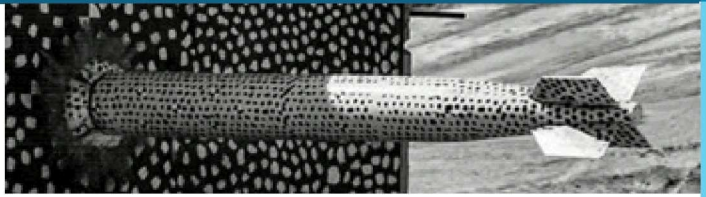
SAND2020-6667PE

LDRD Directors Challenge Review

An Adaptive and Scalable Meshfree Framework for Extreme Deformation and Failure in Solids

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FY20

Mission need

Provide solid mechanics analysts with a Lagrangian method for simulating problems with very large deformation and complex multi-physics

- High velocity impact (~100 – 3000 m/s)
- Impact into soft targets
- Localized melting coupled with mechanical insult

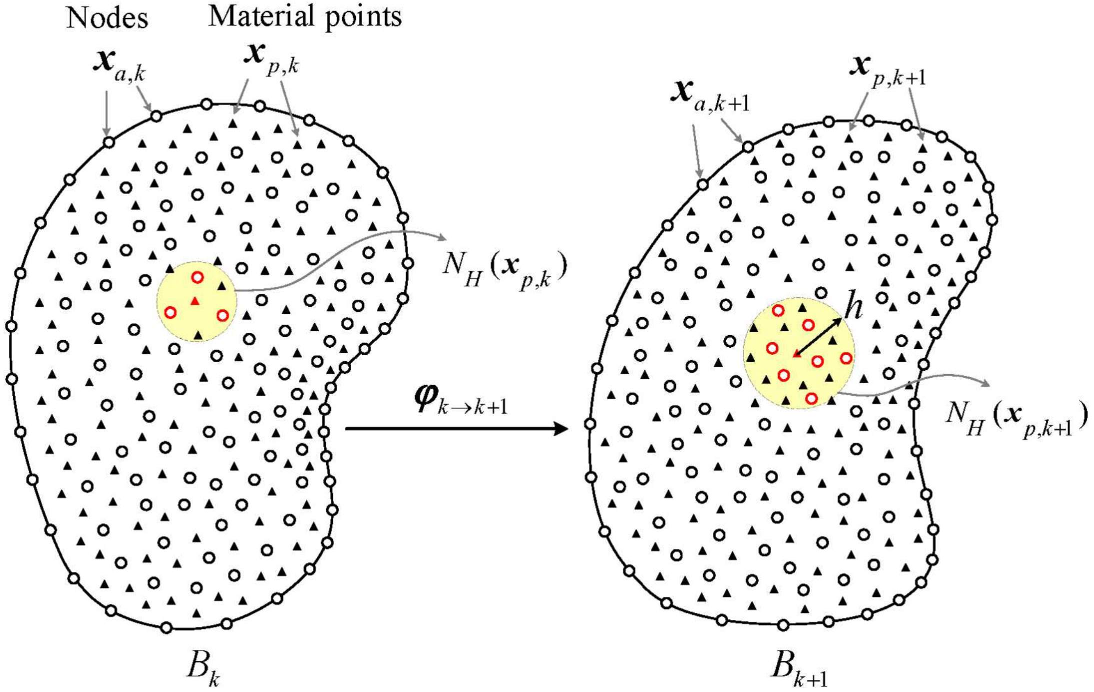
	Eulerian hydrocodes	Lagrangian finite element methods	Lagrangian mesh-free methods
Pros:	Good robustness	Preserve material point identities Unambiguous surface definition	Better smoothness than finite elements. Reconnection easier with no element topology constraints.
Cons:	Smearing of history variables. Difficult to model surface physics (e.g. contact, FSI)	Lack of robustness due to mesh tangling; Reconnection helps (e.g. LGR)	Fixed node & material point set may be insufficient to guarantee accuracy and robustness

Technical approach

New mesh-free adaptivity scheme: **node/point injection within the Optimal Transportation Meshfree (OTM) method**

OTM[1] provides

- Geometrically **exact** updated Lagrangian kinematics
- Exact **conservation** of linear momentum and angular momentum
- **Compatibility** with many mesh-free interpolation schemes, including RKPM. We used local max-ent.
- A variational **formalism**, shared with finite element methods, that provides strong mathematical guarantees.



