PicassoMPM: Massively parallel material point method for additive manufacturing simulations

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NETL Multiphase Flow Science Workshop

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EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

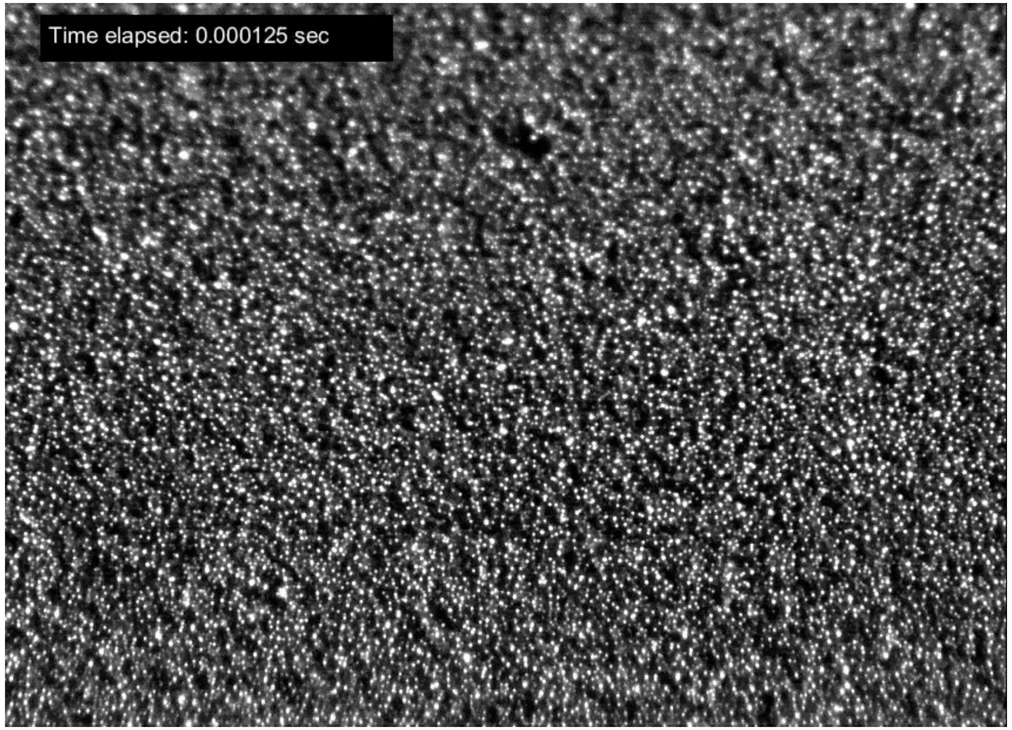
U.S. DEPARTMENT OF ENERGY | Office of Science

An Overview

- ExaAM - applications
- Software stack
  – Cabana/Kokkos
  – Picasso
- PicassoMPM
  – Coupled thermomechanics problems + phase change
  – Examples
  – Performance
- Summary and future work

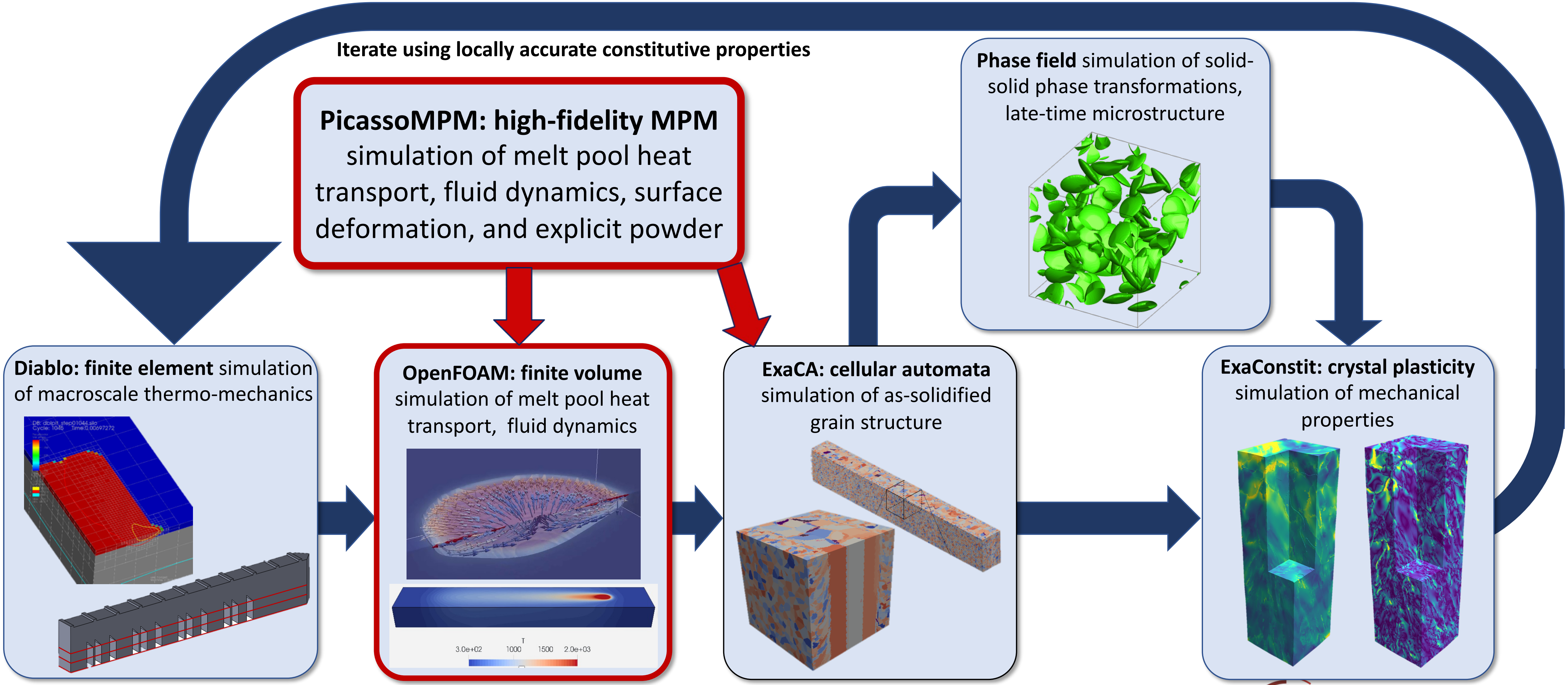
PicassoMPM for additive manufacturing

- Simulation of laser powder bed fusion (LPBF) on Frontier with
  - Thermal (enthalpy formulation), mechanical, and coupled terms
  - Keyhole formation
  - Vapor effects *(no explicit vaporization tracking)*
  - Fully resolved powder bed
    - Size and shape dispersion, dropped and/or raked
  - Laser ray tracing
- Coupling to other parts of the ExaAM workflow
  - Higher fidelity microstructures near defects or in keyholing (CA or PF)
  - Develop models to improve keyhole predictions in additiveFOAM



P. Bidare et al., Acta Materialia, vol 142, pp. 107-120, Jan. 2018.

PicassoMPM in ExaAM



Software Stack

PicassoMPM
MPM app

"CabanaMPM"

ExaMPM
MPM proxy app

Picasso
Performance portable PIC algorithms

Cabana
- *Flexible particle data layout*
- *Performance portable, multi-node **particle** and **particle-grid** motifs*

ArborX
Geometric search

hypre
Structured solvers

MPI
Multi-node computation

Kokkos
On-node performance portability

OpenMP | **CUDA** | **HIP** | **SYCL**

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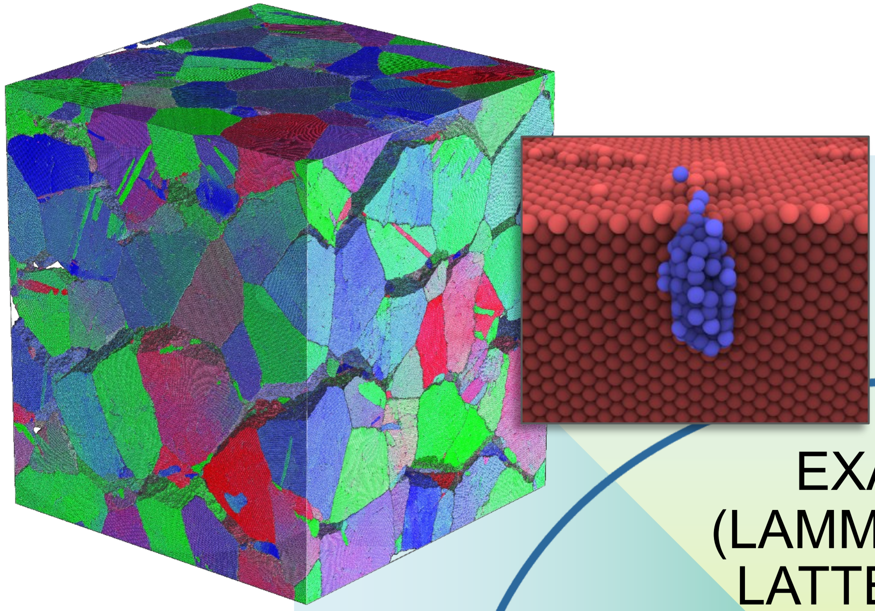
Cabana

