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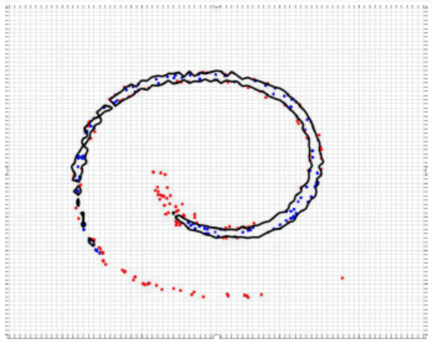
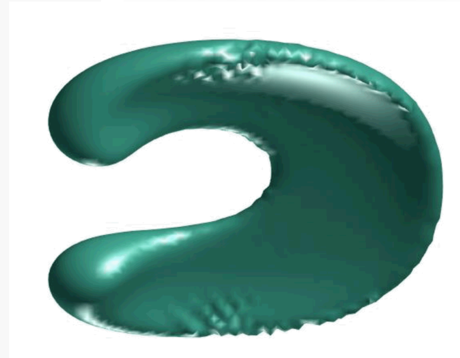
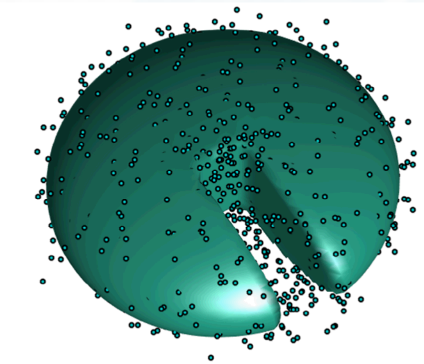






# Simulating Interfacial Multi-Physics Problems Using a Mesh-free Approach

***Lindsay Erickson,***

*K. Morris, and J. Templeton*

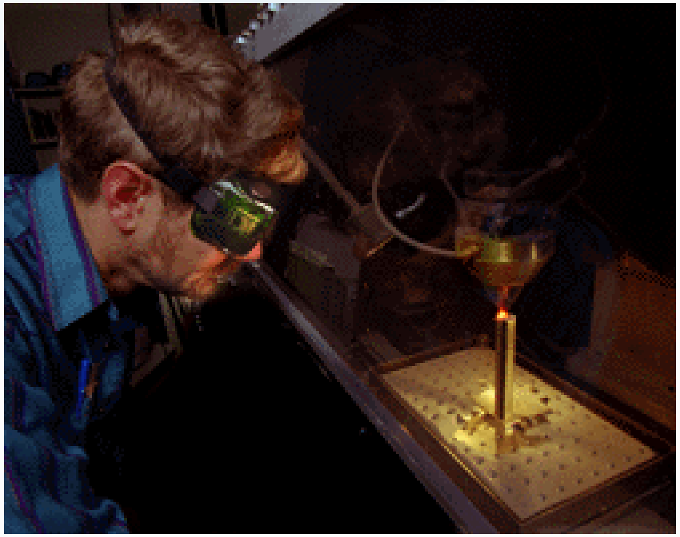
*14th U.S. National Congress on Computational Mechanics*

*July 17th, 2017*

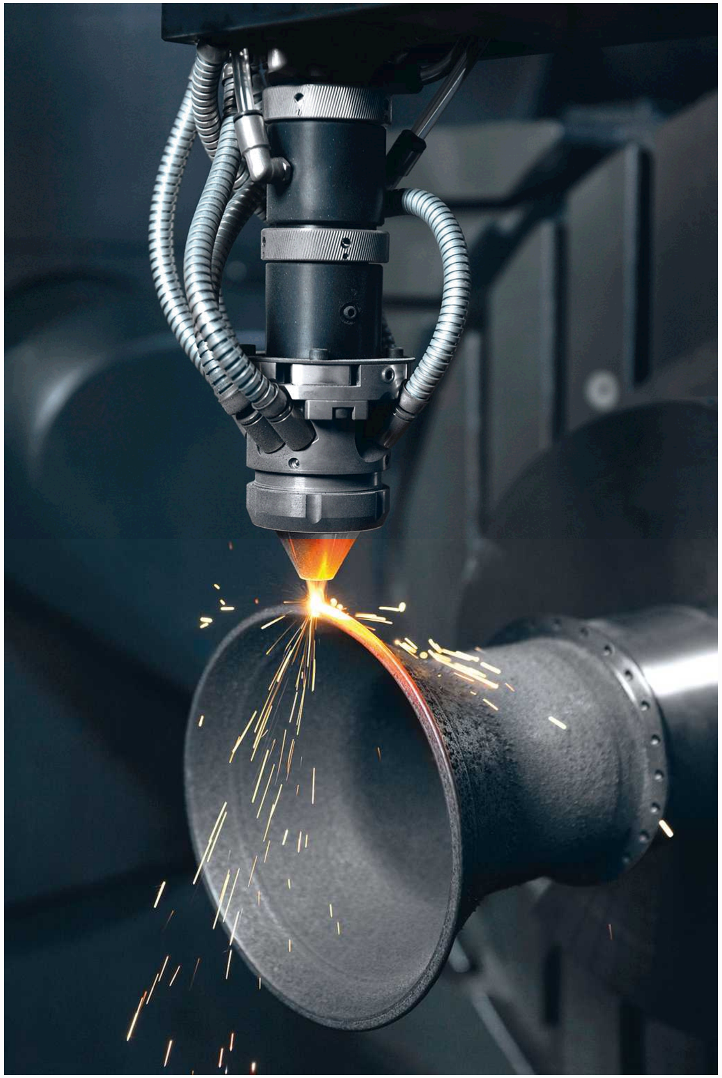
*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.*

# Application: Additive Manufacturing

- Computational modeling for Sandia's Laser Engineered Net Shaping™ (LENS®) technique
- Complicated physics to simulate include:
    - Melting/solidification of metal (i.e. phase transitions)
    - moving interfaces and material relocation

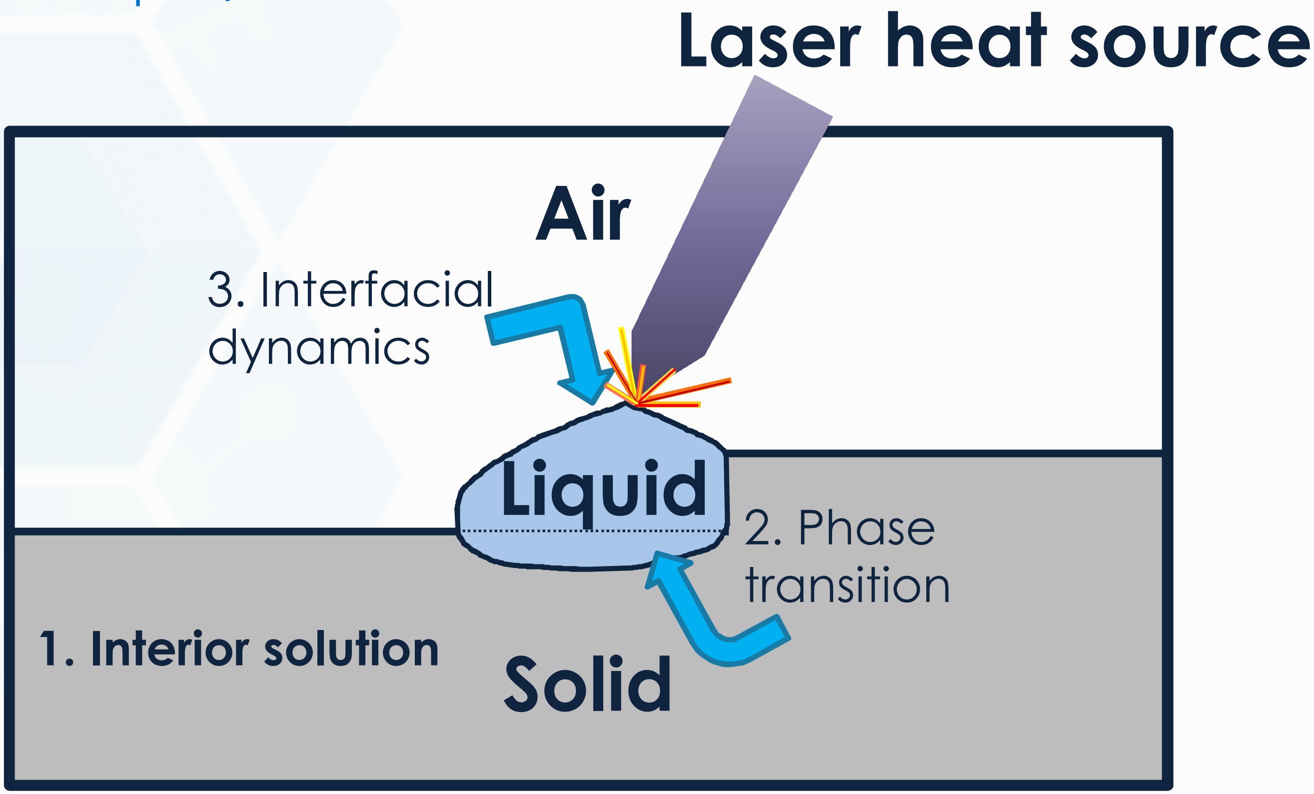


(LENS®) technique



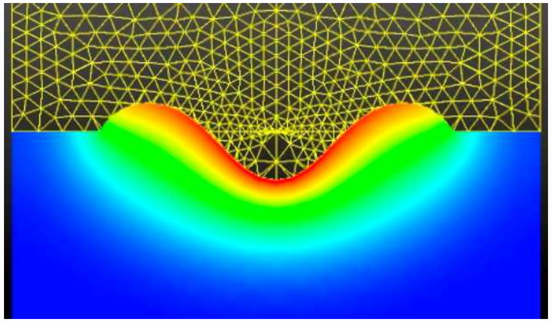
# Functionality required to solve the melt problem