Material (quadrature) points are fully Lagrangian

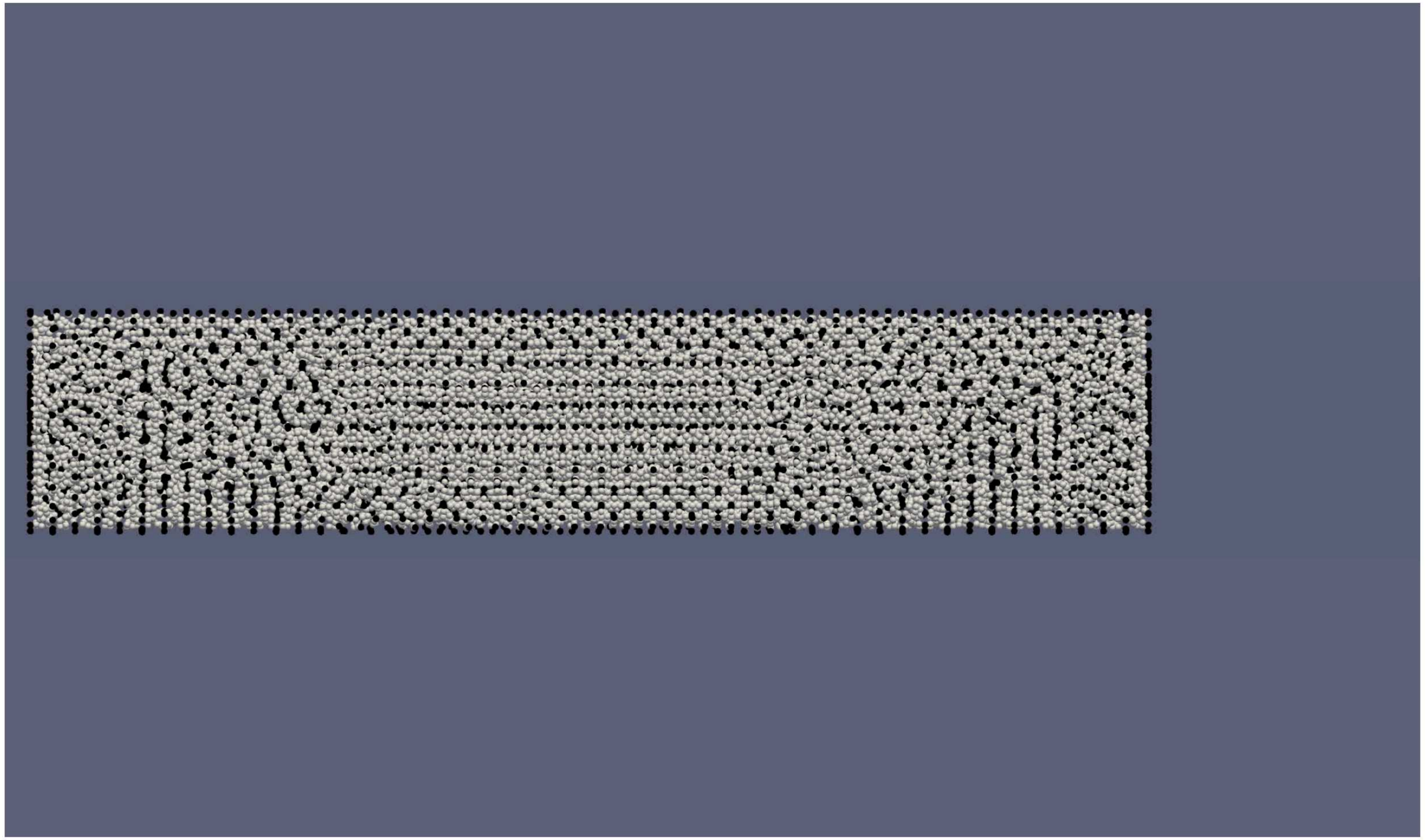
Get reconnection without mapping

$$x_{p,k+1} = \varphi^h_{k\to k+1}(x_{p,k})$$

$$\varphi^h_{k\to k+1}(x) = \sum_a x_{a,k+1} N_{a,k+1}$$

1. Li et al. *Int. J. Numer. Methods Eng.* 2010 (83):1541-1579

OTM: The meshfree Optimal Transportation Method



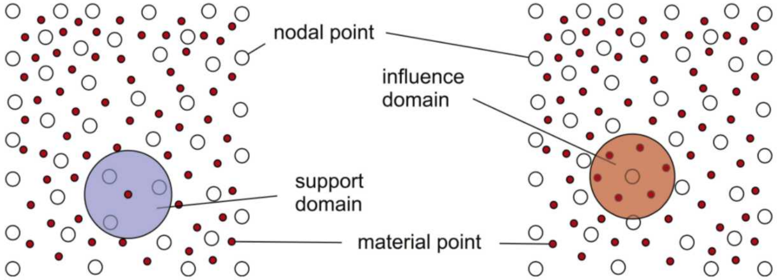
Like FEM, OTM has:

- ● Nodes
- ○ Material Points

Unlike FEM, OTM has no:

- Mesh or Elements

Points have **support** nodes
Nodes have **influence** points



Weißenfels and Wriggers, CMAME, 2017

Adaptivity scheme

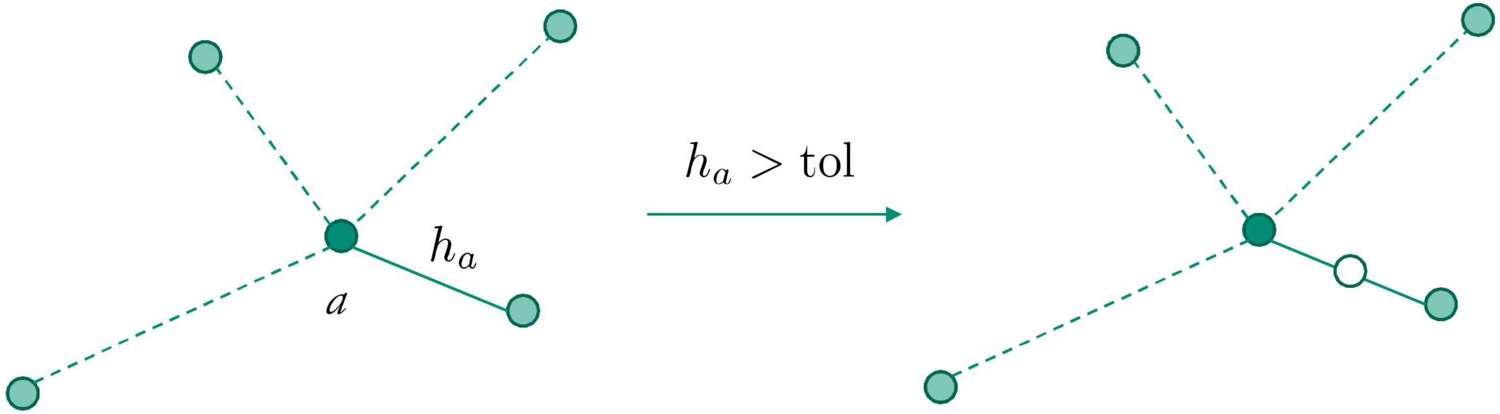
OTM node and point injection

Introduce new nodes and material points on the fly where needed

Existing nodes and material points remain. **No mapping of state variables.**

Do need to interpolate state variables to new material points – we use Lie group interpolation and variational recovery to ensure they stay in their proper manifolds[1]

Initial focus is on capability demonstration. We set a very simple adaptivity metric:



for $a \in$ nodes **do**
  $h_a \leftarrow \min_{b \neq a} |x_a - x_b|$
  if $h_a > \mathrm{tol}$ **then**
    insert node halfway between
    interpolate fields to new node
  end if
end for

- Similar scheme for nodes and material points
- Executed periodically (every N timesteps, say)

[1] Mota et al. *Comp Mech* 2013, 52

Future work on adaptivity metrics

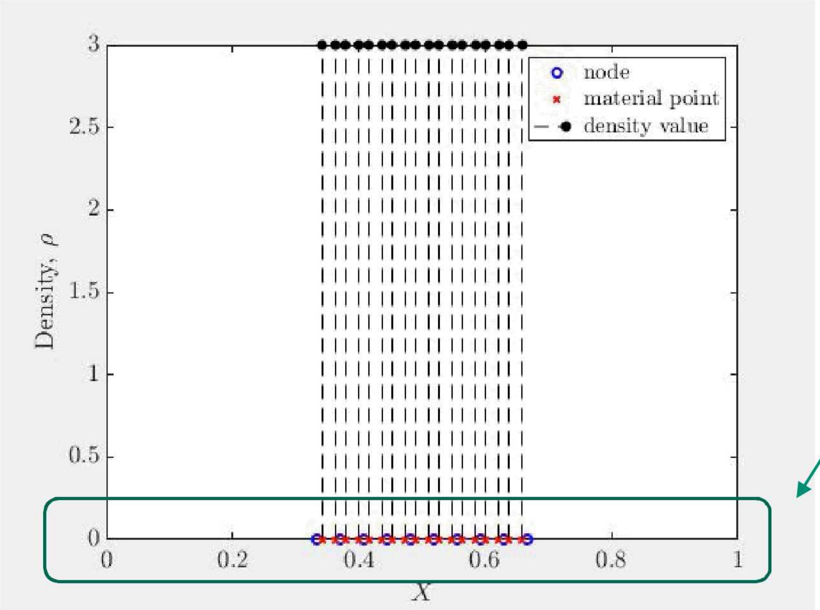
Variational node/point injection

OTM is based on **minimization** of an effective energy functional (true even with history dependence)

Introducing new nodes changes this energy, depending on position. Similar to diffusion of species.

Explore using this analogy to optimize new nodal locations (and choose optimal number of nodes given a cost). Use **physics** of problem to **drive adaptivity** directly.