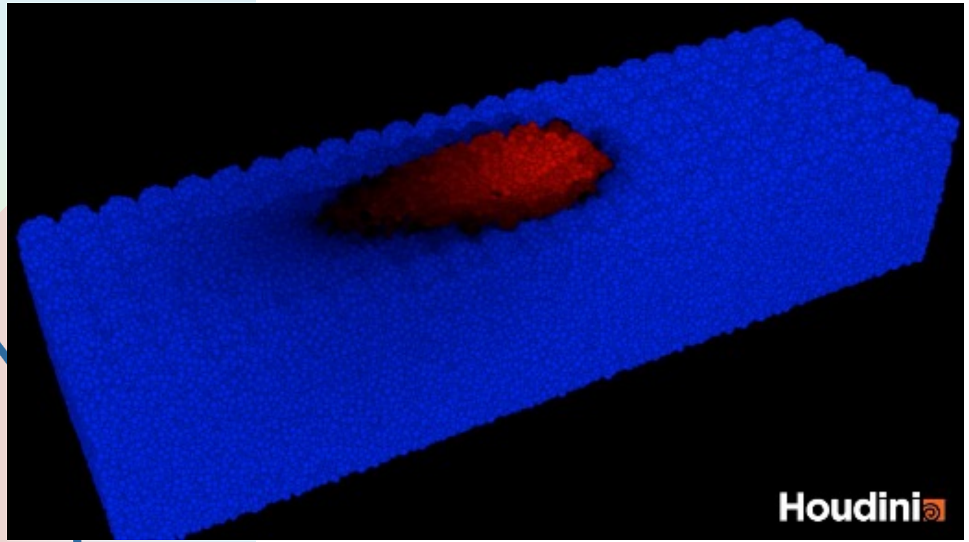
Particle library

Slattery et al., (2022). Cabana: A Performance Portable Library for Particle-Based Simulations. Journal of Open Source Software, 7(72), 4115, https://doi.org/10.21105/joss.04115

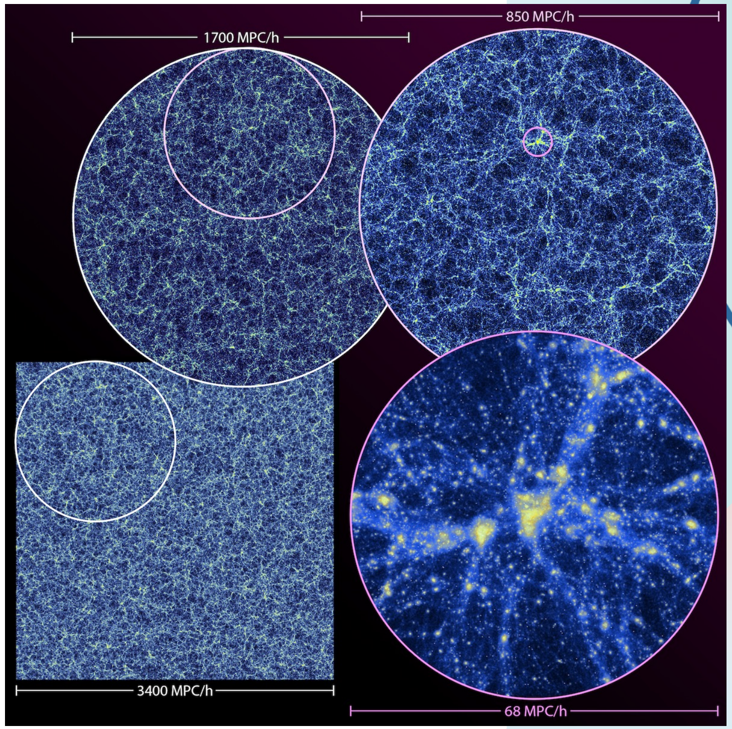
CoPA application partners



EXAALT
(LAMMPS MD,
LATTE QMD)

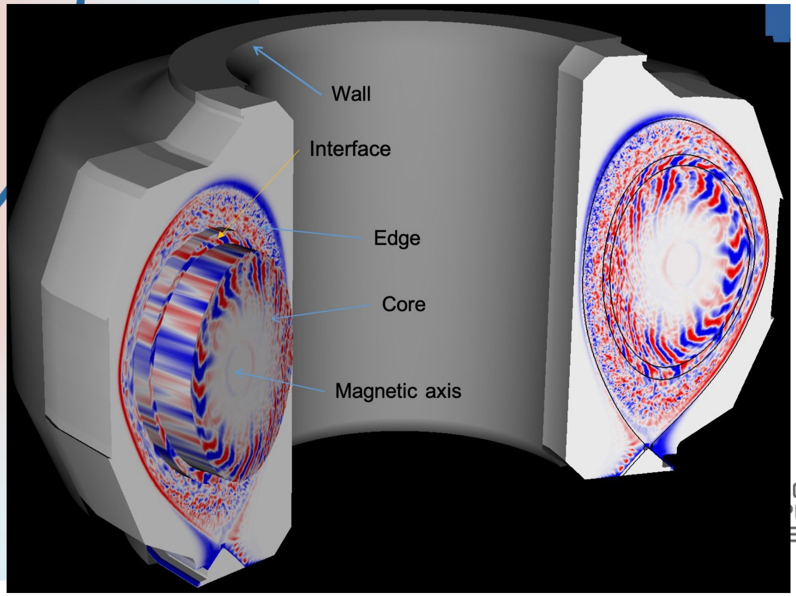


ExaAM
(Picasso
MPM)



ExaSky
(HACC
N-body)

Fusion WDM
(XGC PIC)



Cabana functionality **(MPM relevant)**

- Core library
  - **Particle/neighbor parallelism**
  - Neighbor lists
  - Linked cell lists
  - Binning/sorting
  - **Particle migration**
  - Particle halo
  - Particle I/O
- Cajita (structured grids)
  - **Grid parallelism**
  - **Grid halo**
  - **Particle-grid interpolation**
  - FFTs
  - Structured solvers
  - **Grid load balancing**
  - ***Sparse grids****
- Proxy apps (MD, PIC, **MPM**, N-body)