1. **Solving systems of equations in the solid, liquid and air regions with moving boundaries**
2. Solving the phase transition problem
3. Tracking the liquid/air interface

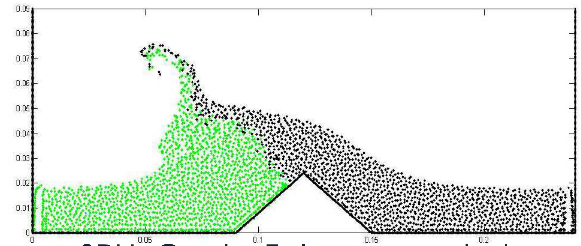


# Mesh-based versus Mesh-free

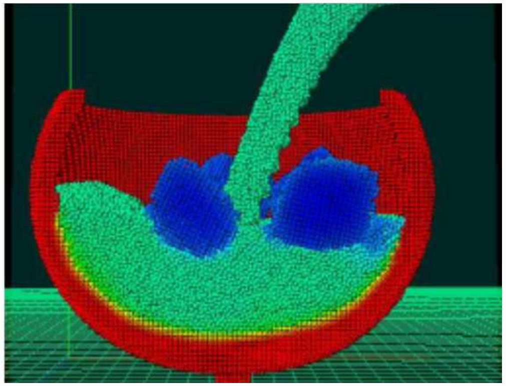
- Mesh-based
  - Advantages
    - Can design mesh to minimize discretization errors
    - Clear theories regarding mesh convergence and numerical errors
  - Challenges
    - Difficult to account for large topological changes
    - Retaining high-quality elements as mesh deforms
- Mesh-free
  - Advantages
    - Capable of tracking large deformations
    - Straightforward to model free-surface effects
  - Challenges
    - Limited error analysis
    - Difficulty maintaining high-order quadrature through flow



CDFEM of Laser Weld, D. Noble



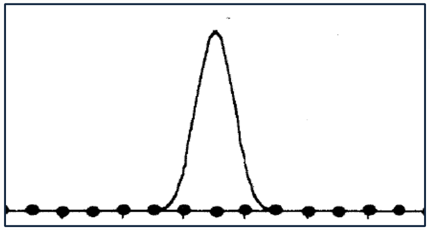
SPH Cueto-Felgueroso et al., 2003



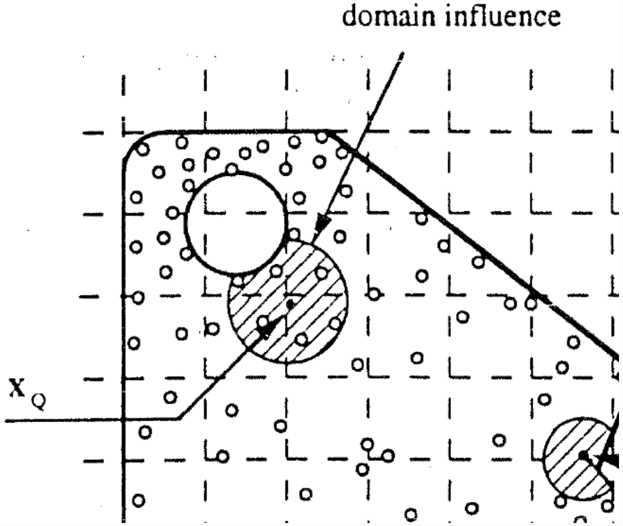
SPH of melting ice, Iwasaki *et al.*, 2010

# Reproducing Kernel Particle Method

$$u^a(x,y) = \sum_{I=1}^{NP} N_I(x,y)\,u_I$$



$$N_I(x,y) = C(x-x_I, y-y_I)\,w_d(x-x_I, y-y_I)\,\Delta V_I$$

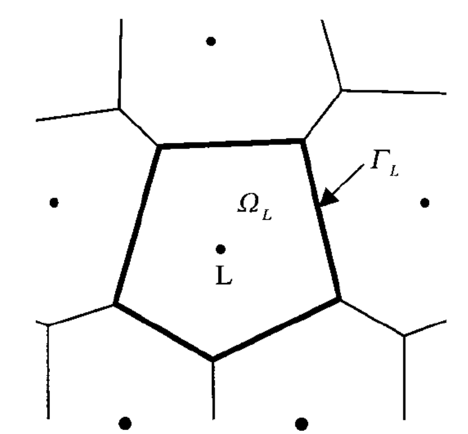



$$\mathscr{L}u^a = f \quad \text{in } \Omega$$

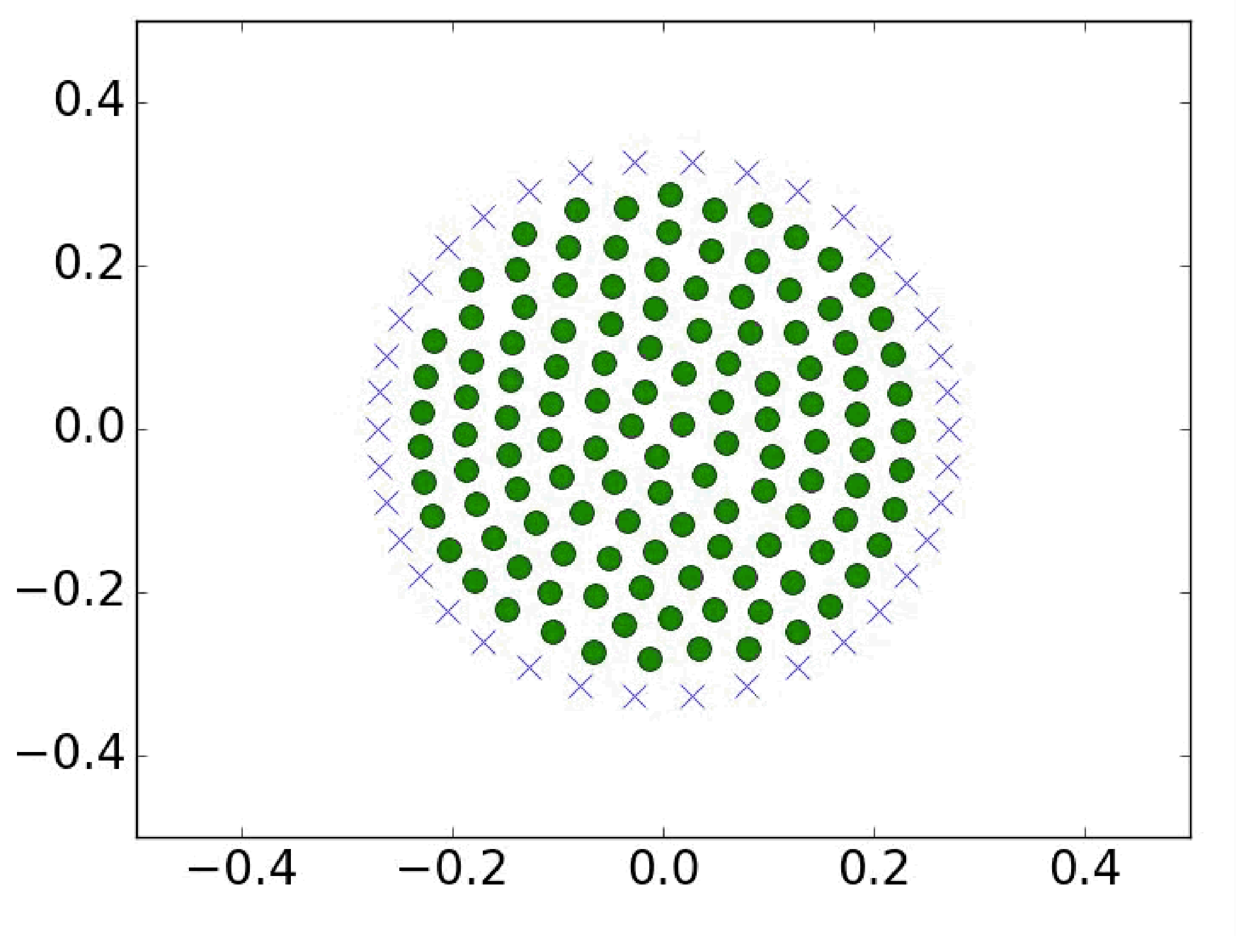
$$u^a = g \quad \text{on } \Gamma_g$$

$$\frac{\partial u^a}{\partial n} = h \quad \text{on } \Gamma_h$$

- RKPM Choices
  - point collocation (requires higher order shape functions and voronoi tesselation)
  - Gaussian quadrature (lower order shape functions, background mesh)