Use recent OTM treatment of diffusion[1] to drive nodes to **optimal locations** during adaptation step



- Nodes and points initially clustered in center of domain
- Distribute themselves uniformly due to entropy of mixing
- Combining with mechanical energy functional would bias them towards under-resolved features

1. Fedeli et al. *Int J Numer Methods Eng* 2017; 112

LGR: a performance-portable Lagrangian remeshing code toolkit

LGR: Toolkit for Lagrangian Grid Reconnection, Dan Ibañez 1443

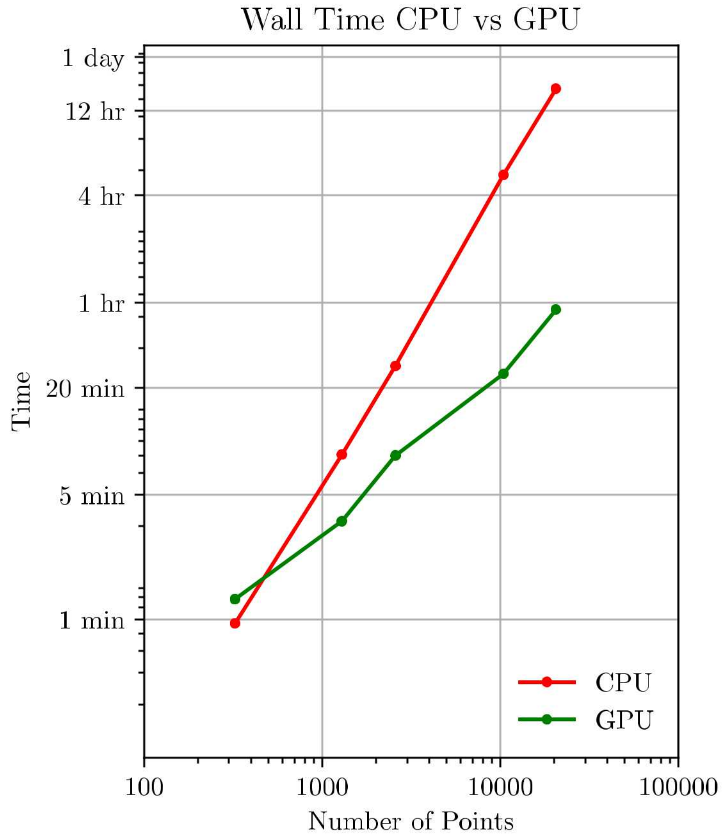
- **Open-source** on Github
- Fundamentally designed from the ground up for **adaptivity**, a key component of our project
- Has minimal dependencies, enabling **rapid prototyping of ideas** and quick build-test turnaround times

LGR on NVIDIA GPUs

- **Performance portability** based on raw CUDA code, Thrust library, and C++14 **standard** constructs
- **Interoperable** with other CUDA-enabled libraries (Kokkos, ArborX…)
- Data access patterns designed for **fast access** and **minimal data race conditions** on threaded architectures

Our team

- Gained valuable experience **developing portable algorithms and testing complex code** for correctness and performance on both the CPU and GPU **without any algorithm duplication**
- Found that OTM methodologies are amenable to **performance on GPU architectures**—further exploration and optimization required!
- Utilization of GPU for our code is **above 90%** most of the time.



github.com/SNLComputation/lgrtk

ArborX: enabling geometric search algorithms in LGR

Geometric search

- is at the core of meshfree methods to establish node/point relationships (akin to connectivities in FEM)
- has broader applicability, e.g., in **contact algorithms**

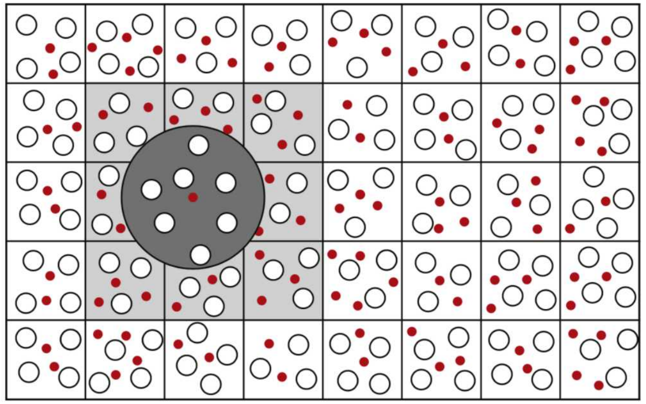


Fig. 4. Subdivision of the domain into static cells.

ArborX: an open-source library designed to provide performance portable algorithms for geometric search

- Hosted on Github
- Based on Kokkos and Thrust libraries to deliver performance on both CPU and GPU architectures
- Currently under investigation in other Sandia apps (ATDM and IC: Sierra, NimbleSM…)

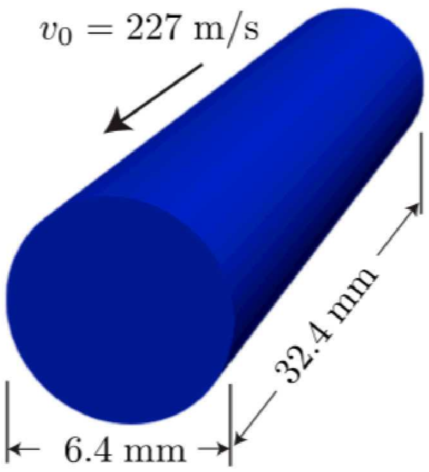
We developed a **reusable, performance-portable search library interface** for LGR