** In progress*

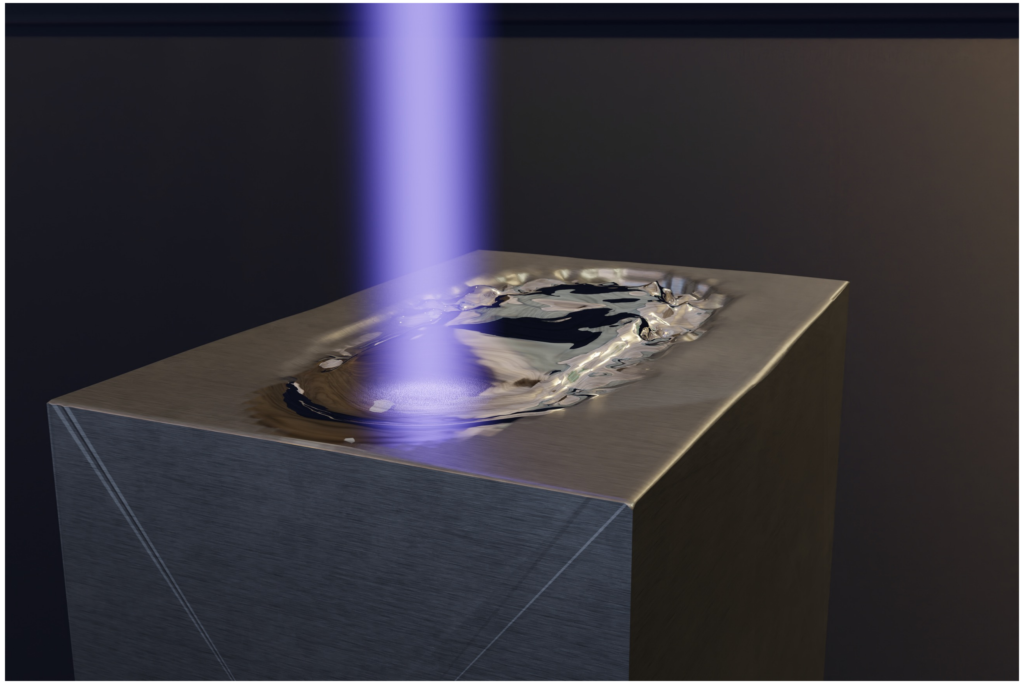
Picasso

PIC Library

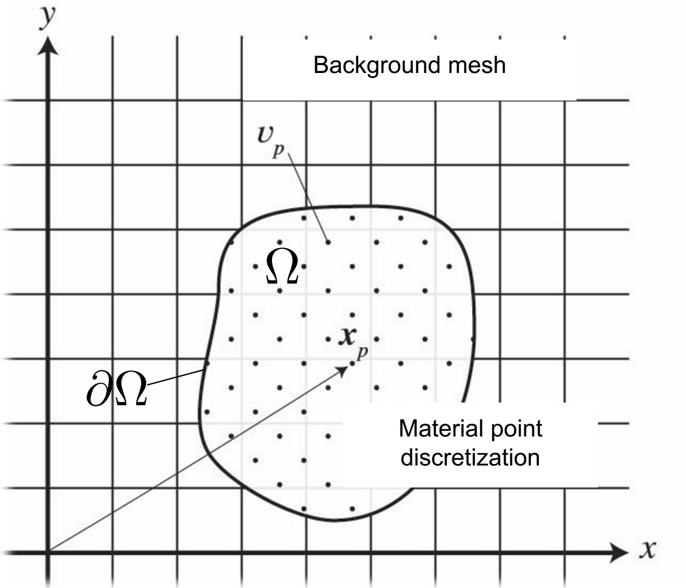
+

PicassoMPM

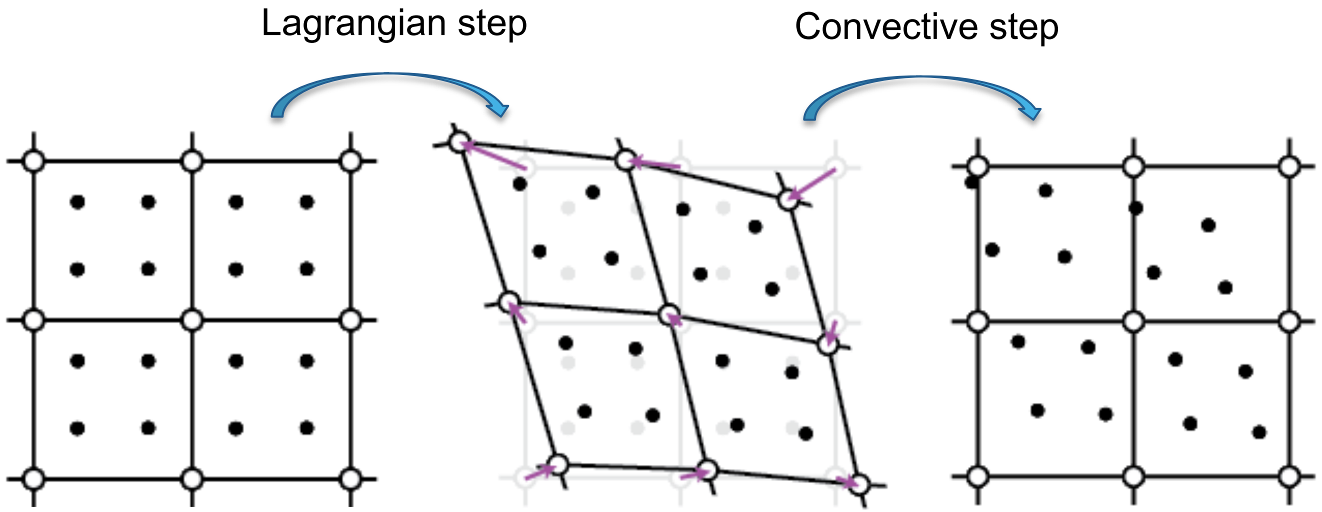
Additive manufacturing application



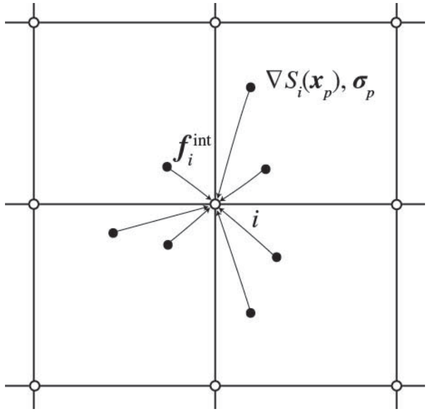
MPM



Picasso
- Interpolation/basis functions
- Field management
- Batched linear algebra
- PolyPIC
- APIC
- Level set utilities

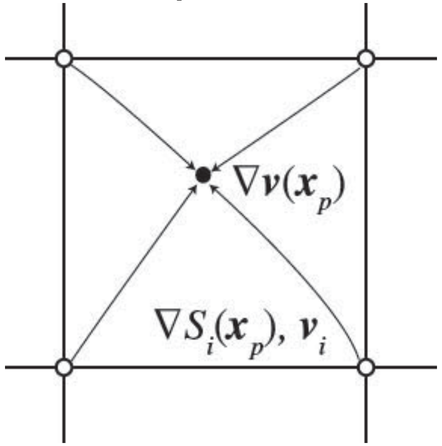


1.) P2G



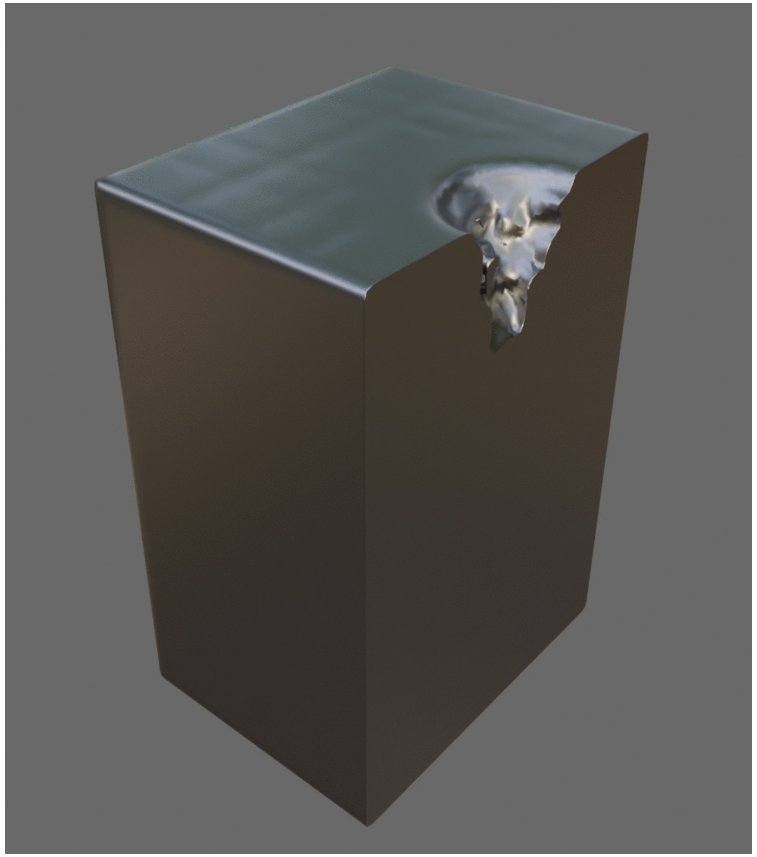
2.) Field Solve

3.) G2P



PicassoMPM development

- Coupled Thermal+Momentum+Surface single-velocity explicit flow solver
- Latent enthalpy phase change
- Surface physics (ArborX)
  - Tree construction/traversal
- How do these components use Cabana?
  - Particle and grid data structures and parallel iteration
  - Particle-to-grid and grid-to-particle interpolation
  - Grid halo communication/exchange



Model equation system

Energy:

$$\rho \frac{DH}{Dt} = \nabla \cdot (\kappa \nabla T) + \dot{q}^s$$

Liquid volume fraction

$$\alpha = \begin{cases} 0, & H < H_s \\ \frac{H-H_s}{H_l-H_s}, & H_s \leq H < H_l \\ 1 & H \geq H_l \end{cases}$$

$H_l = H_s + \Delta H_{sl}$ Latent heat

Discretized weak form:

$$\sum_p m_p w_{ip} \frac{(H_i^{n+1} - H_i^n)}{\Delta t} = -\sum_p \kappa_p v_p^n \nabla w_{ip} \cdot \left(\sum_j \nabla w_{jp} T_j^n \right) + \sum_p v_p w_{ip} \dot{q}^s + \int_{\partial\Omega^n} w_i(\boldsymbol{x}) q^b ds(\boldsymbol{x})$$

Phase averaged properties

$$\rho = \alpha \rho^l + (1-\alpha)\rho^s$$

$$c = \alpha c^l + (1-\alpha) c^s$$

$$\kappa = \alpha \kappa^l + (1-\alpha)\kappa^s$$

Momentum:

$$\rho \frac{D\boldsymbol{u}}{Dt} = \underbrace{\nabla \cdot \boldsymbol{\sigma}}_{\boldsymbol{f}_i} + \rho \boldsymbol{f}$$

Discretized weak form:

$$\sum_p m_p w_{ip} \frac{(\boldsymbol{u}_i^{n+1} - \boldsymbol{u}_i^n)}{\Delta t} = \underbrace{-\sum_p \boldsymbol{\sigma}_p \cdot \nabla w_{ip} v_p + \sum_s \boldsymbol{t}_s w_{is} A_s}_{\nabla \cdot \boldsymbol{\sigma}} + \underbrace{\sum_p m_p w_{ip} \boldsymbol{f}_p}_{\rho \boldsymbol{f}}$$

Surface tension physics

Surface tension potential energy:

$$\psi^s = \int_{\partial\Omega} k^\sigma |\hat{J}\hat{F}^{\text{-T}}\hat{\boldsymbol{n}}| ds$$

Picasso::P2G::divergence(spline, **st_p**, du_surface_i)

Node force due to surface tension energy quadrature:

$$f_{i,d} = -\sum_p \frac{\partial \psi^s}{\partial \hat{F}_{dj}}(\hat{F}(x_p), dA_p)\frac{\partial N_i(x_p)}{\partial x_j}$$

Chen et al. A Momentum-Conserving Implicit Material Point Method for Surface Tension with Contact Angles and Spatial Gradients. ACM TOG. 2021

Tensor gradient form:

$$\frac{\partial \psi_s}{\partial \hat{F}_{\alpha\beta}} = 2k\frac{C_{\gamma\alpha\beta\kappa\lambda}\hat{F}_{\kappa\lambda}(\mathbf{CF})_\gamma}{||\mathbf{CF}||}$$

$$C_{\alpha\gamma\epsilon\delta\zeta} = \frac{1}{2}\epsilon_{\alpha\gamma\delta}\epsilon_{\beta\epsilon\zeta}\underline{dA_\beta}$$

Unit surface normal vector

Hyde et al., *ACM Trans. Graph* (2020).