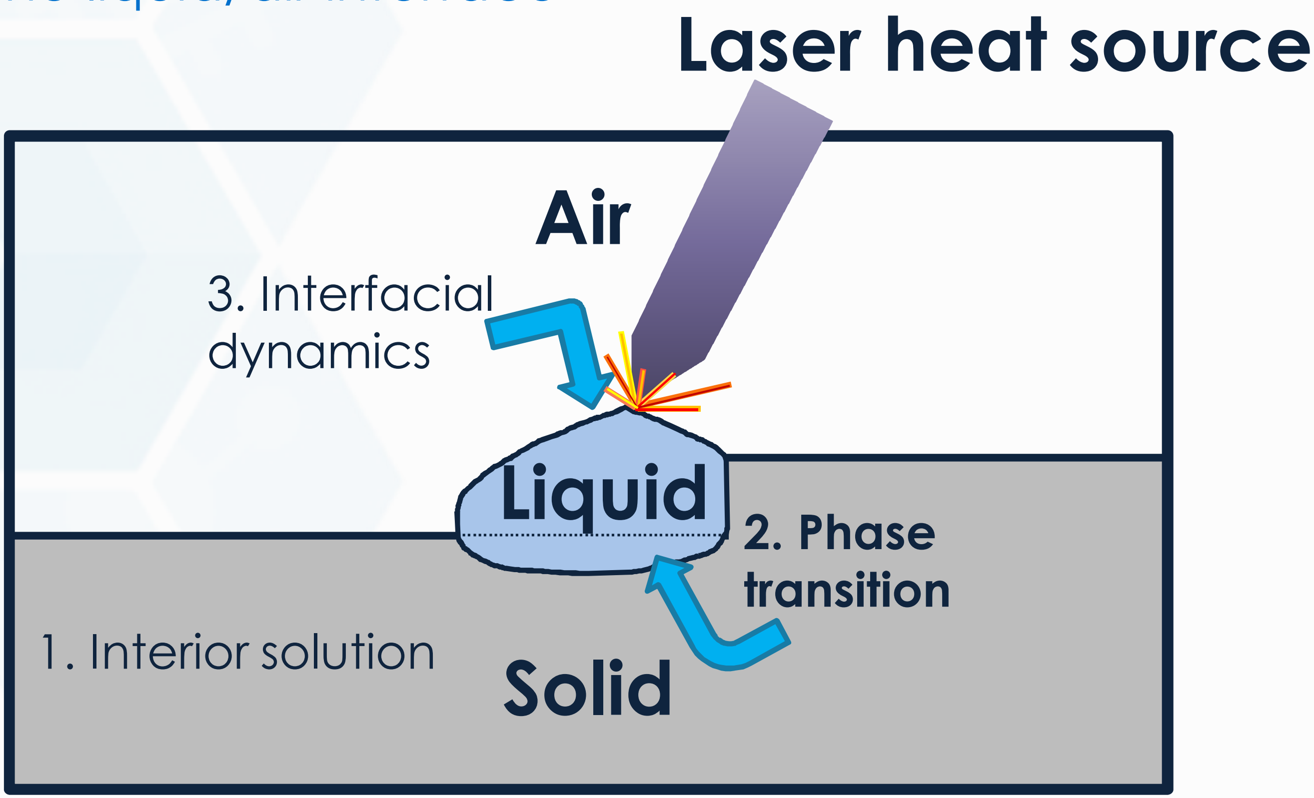
# Particle configuration can be updated based on moving interface




- A molecular dynamics-inspired error minimization technique is used here to adjust the interior particles (o's) based on the interfacial particles (x's)

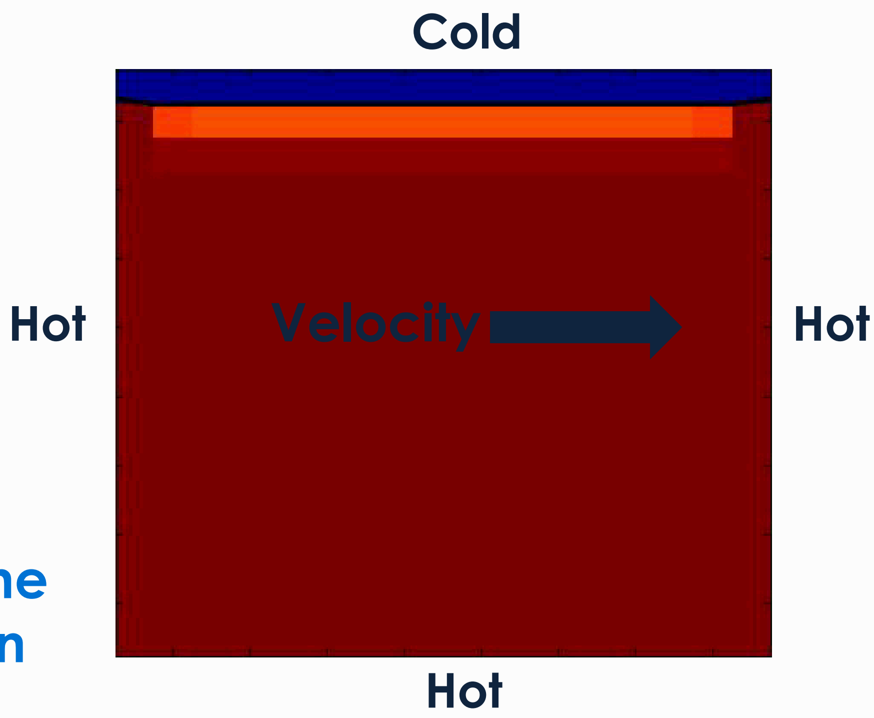
# Functionality required to solve the melt problem

1. Solving systems of equations in the solid, liquid and air regions with moving boundaries
2. **Solving the phase transition problem**
3. Tracking the liquid/air interface



# Solving melting/solidification problems

- One could solve the heat equation for a solidifying liquid and melting solid as one continuous domain with variable coefficients
- The interface can be defined implicitly at the melt temperature

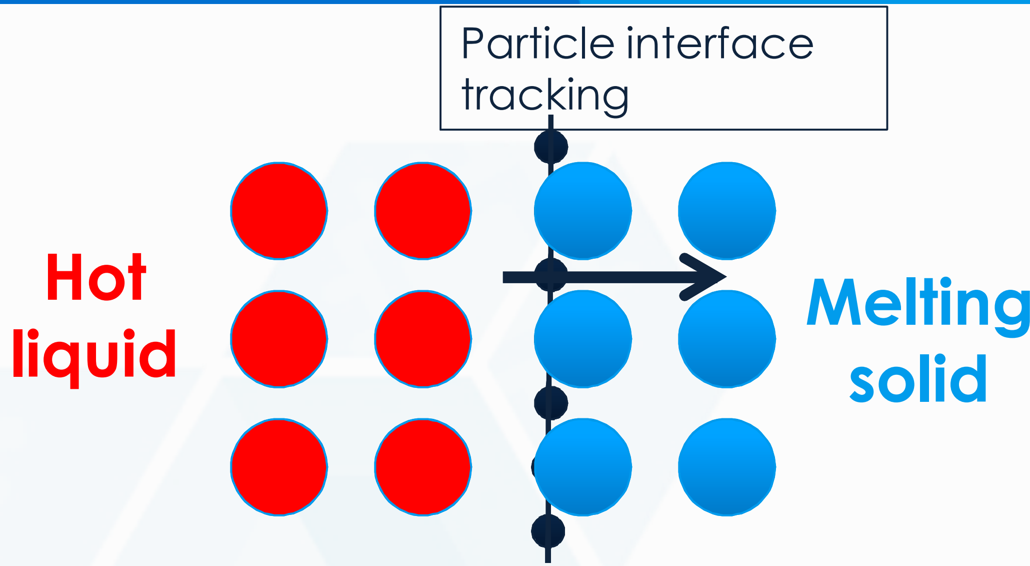


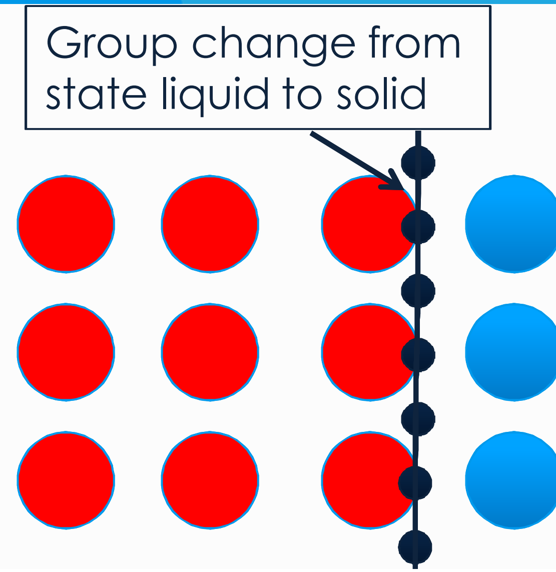

- **Alternatively, one can define the interface explicitly and solve for the interfacial velocity using the Stefan condition:**

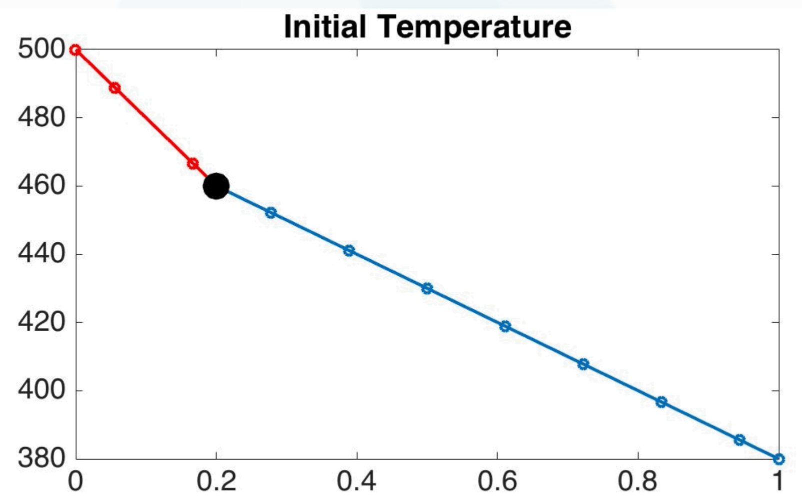
$$T_t = \alpha_L T_{xx}$$
$$T_t = \alpha_S T_{xx}$$

$$\rho_s L \frac{\partial X}{\partial t} = k_s \frac{\partial T}{\partial x}|_{solid} - k_l \frac{\partial T}{\partial x}|_{liquid}$$

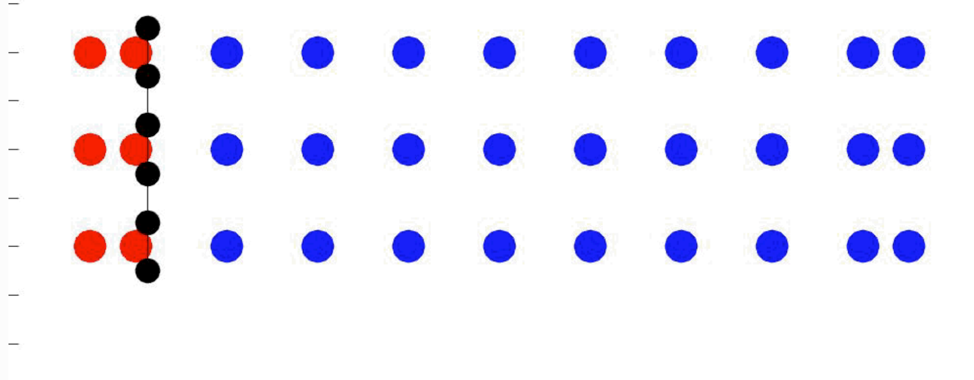
# Solving melting/solidification problems