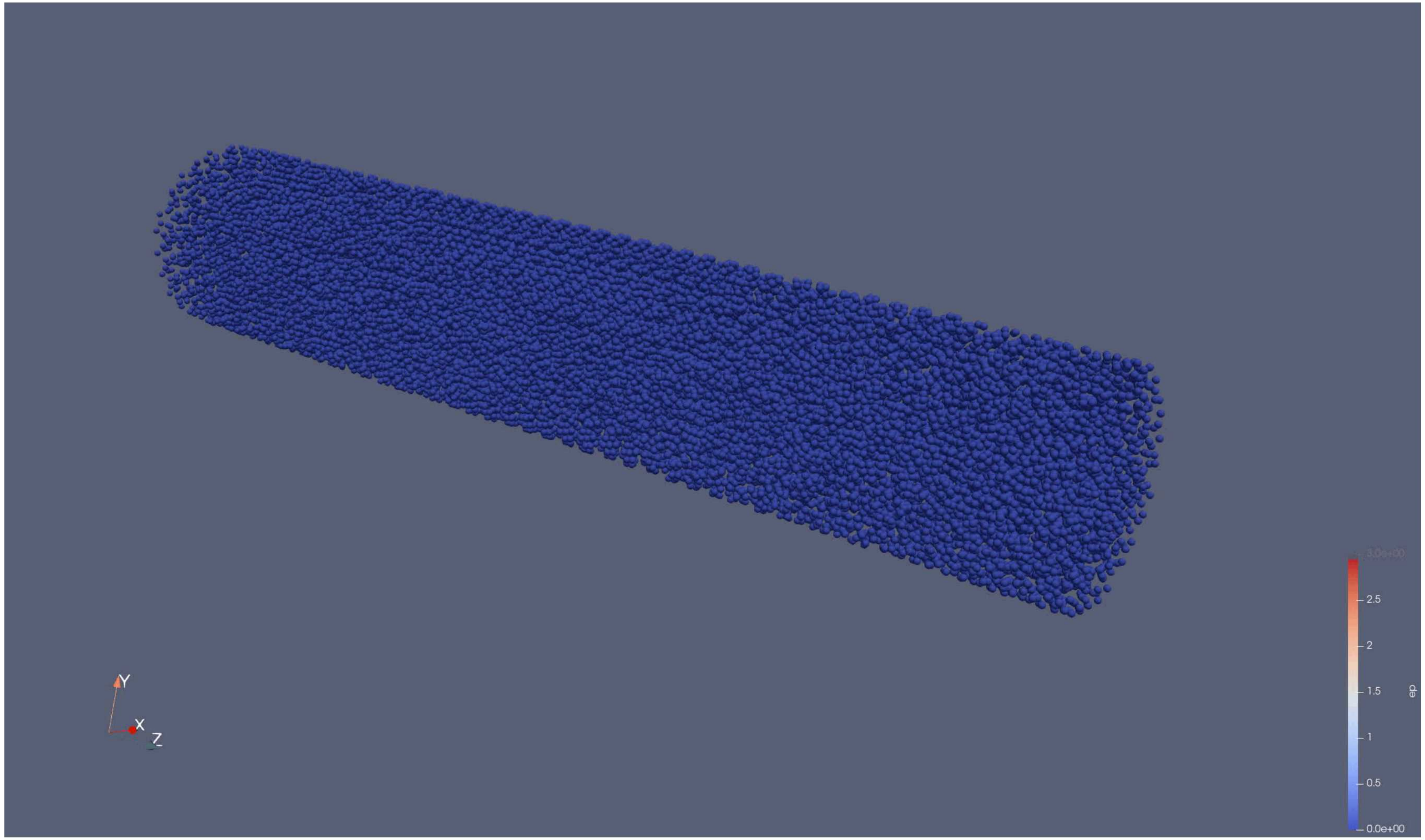
github.com/arborx/ArborX

Weißenfels and Wriggers, CMAME, 2017

Taylor Bar with OTM running on LGR v3 on the GPU

Copper Taylor bar of length 32.4 mm and diameter 6.4 mm impacting a rigid wall with an initial velocity of 227 m/s. Common example for testing numerical methods for large deformation (Li, Habbal & Ortiz 2010).