PicassoMPM (thermomechanics + surface tension)

Communication

Memory/ flop kernel

1. Particle to grid x2
2. Get grid temperature from enthalpy constitutive relation
3. Compute grid enthalpy change/internal force contributions from stress and surface tension
4. Grid update x2
5. Add boundary conditions
6. Grid to particle x2

1. **Picasso::p2g::value**(m_p, v_p, h_p, h_i, m_i, dt, spline);
   Picasso::p2g::value(m_p, v_p, u_p, u_i, m_i, dt, spline);

2. **PicassoMPM::Constitutive::MaterialModel**<TProps>::updateTemperature(…)
   Picasso::G2P::gradient(spline, t_i, **grad_t_p**);
   Picasso::G2P::gradient(spline, v_i, **grad_v_p**);
   Picasso::G2P::gradient(spline, x_i, **F_p**);

3. **PicassoMPM::StressModel**<StressFunc>::computeStress (…)
   PicassoMPM::SurfaceTensionModel<SurfaceTensionFunc>::getSurfaceTension(…)
   Picasso::P2G::divergence(spline, **grad_t_p**, dh_i);
   Picasso::P2G::divergence(spline, **s_p**, du_i);
   Picasso::P2G::divergence(spline, **st_p**, du_surface_i);

4. **h_i**(i, j, k) += **dt** * **dh_i**(i, j, k) **/ m_i**(i, j, k);
   u_i(i, j, k) += **dt** * **(du_i**(i, j, k) + **du_surface_i**(i, j, k) + **du_gravity_i**(l, j, k) + **du_recoil_i**(l,j,k)) **/ m_i**(i, j, k);

5. **PicassoMPM::BoundaryCondition**<BCFunc>::apply(…);
   PicassoMPM::BoundaryCondition<BCFunc>::applyParticle(…);

6. **Picasso**::**g2p::value**(h_i, h_p, spline);
   Picasso::**g2p::value**(u_i, u_p, spline);

Each kernel is called by **Cabana::simd_parallel_for** (particles) or **Cajita::grid_parallel_for** (grid) (**Cajita::Halo** as needed)

Surface particle generation

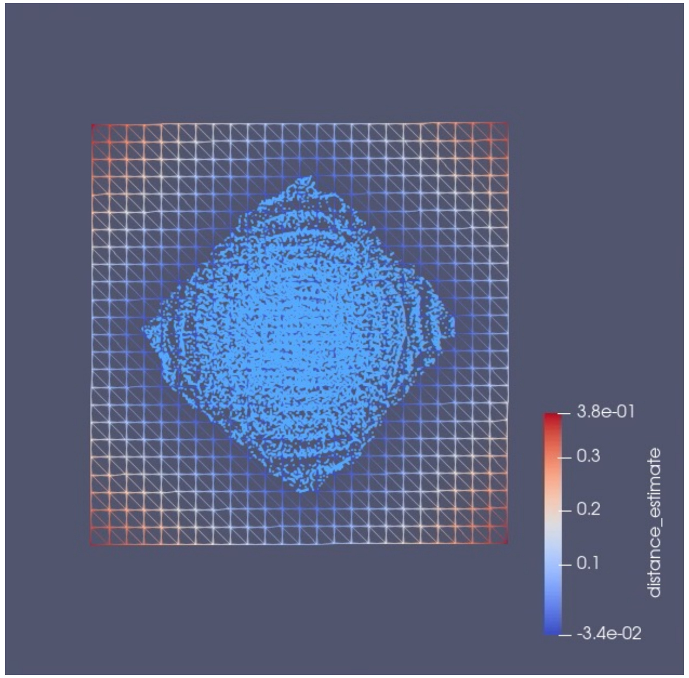
Level set calculation:

Signed distance function: $|\nabla \phi(x)| = 1$

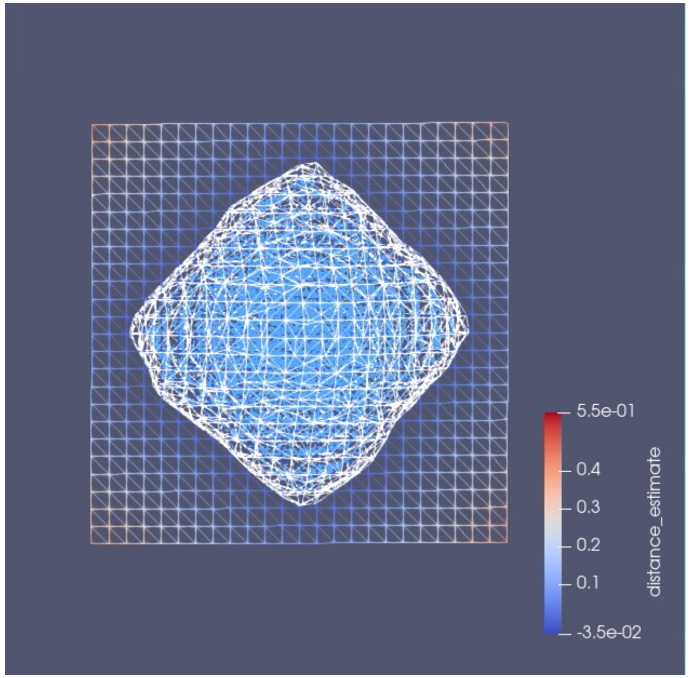
Eikonal equation:

$$\frac{\partial \phi(x,t)}{\partial t} + ||\nabla \phi(x,t)||_2 = 0$$

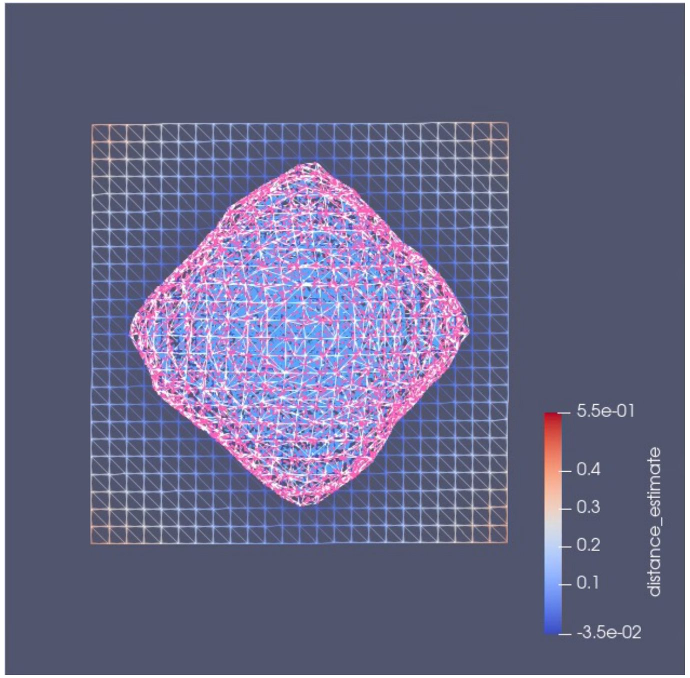
Zero level set isocontour:



Marching cubes triangle mesh:

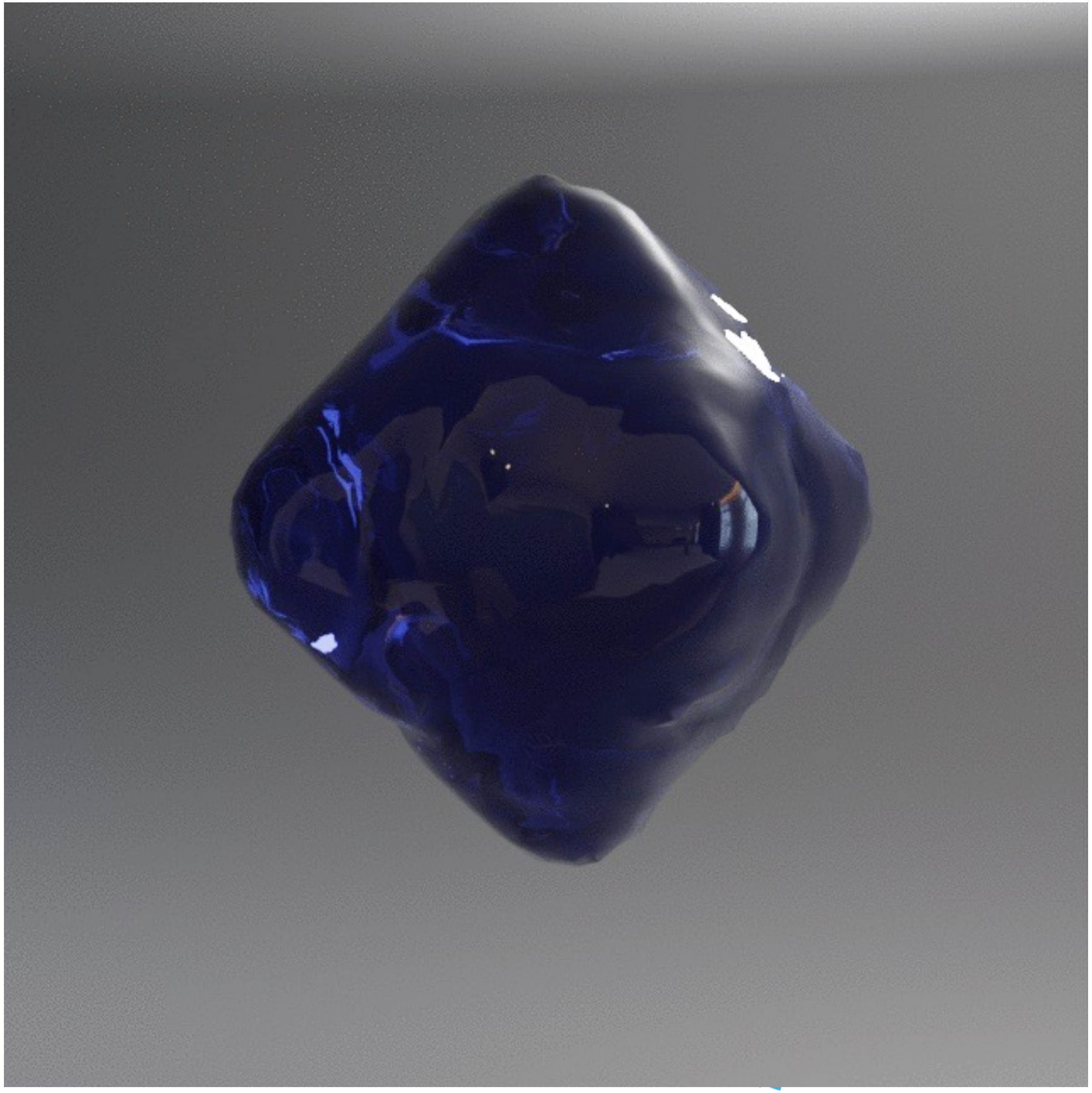


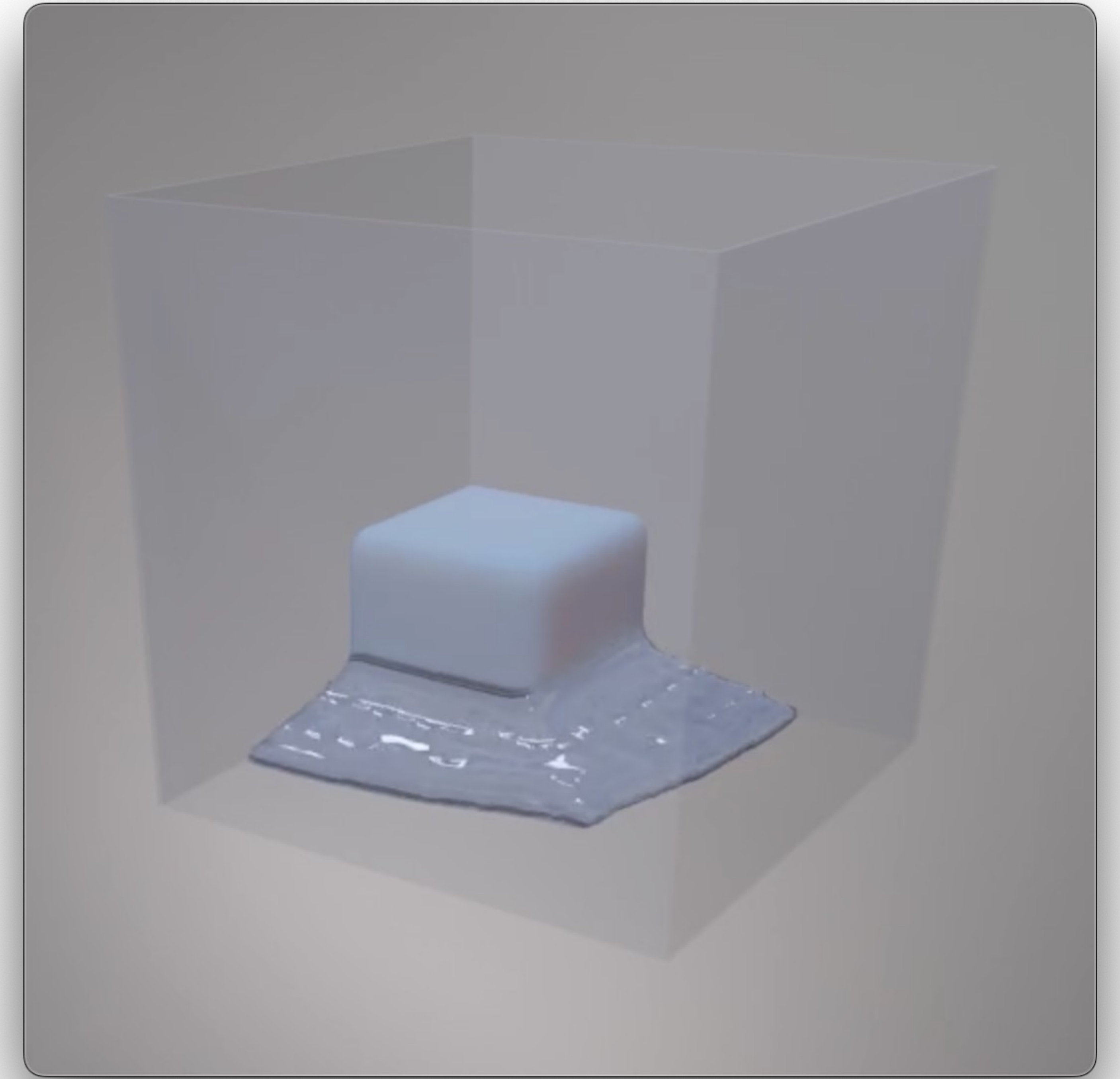
Surface particle generation:



Example problems

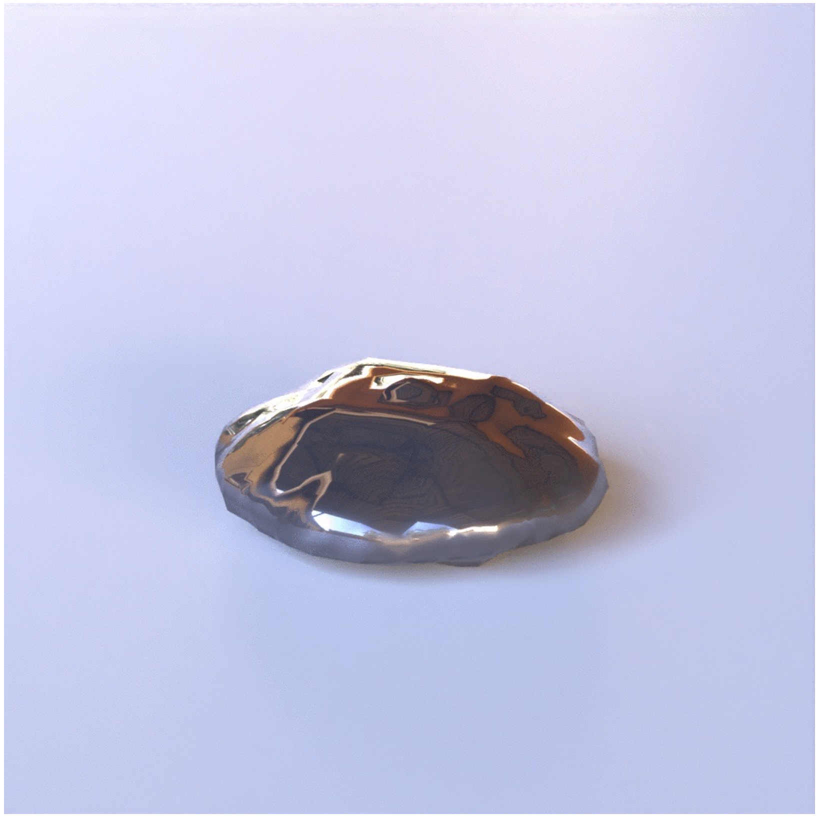
- **Oscillating cube**
- Dam break
- Spot melts