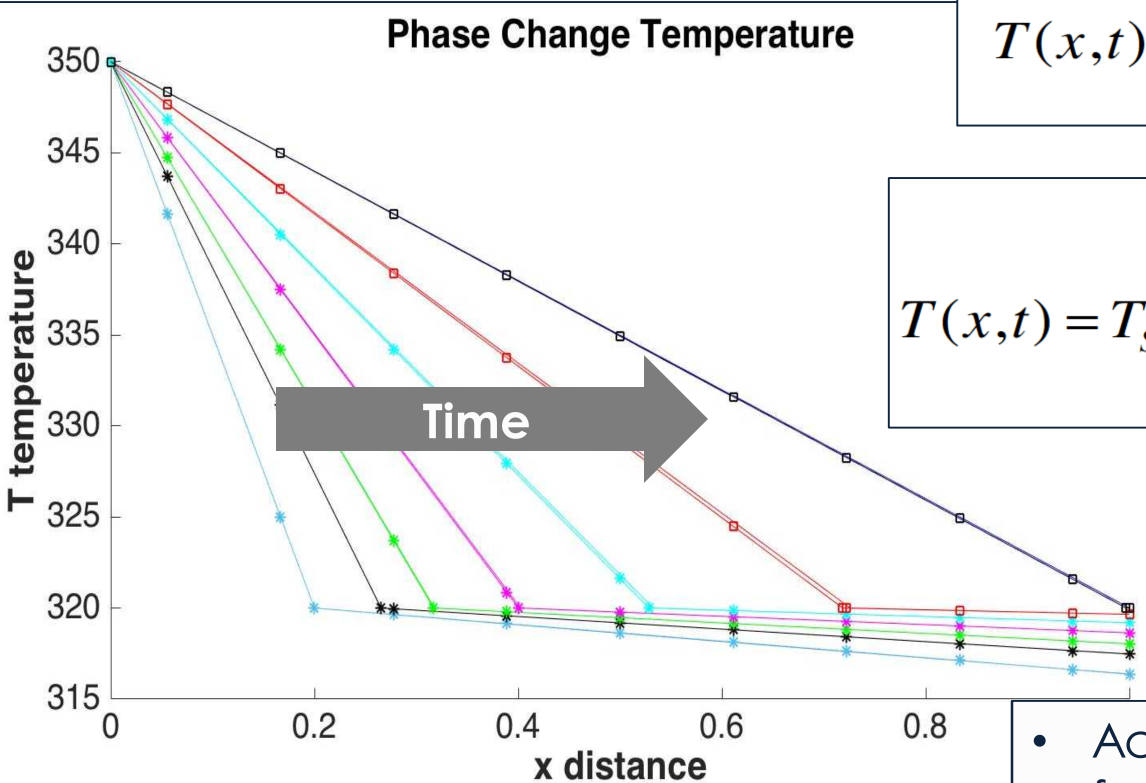




$$\rho_s L \frac{\partial X}{\partial t} = k_s \frac{\partial T}{\partial x}|_{solid} - k_l \frac{\partial T}{\partial x}|_{liquid}$$



# Analytic Solution for Stefan Problem and convergence study




$$T(x,t) = T_L - (T_L - T_m)\frac{erf\left(\frac{x}{2\sqrt{\alpha_L t}}\right)}{erf\,\lambda}$$

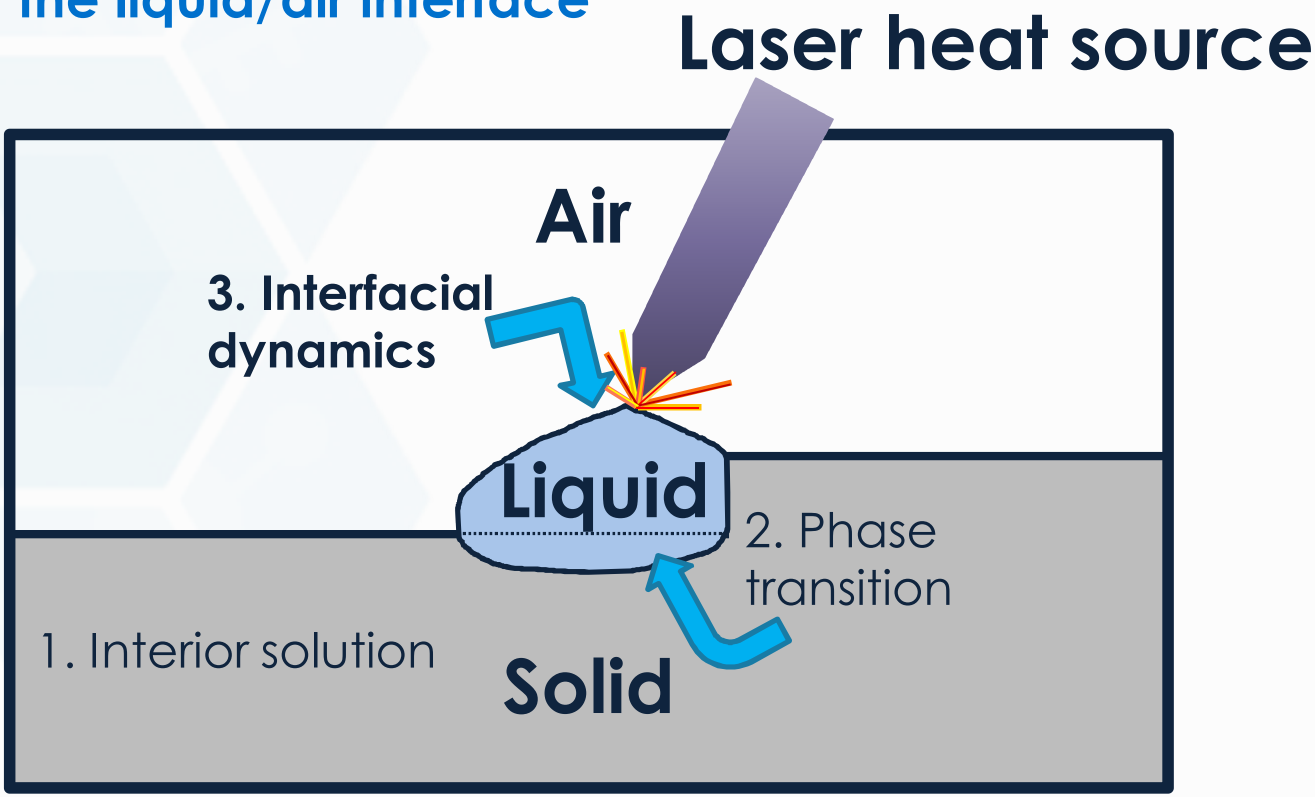
$$T(x,t) = T_S + (T_m - T_S)\frac{erfc\left(\frac{x}{2\sqrt{\alpha_S t}}\right)}{erfc(\lambda\sqrt{\alpha_L / \alpha_S})}$$

$$X(t) = 2\lambda\sqrt{\alpha_L t}$$

- Accurate but not convergent for the interfacial velocity
- Convergent in time (1st order BE) and space (2nd order) for the heat equation solution

# Functionality required to solve the melt problem

1. Solving systems of equations in the solid, liquid and air regions with moving boundaries
2. Solving the phase transition problem
3. **Tracking the liquid/air interface**

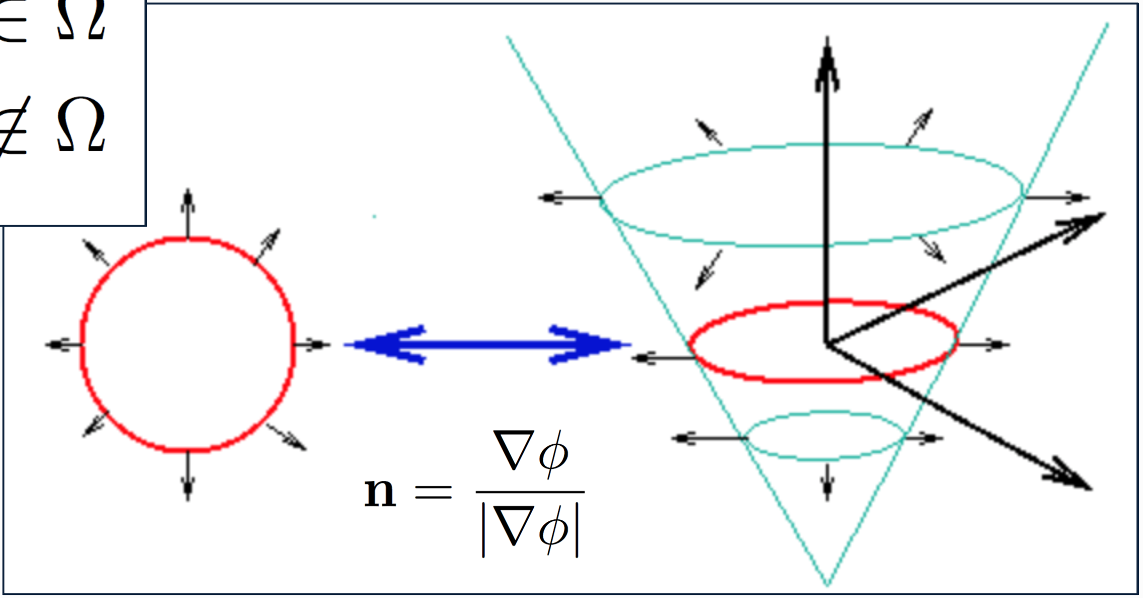


# Interface Method Options

- Interface capturing (Eulerian, e.g. level set methods)
  - ✓ Natural merging and pinch-off
  - ✓ Normal vector and curvature calculations
  - x Mass conservation problems
  - x Limited by grid size
- Interface tracking (Lagrangian particle methods)
  - ✓ Conservative by design
  - ✓ Excellent at resolving fine scale dynamics
  - x No connectivity/difficult to define normal vector/curvature
  - x Needs reseeding under distorted velocity conditions