Taylor Bar with OTM running on LGR v3 on the GPU

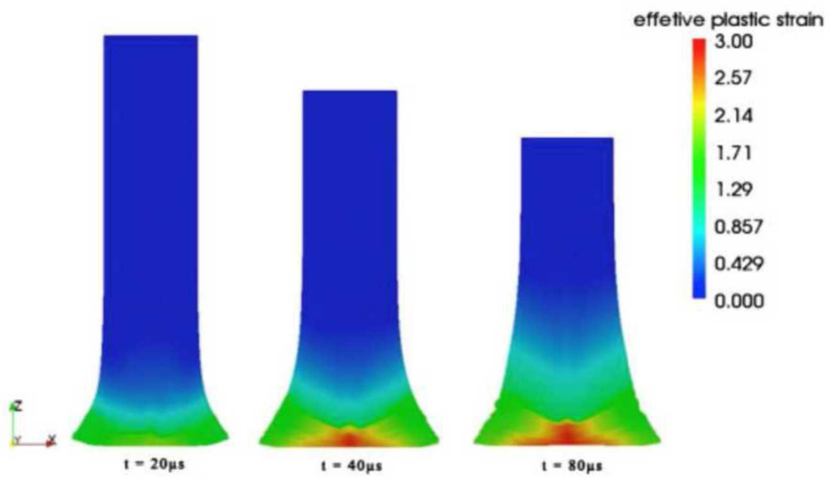
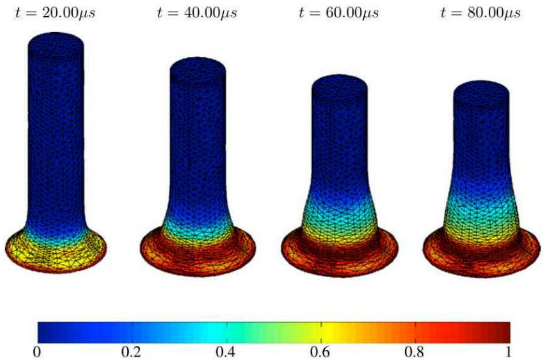
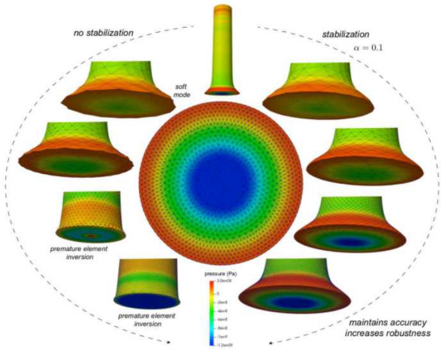


Figure 14. Taylor-anvil impact test of copper specimen at 227 m/s impact velocity. Distributions of effective plastic strain at 20, 40 and 80 µs.

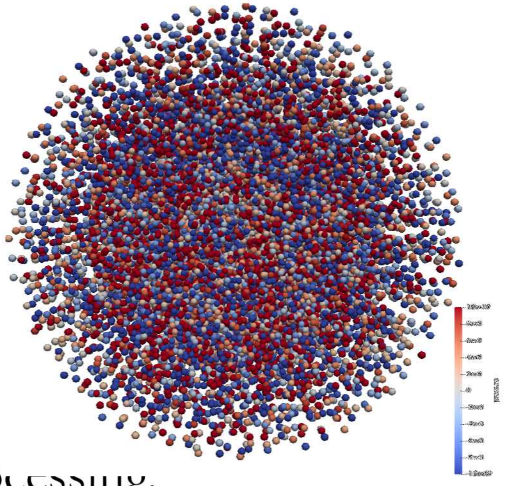
Li, Habbal & Ortiz (2010) eqps results
t = 20us, 40us, 80us
5174 nodes, 26741 points
They look very smooth.
Postprocessed from point data?