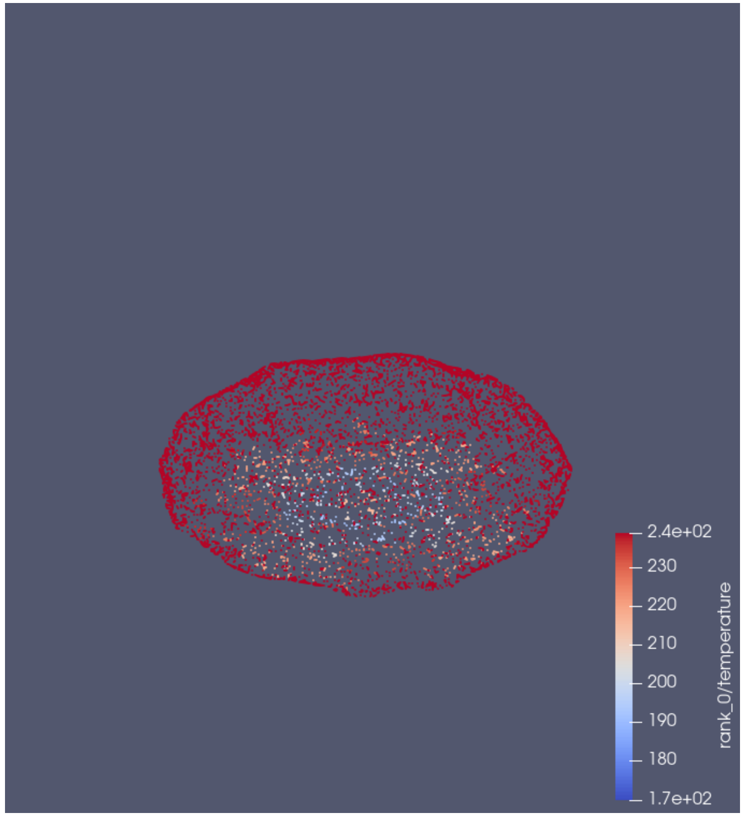


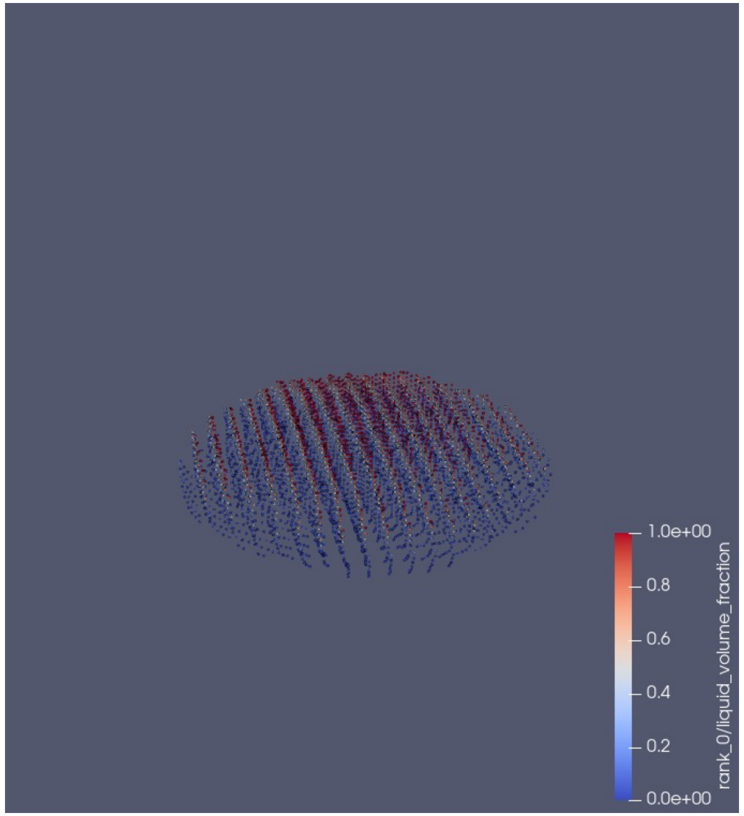


Melting cube dam break

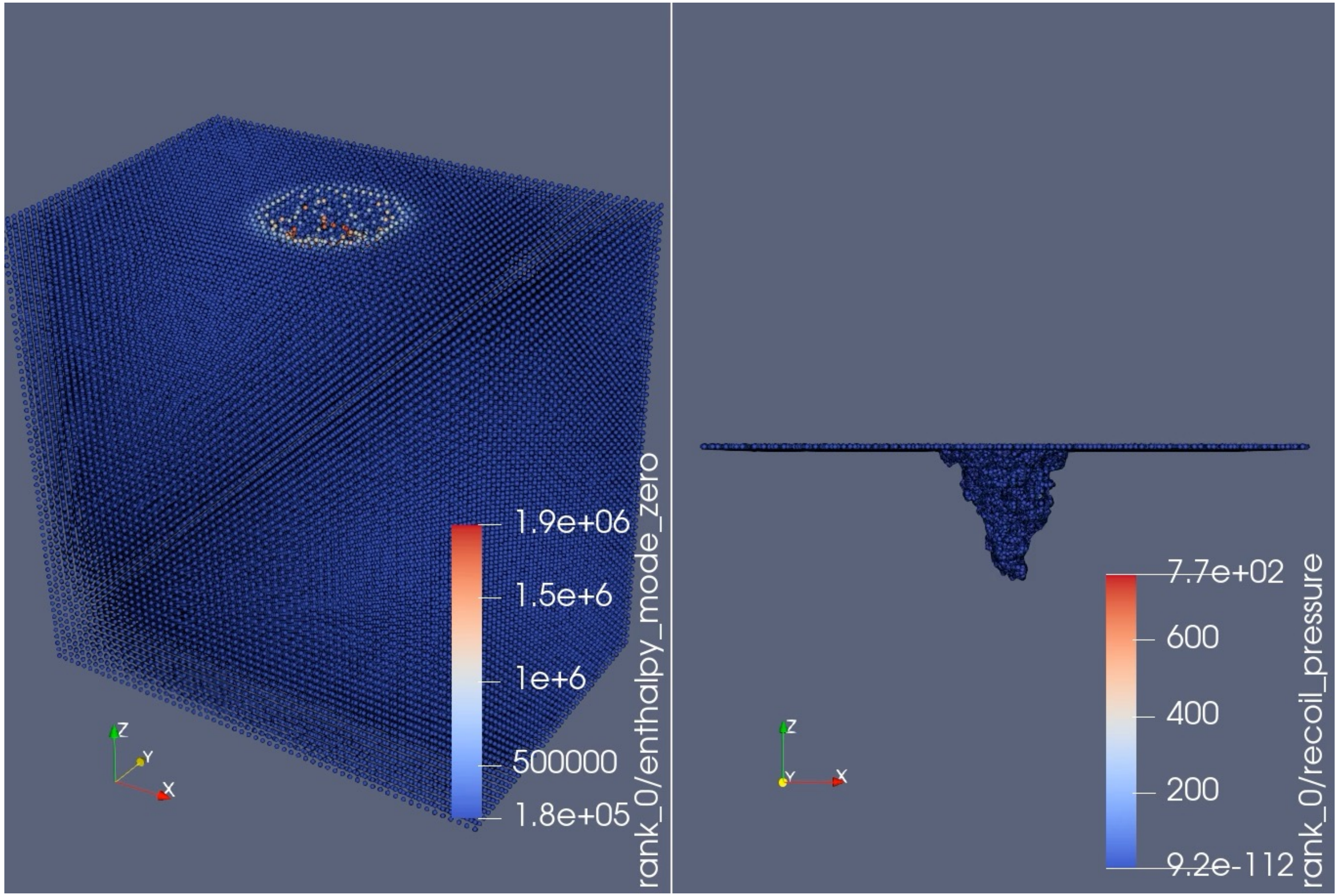
Liquid metal solidifying on a chilled surface