# Level set (signed distance) method

$$\phi(\mathbf{x},t) > 0 \quad \text{for} \quad \mathbf{x} \in \Omega$$
$$\phi(\mathbf{x},t) \le 0 \quad \text{for} \quad \mathbf{x} \notin \Omega$$



- 5th order HJ-WENO scheme for the gradient operator
- 2nd order TVD RK for the time derivative

Re-initialization equation

$$\frac{\partial \phi}{\partial \tau} + S(\phi_0)(|\nabla\phi| - 1) = 0$$

$$S(\phi_0) = \frac{\phi_0}{\sqrt{\phi_0^2 + (\Delta x)^2}}.$$

# Hybrid particle-level set method

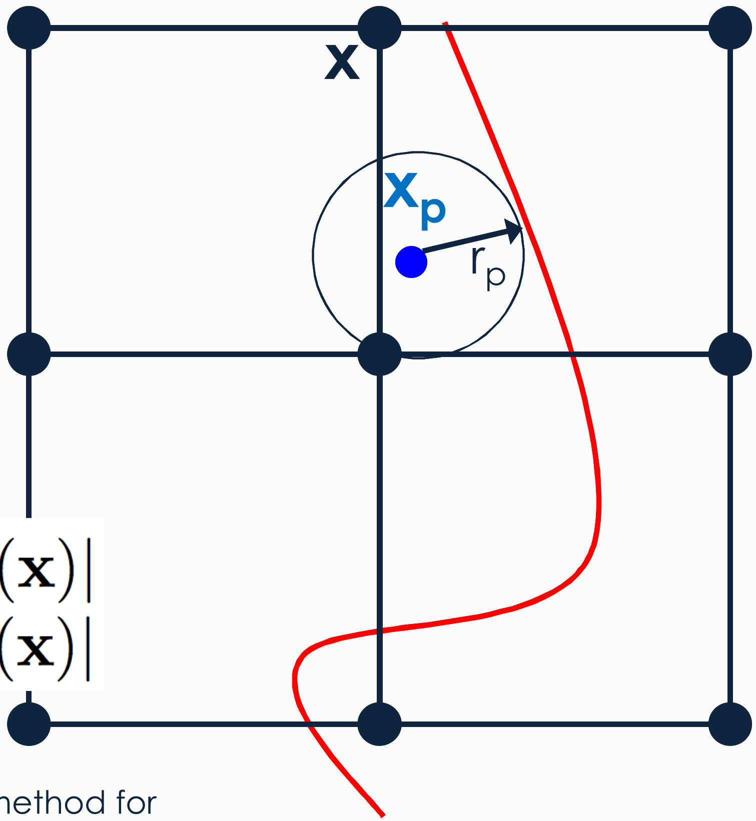
- Particles are placed near the interface and initialized with a sign and distance from the interface
- This information is used to update the level set field

$$\phi_p(\mathbf{x}) = s_p(r_p \pm |\mathbf{x} - \mathbf{x}_p|)$$

$$\phi^+(\mathbf{x}) = \max_{p \in E^+}(\phi_p, \phi)$$

$$\phi^-(\mathbf{x}) = \min_{p \in E^-}(\phi_p, \phi).$$

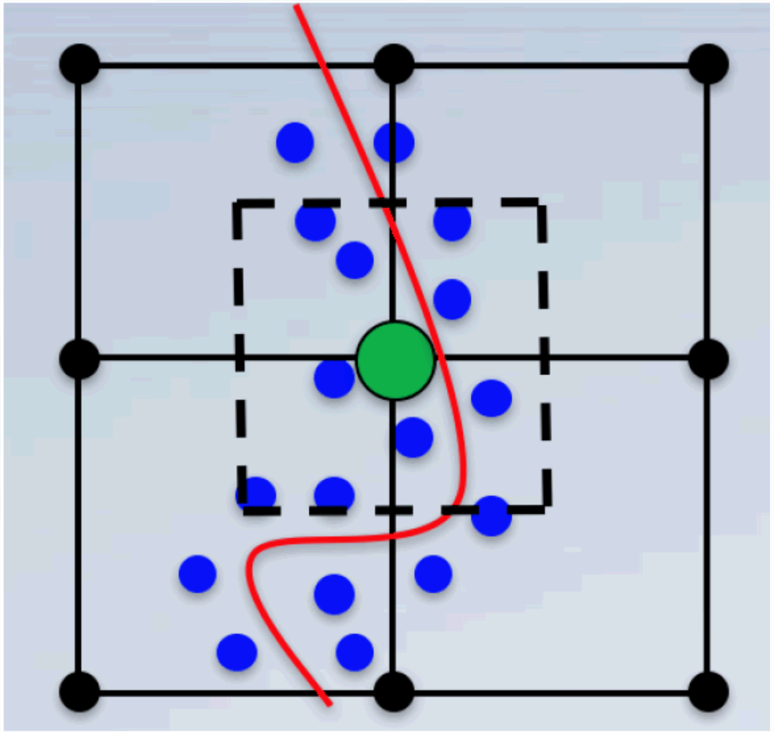
$$\phi(\mathbf{x}) = \begin{cases} \phi^+(\mathbf{x}) & \text{if} \quad |\phi^+(\mathbf{x})| \le |\phi^-(\mathbf{x})| \\ \phi^-(\mathbf{x}) & \text{if} \quad |\phi^+(\mathbf{x})| > |\phi^-(\mathbf{x})| \end{cases}$$

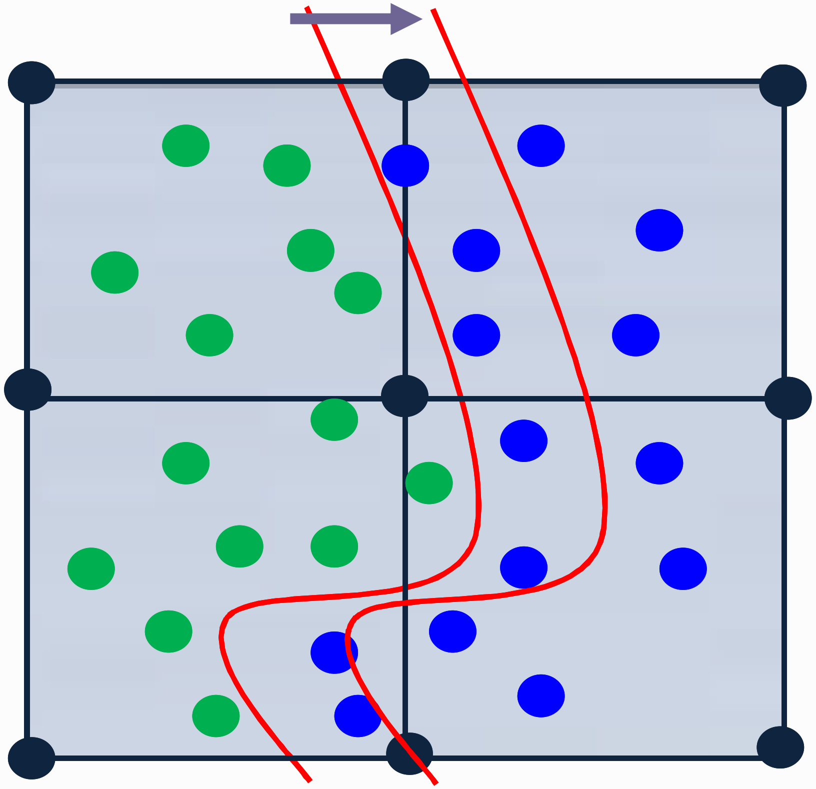



D. Enright, R. Fedkiw, J. Ferziger, I. Mitchell, A hybrid particle level set method for improved interface capturing, Journal of Computational Physics 183 (1) (2002) 83–116.