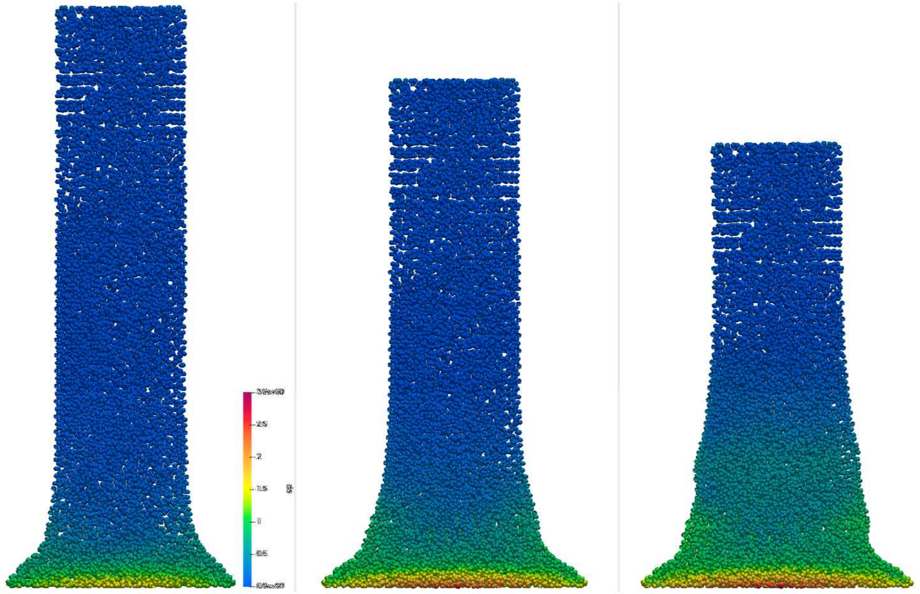


Aguirre et al., JCP, 2014



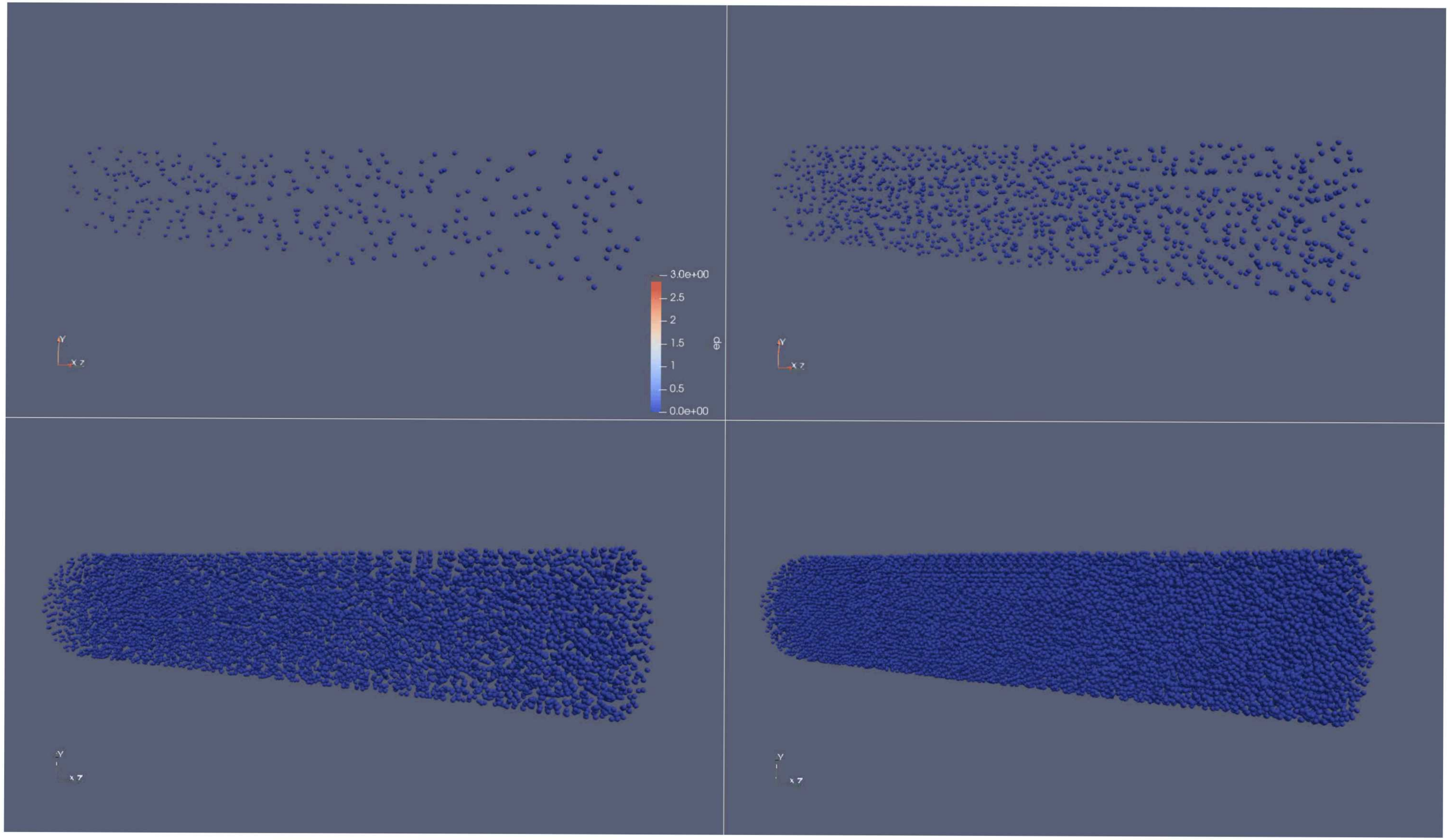
Foulk et al., IJNME, 2020?