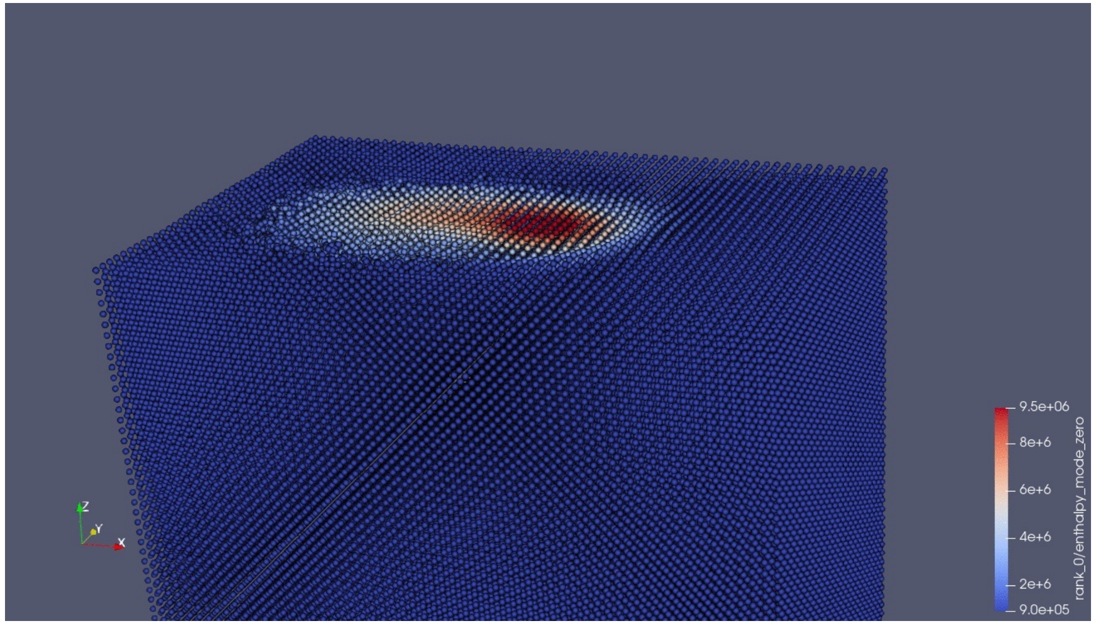


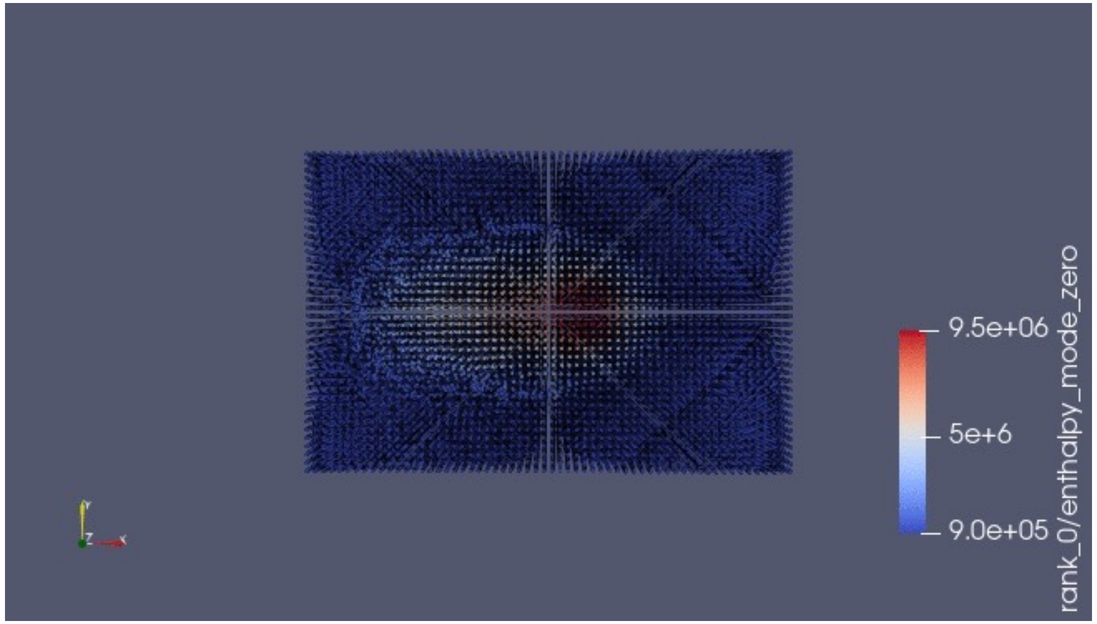
Spot melts



1.9e+06
1.5e+6
1e+6
500000
1.8e+05
rank_0/enthalpy_mode_zero
Z
Y
X
7.7e+02
600
400
200
9.2e-112
rank_0/recoil_pressure
Z
Y
X

Laser tracking





Performance / Exascale readiness

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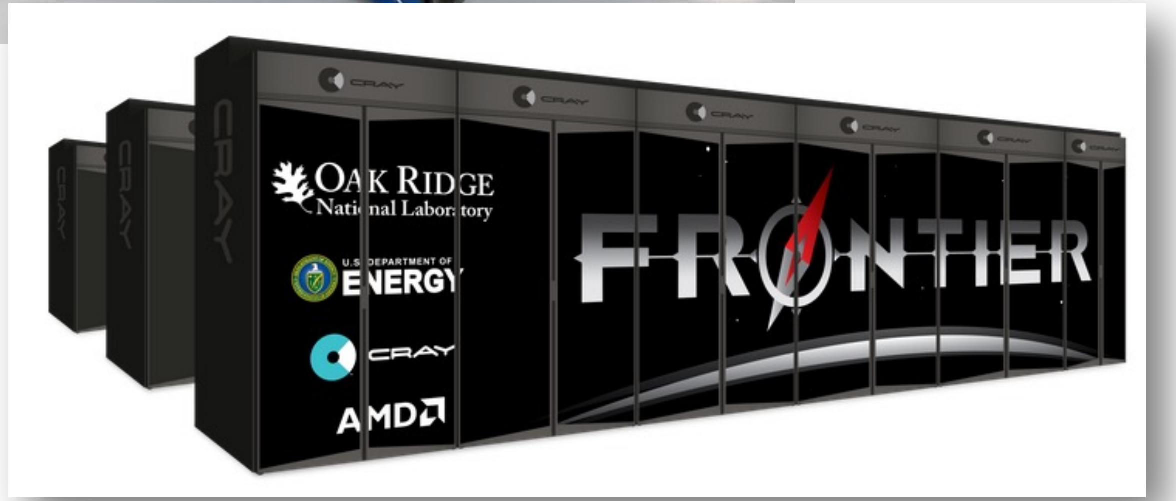
Performance comparison hardware

- Summit node
  - 6 NVIDIA V100 GPU
  - 42 IBM POWER9 CPU cores
- Crusher pre-Frontier testbed
  - 8 AMD MI250X GPU (GCD)
  - 64 AMD EPYC CPU cores

https://www.ornl.gov/news/ornl-launches-summit-supercomputer



https://www.ornl.gov/news/us-department-energy-and-cray-deliver-record-setting-frontier-supercomputer-ornl

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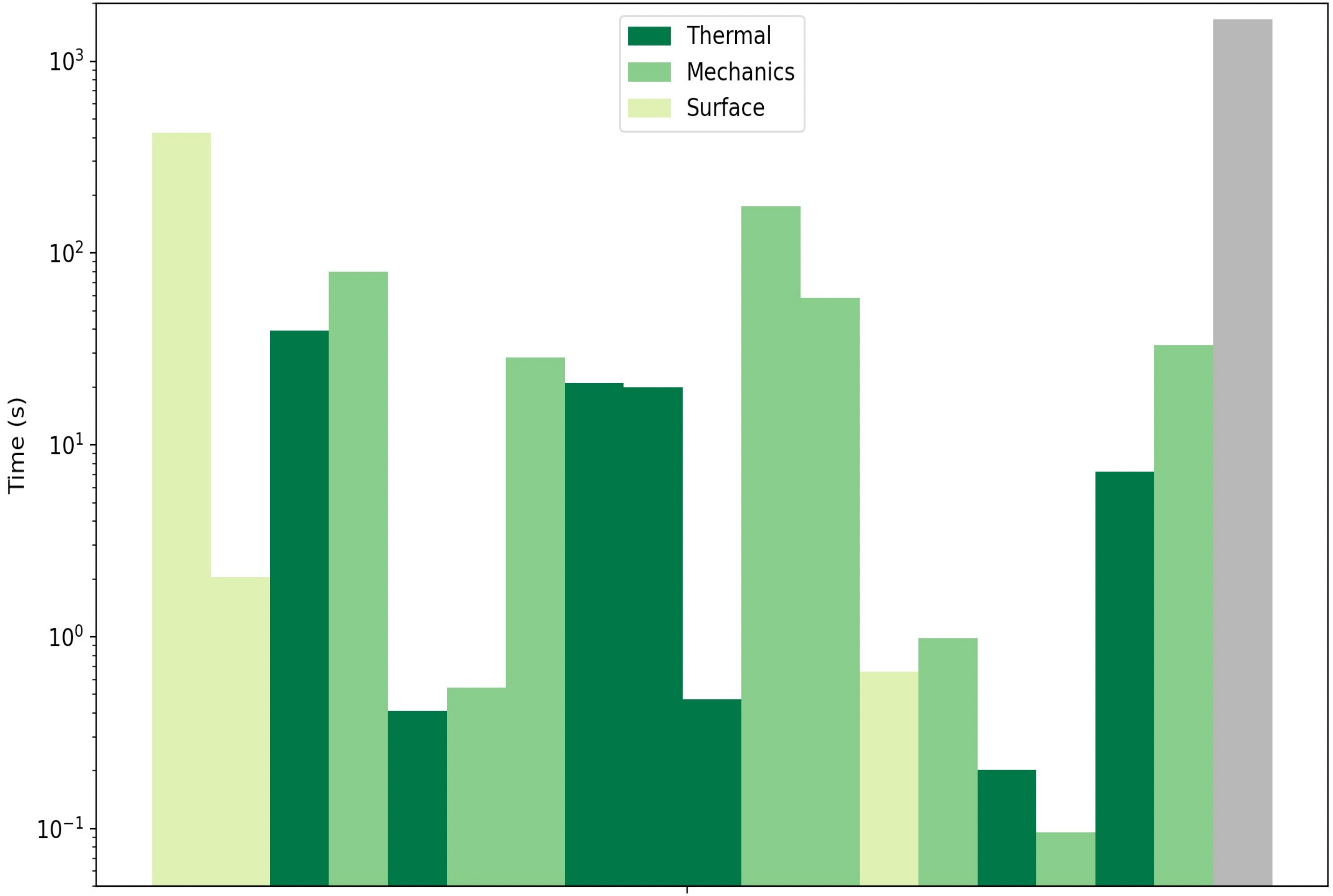
Crusher performance: kernel view