# Interpolative Particle Level Set Method

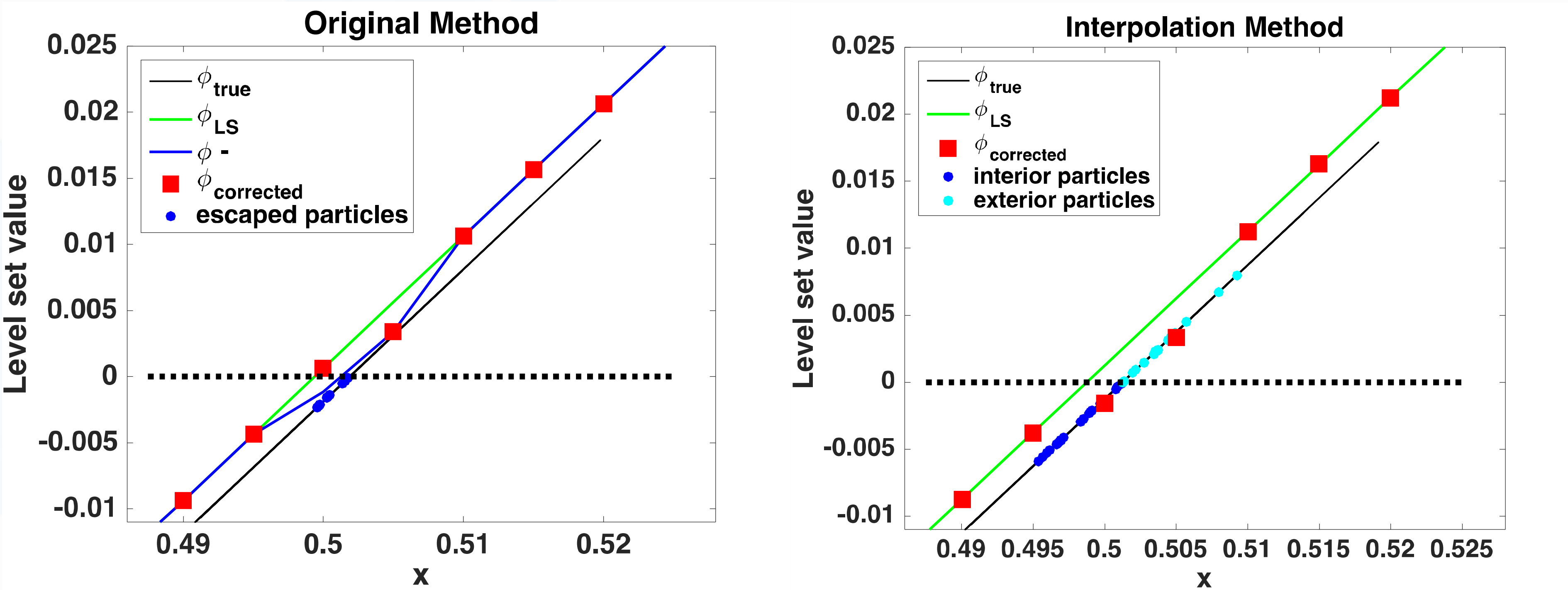
- We treat the particles as a form of Lagrangian refinement around the interface and use (bi/tri) linear interpolation to update the 'coarse' level set field on the grid, provided the number of particles near a grid point is sufficiently large.





# Particle Level Set Method Comparison

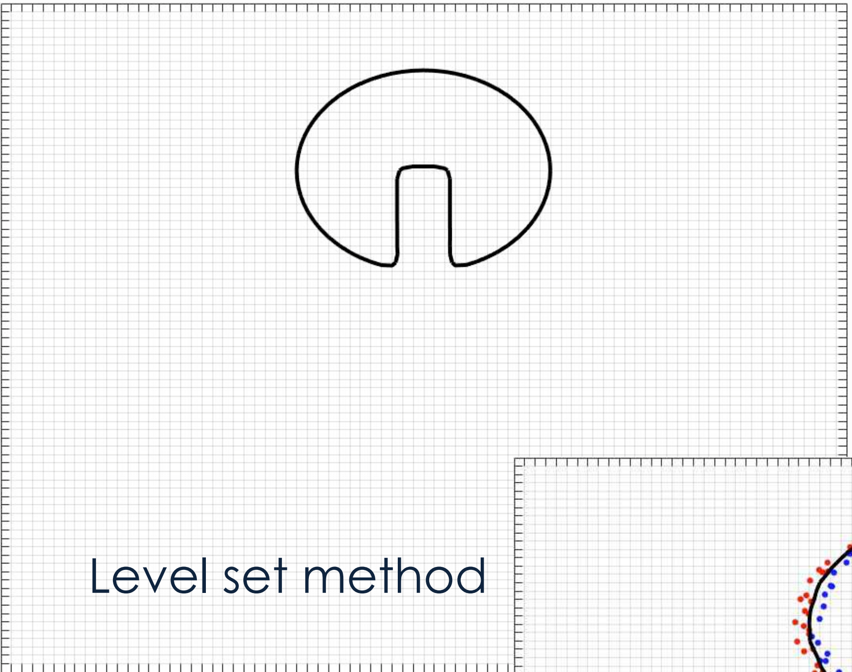
## Particle Level Set (PLS) Method[1] versus Interpolative PLS[2]

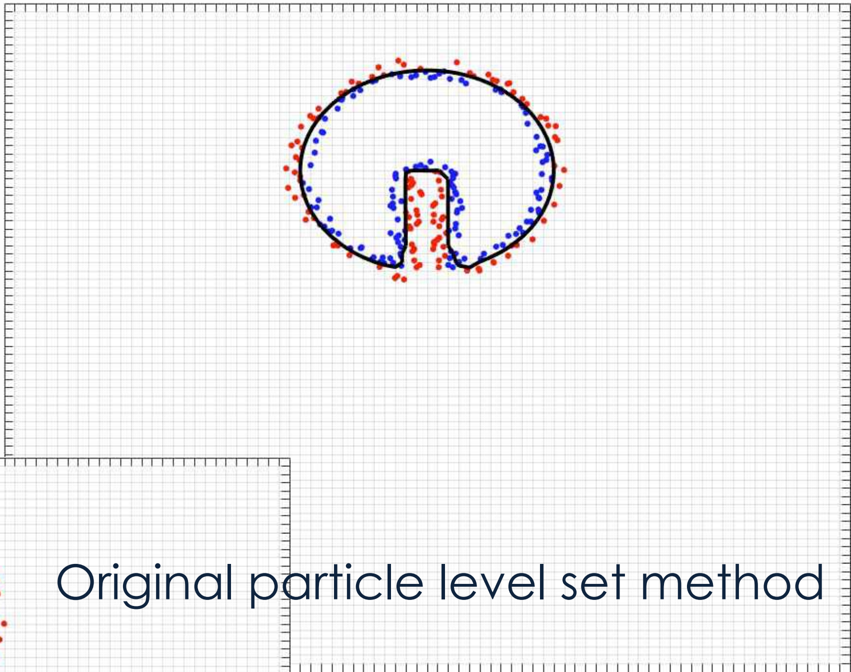


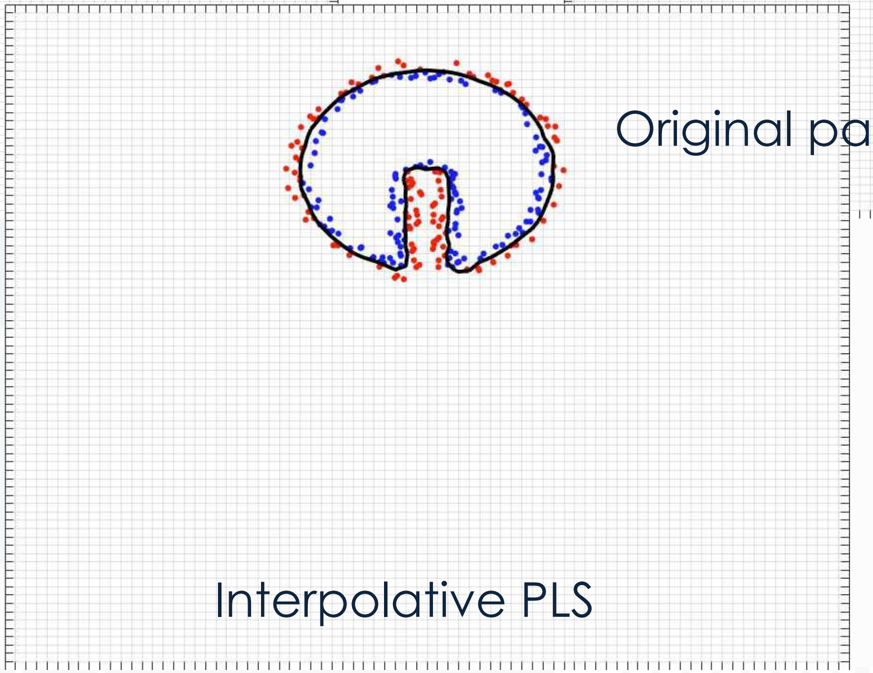

[1] Enright, Fedkiw, Ferziger, Mitchell, "A hybrid particle level set method for improved interface capturing," J. Comp. Phys. (2002).

[2] Erickson, Morris, Poliakoff, Templeton, "An interpolative particle level set method," in preparation.

# Slotted disk test for numerical diffusion (rigid body rotation)



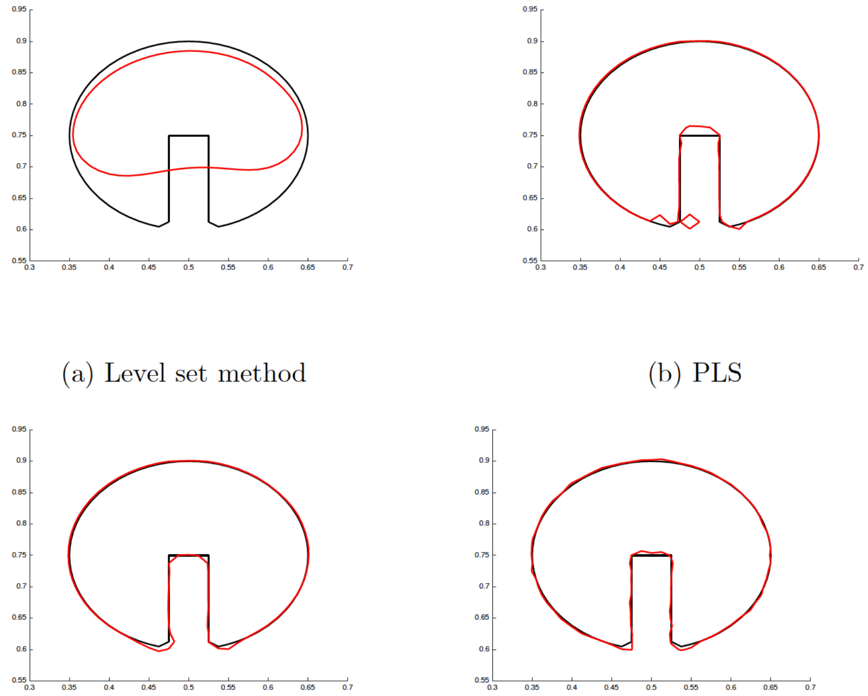




Test for the method's ability to resolve sharp corners. (80 x 80 grid)