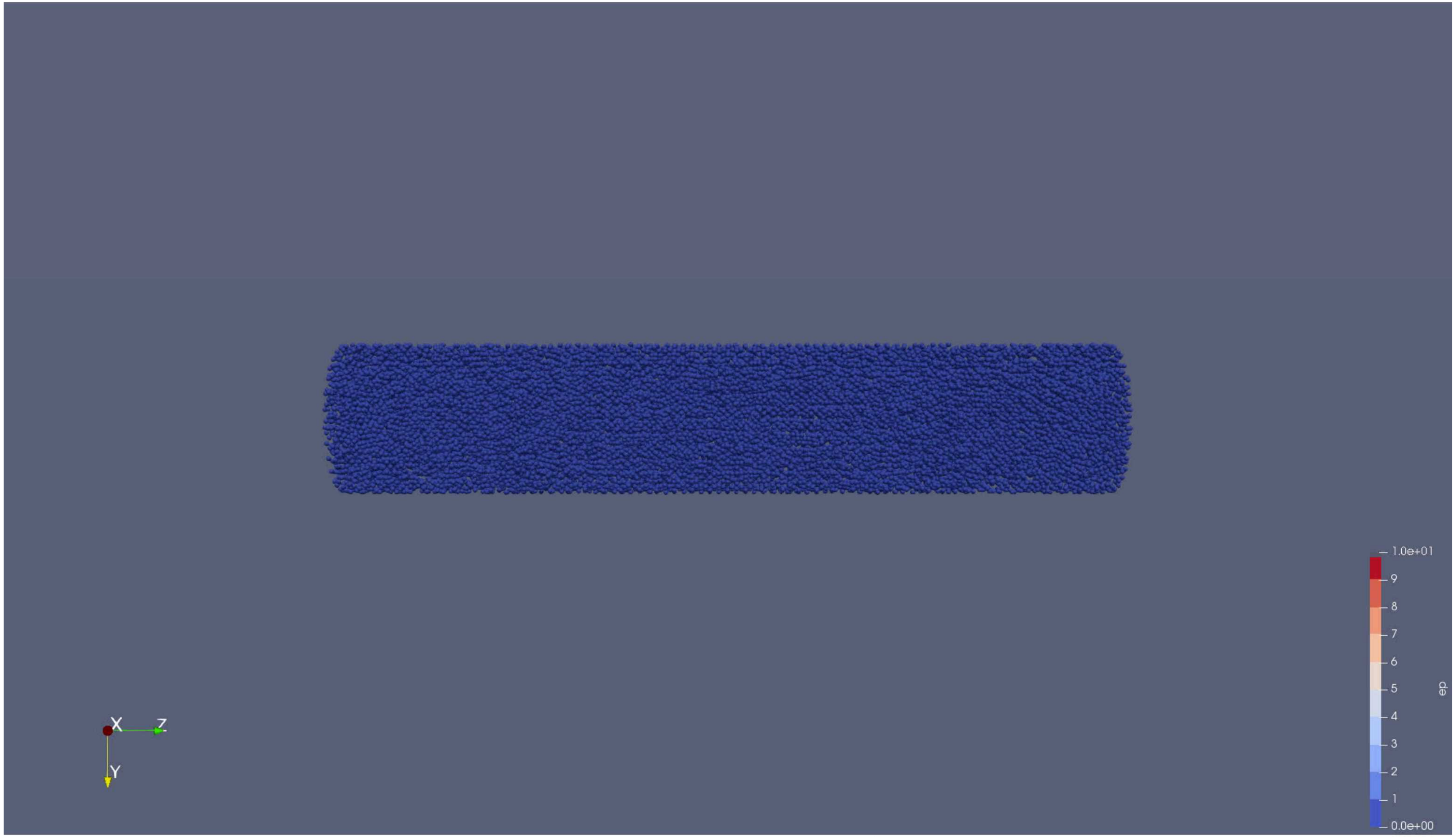
Our eqps results
t = 20us, 40us, 80us
5179 nodes, 26488 points
These are raw point results without postprocessing.
They are not perfectly symmetric because we initialized with an unstructured mesh generated by Cubit.
The view is from a slice down the middle.
Pressure oscillations due to locking. Mitigate (Tupek & Koester).

Taylor Bar with meshfree OTM and adaptation



Nodes: 110, 339, 2174, 5179
Points: 324, 1290, 10428, 26488

Taylor Bar at Extreme Deformation



Initial Velocity: 750m/s
Nodes: 5179, Points: 26488

Key Accomplishments

- Developed and implemented a framework for ***meshfree*** simulation.
- Leveraged the theory of the Optimal Transportation Method for ***extreme deformation***.
- Introduced ***adaptivity*** to meshfree simulations.
- Leveraged the LGR code for ***scalability*** and execution on the GPU.
- Our team achieved the first year objectives.

Lessons Learned

- Holistic synergy between 1400, 1500, and 8300.
- Strong, extremely capable team.
- Can achieve regimes of extreme deformation naturally.
- Can introduce adaptivity with relative ease.
- OTM inherits many fundamentals from FEM.
- Created a tool for further exploration of meshfree methods, adaptivity, and extreme deformation.

Risks, Issues, and Mitigations

- Old habits are hard to break (no mesh, no elements).
- Some things look hard but are easy and vice versa.
- Develop new intuition through experience.
- Better adaptivity metrics (variational, energy based).
- Shape functions and adaptivity at extreme deformation (use of different schemes).
- Locking in isochoric deformation (Mike Tupek and Jake Koester looking at this).

Future Promise

- Keep our team.
- Formulate novel, meshfree adaptivity metrics.
- Access regimes currently inaccessible with existing technology:
  - impact on hard, soft targets
  - simulation of subtractive and additive manufacturing
  - phase changes, melting
  - pervasive fracture and fragmentation
  - fire scenarios and others