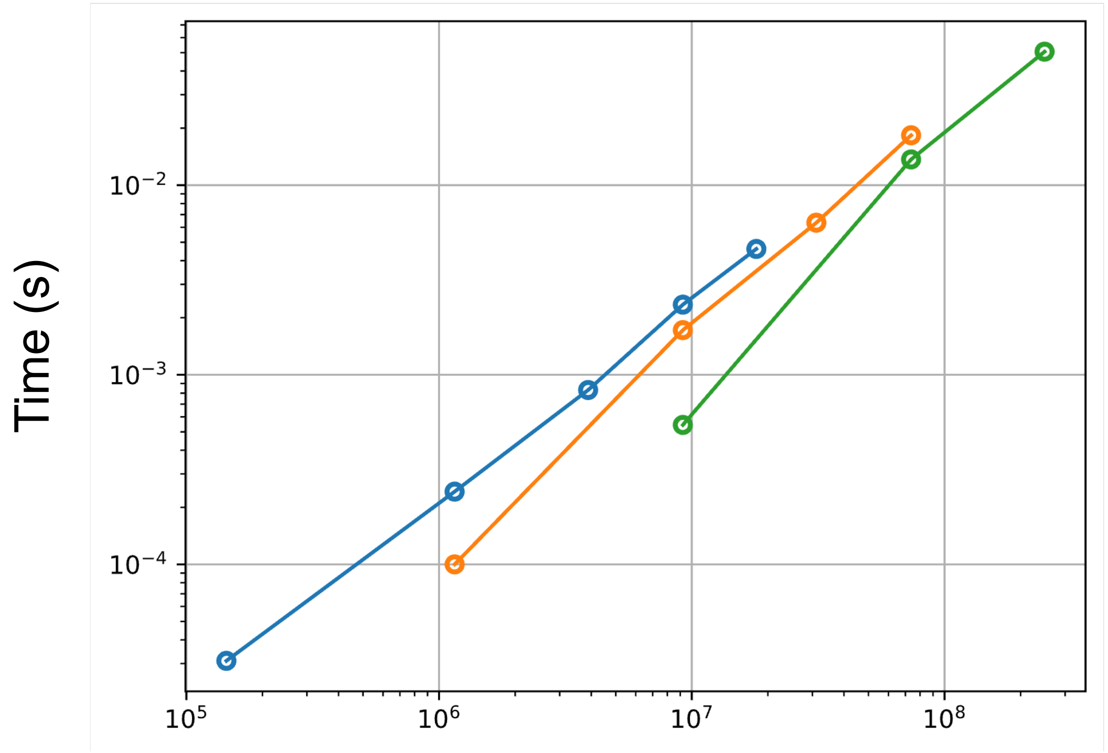


- Run case:

  Spot melt with 9M grid points, 250M particles

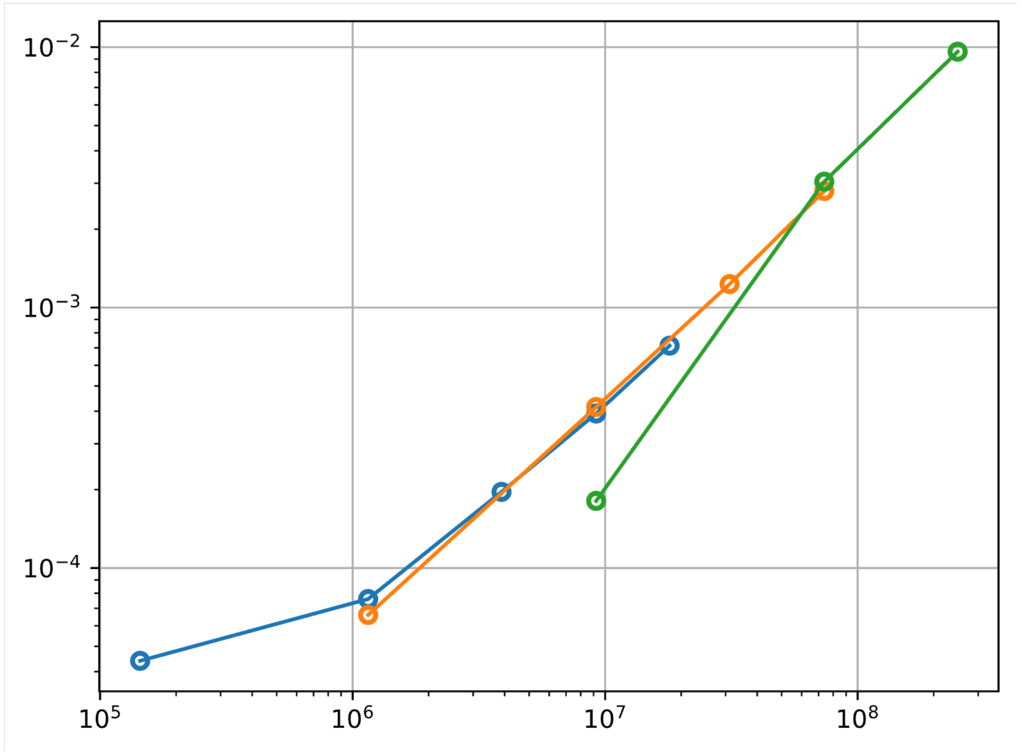
Crusher results – size scaling for representative kernels

p2g: divS



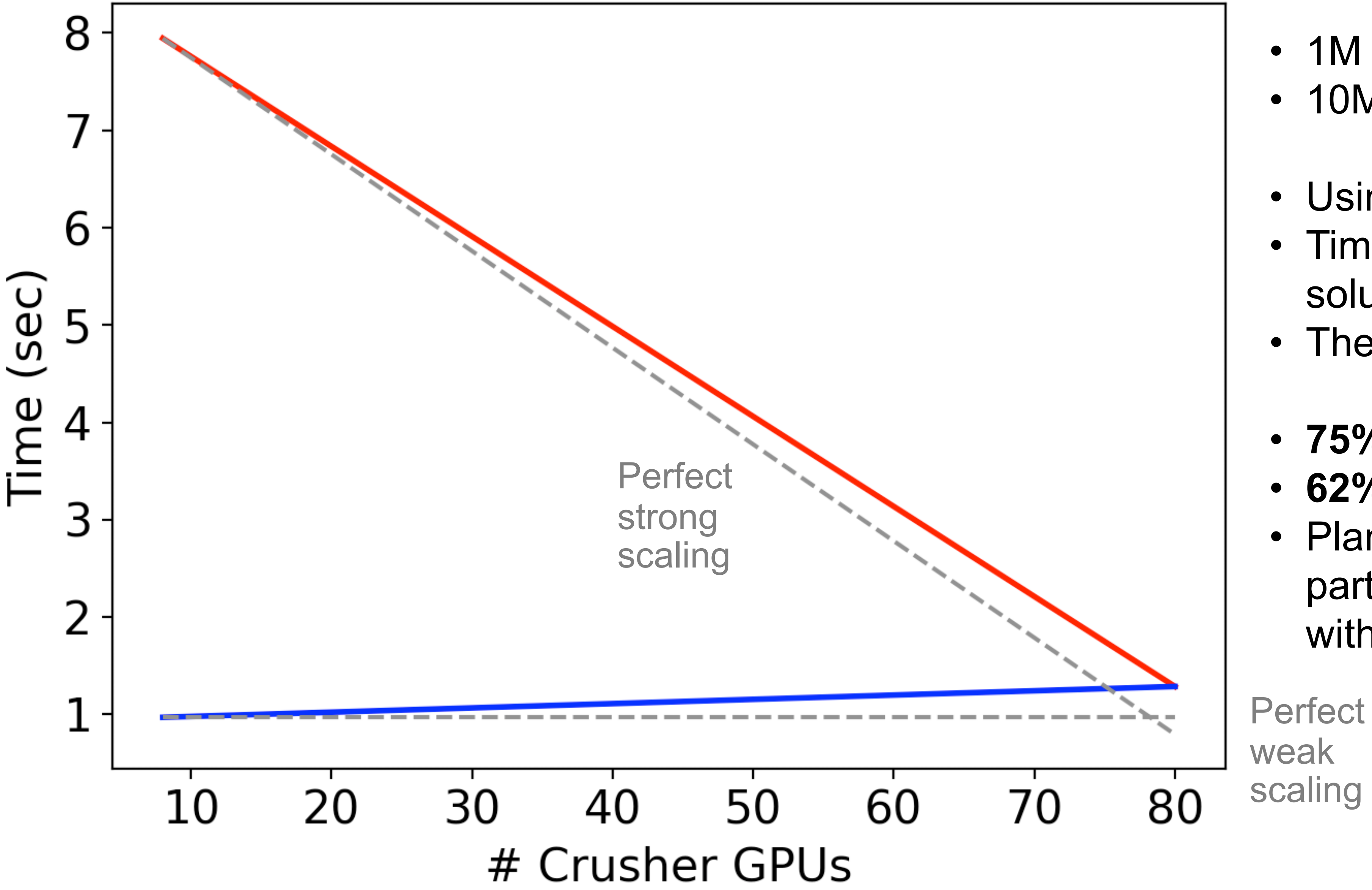
Np

g2p: U



Np

Crusher scaling with 1 & 10 nodes (APIC)



- 1M grid & ~31M particles
- 10M grid & ~330M particles

- Using 1 & 10 Crusher nodes
- Time for 200 steps (not time to solution)
- Thermal-only spot melt

- **75% weak scaling eff.**
- **62% strong scaling eff.**
- Plan to run much larger particle counts (especially with powder)

Summary/On-going work

- PicassoMPM is a performance portable high fidelity multi-physics MPM application for additive manufacturing, built on the Cabana, Picasso, and ArborX libraries.
- In-progress comparisons with UTK MURI experimental and OpenFOAM simulation results for direct numerical simulations of LPBF
- Additional physics capabilities and on-going performance optimizations
  - **Implicit solvers**
  - Sparse grid
  - Ray tracing

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Site Lead: Steve Plimpton, SNL
Site Lead: Stuart Slattery, ORNL
FFTX Lead: Phil Collela, LBNL

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  - **Chenfanfu Jiang**, Yuxing Qui, Yu Fang (UCLA)
  - **Duan Zhang** (LANL)
- Experimental comparison, understanding, and validation
  - **Hahn Choo**, Rakesh Kamath, Ryan Heldt (UTK), Naren Raghavan (LANL)
- Solidification modeling:
  - John Coleman, Gerry Knapp, Alex Plotkowski (ORNL)