# Slotted disk grid refinement study results

| Grid size | 40x40 | 80x80 | 160x160 |
|---|---|---|---|
| Initial LS Volume | 0.0623 | 0.0630 | 0.0632 |
| Level Set Method | 0.000 | 0.0451 | 0.0482 |
| Particle Level Set | 0.0680 | 0.0638 | 0.0509 |
| Corrected PLS | 0.0657 | 0.0645 | 0.0640 |
| Interpolative PLS | 0.0625 | 0.0633 | 0.0631 |

| Time step | 0.01 | 0.005 | 0.0025 | 0.00125 |
|---|---|---|---|---|
| LS | 0.0270 | 0.0346 | 0.0415 | 0.0451 |
| PLS | 0.0337 | 0.0482 | 0.0753 | 0.0638 |
| CPLS | 0.0684 | 0.0661 | 0.0651 | 0.0645 |
| IPLS | 0.0634 | 0.0633 | 0.0633 | 0.0633 |

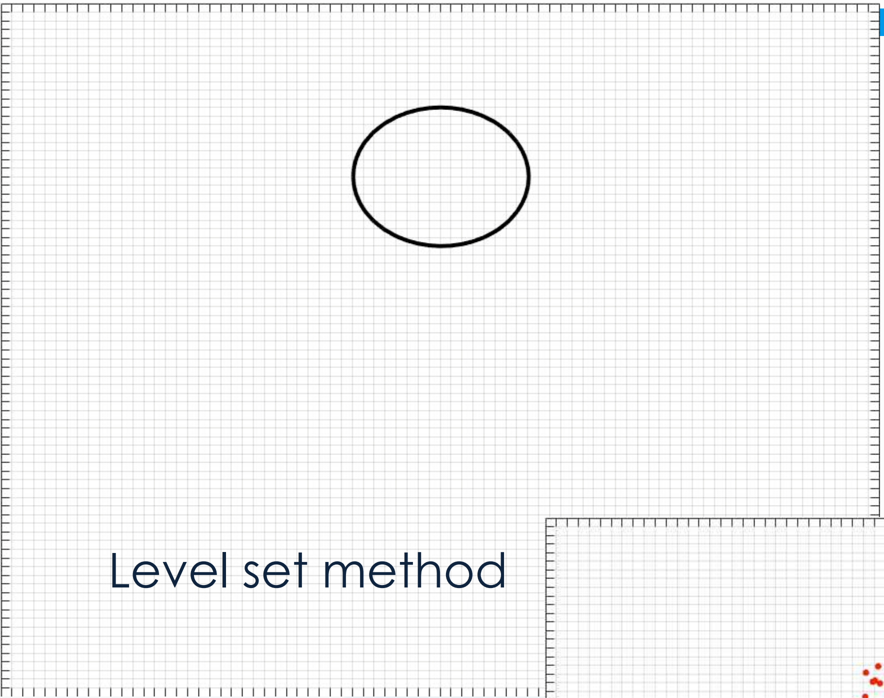


(a) Level set method (b) PLS

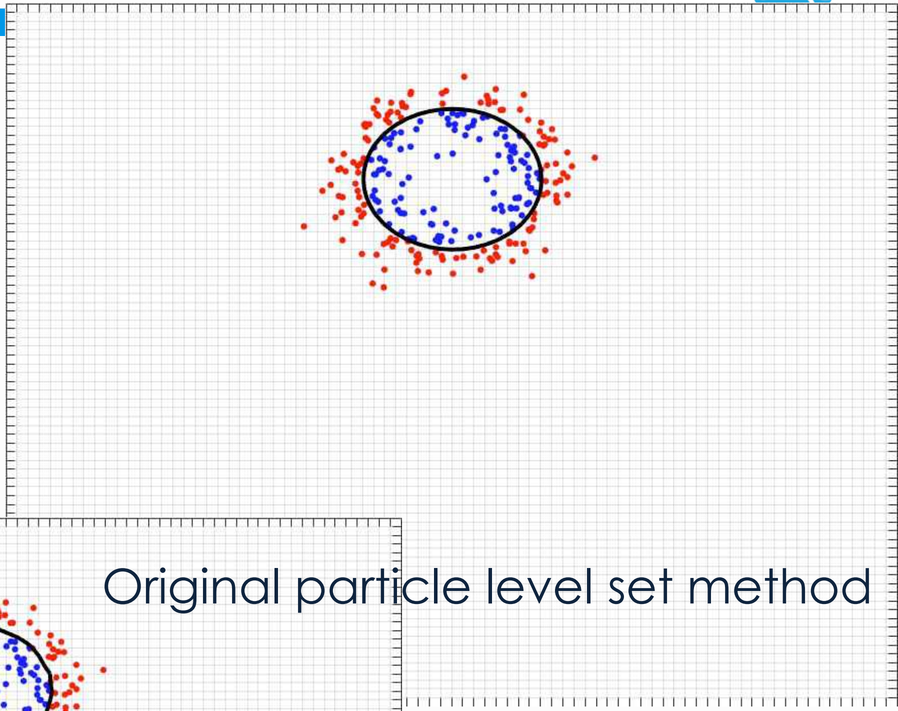
(c) Corrected PLS (d) IPLS

Initial volume versus volume after a full rotation for three different levels of grid refinement. For both particle methods we use 5000 particles. The initial volumes are listed in this table, since this is a function of spatial discretization. The analytic volume of the slotted disk is 0.0632.

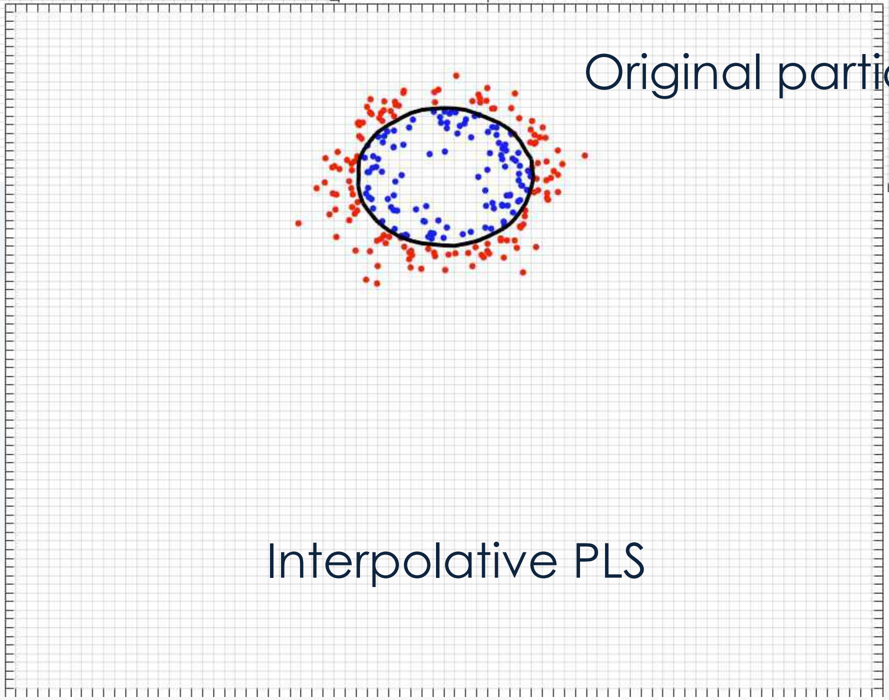
# Circle in a vortex flow test for resolving thin filaments (shearing)



Level set method



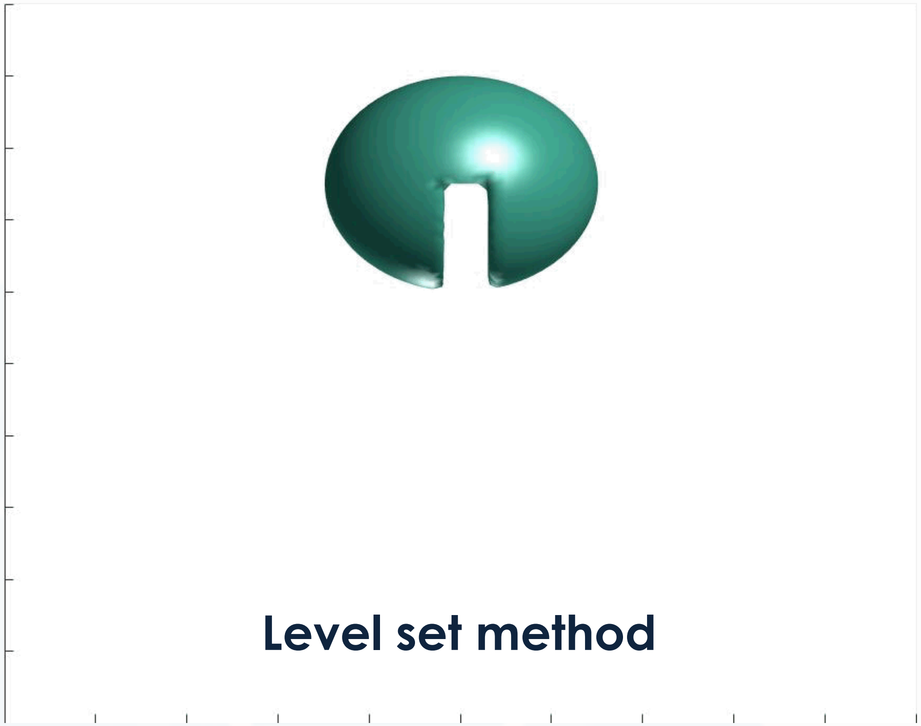
Original particle level set method

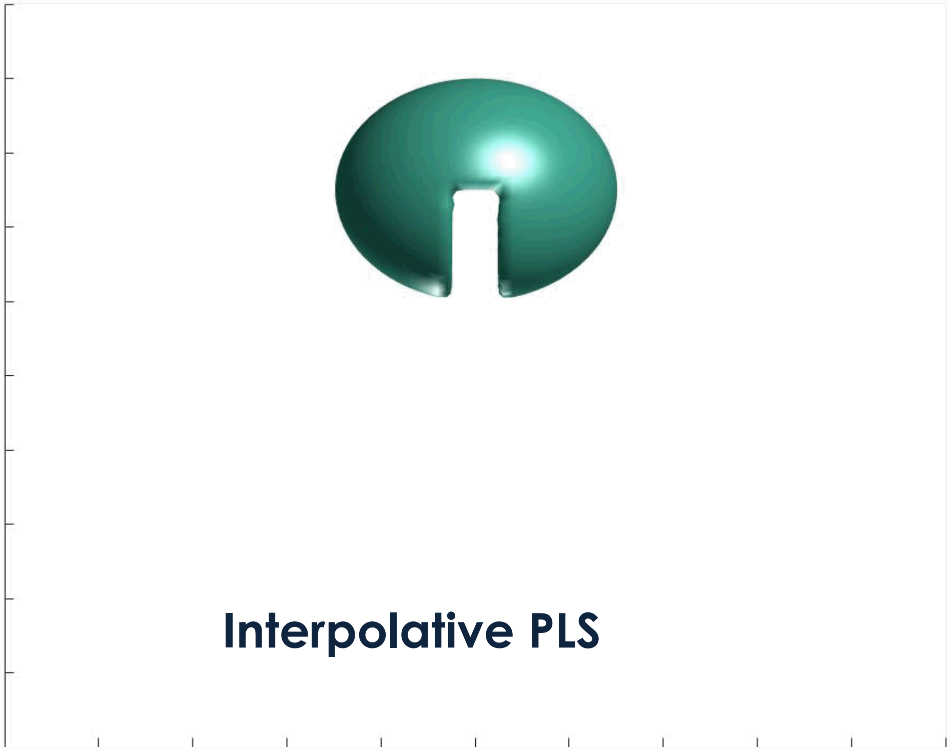


Interpolative PLS

Test for the method's ability to resolve thin filaments. (80 x 80 grid) Interpolative PLS is better able to capture the interface below the grid resolution

# 3D Slotted disk: Level set versus IPLS

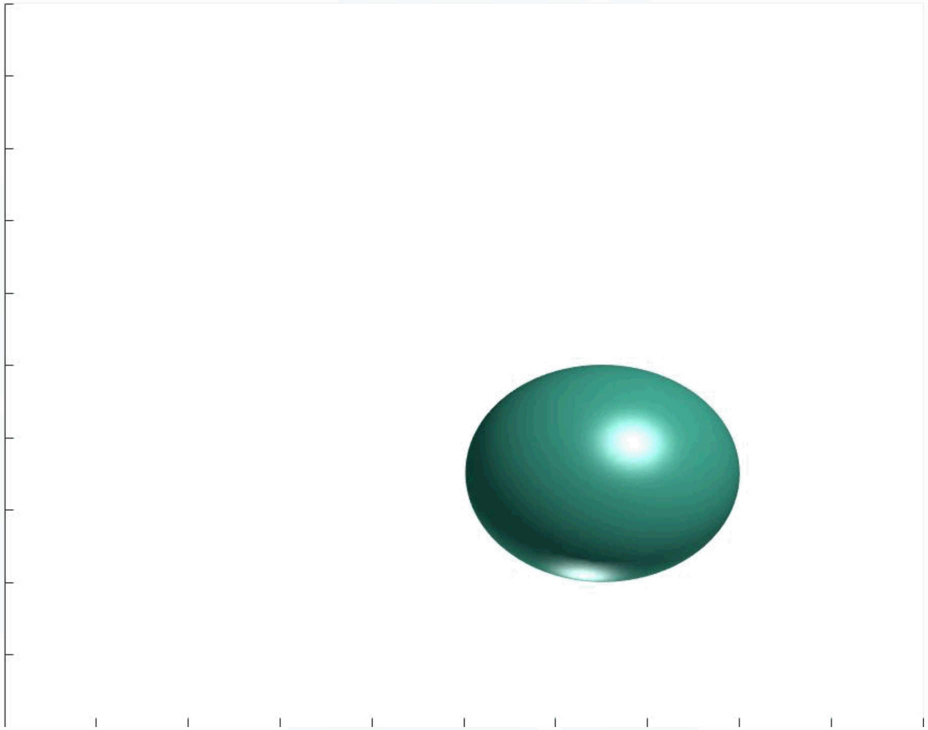


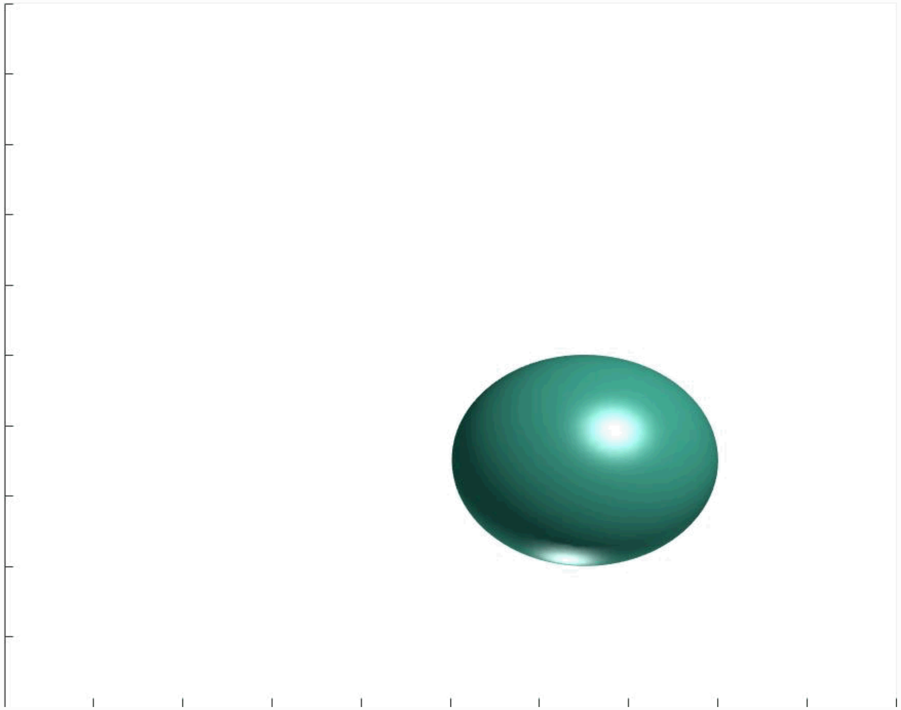

Test for the method's ability to limit the effects of numerical diffusion (100 x 100 x 100 grid)

# 3D vortex flow: Level set versus IPLS

**Level set method**



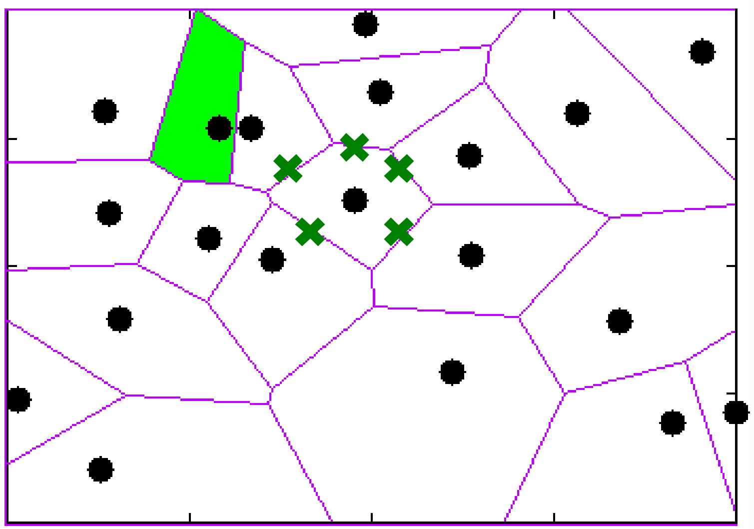
**Interpolative PLS**



Test for the method's ability to resolve thin filaments(100 x 100 x 100 grid)

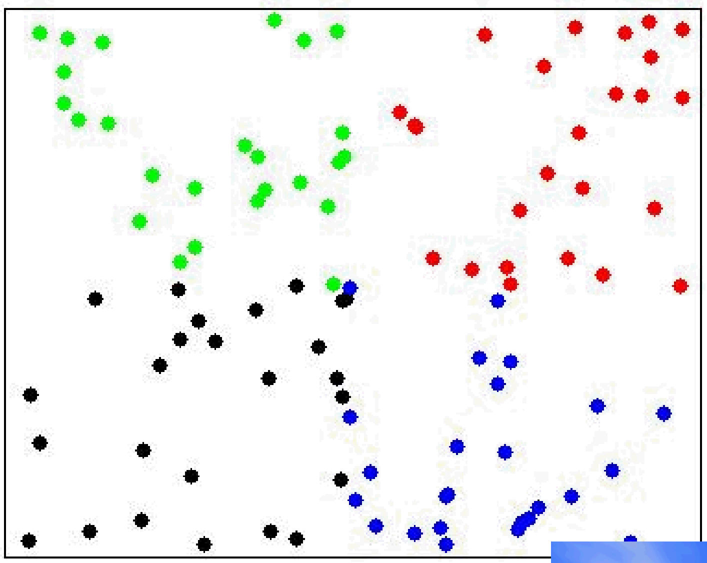
# Our mesh-free Moab software package

- Neighbor search and volume calculations: voronoi tesselation software (Voro++)
  - C++ software library for cell-based calculations
  - solve for cell volumes and stress point locations
  - nearest neighbor lists
  - has been successfully employed on very large particle systems
- Uses Trilinos (open source libraries developed at Sandia) packages for linear solvers and domain decomposition for parallel computations



Voro++ voronoi tesselation

http://math.lbl.gov/voro++/



Zoltan2 repartitioning in Trilinos

https://trilinos.org