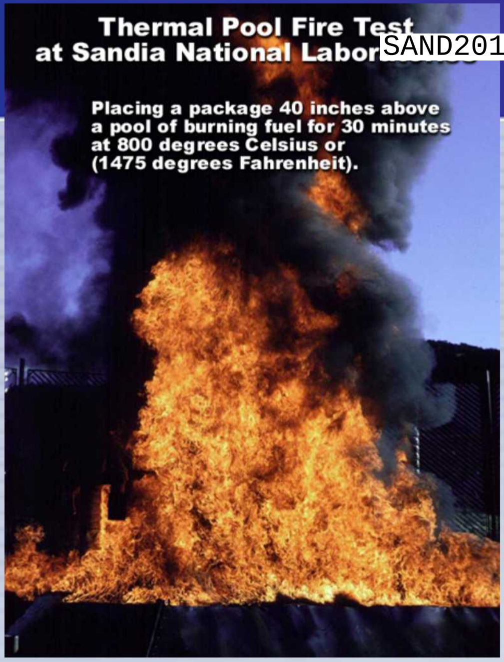
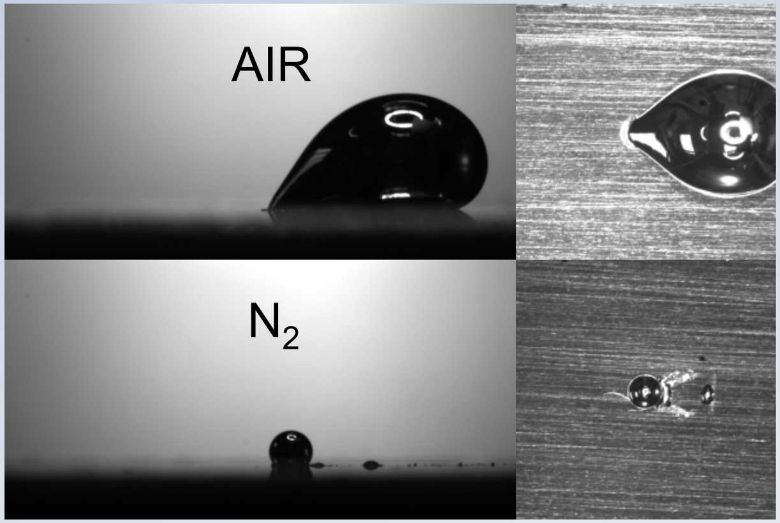
Motivation

SAND2015-7376PE

- **Sandia has the responsibility to design and qualify NW system safety in abnormal thermal environments**
  - This is a unique engineering challenge
- **Probabilistic assessments require a high degree of confidence in simulation results**
- **We must model extremely challenging environments with many complicated, interacting physical phenomena**
  - Melting and decomposition are two important examples





Cerrolow-117 metal droplets on incline, C. Brooks (2012)

Point Collocation RKPM

$$u^{\mathrm{a}}(x, y) = \sum_{I=1}^{\mathrm{NP}} \bar{w}_{\mathrm{d}}(x - x_I, y - y_I) u(x_I, y_I) \Delta V_I$$

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

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

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

Novel Convolution-based Approach

- **Compare math, meets Q2 milestone, prototype results, 1D FD consistency, relationship between filtered and un-filtered, stress points**

$$\int_{\partial\Omega} w(\mathbf{y}-\mathbf{x})\nabla u(\mathbf{y})\cdot\mathbf{n}\,dS_{\mathbf{y}} - \int_{\Omega}\nabla_{\mathbf{y}} w(\mathbf{y}-\mathbf{x})\cdot\nabla u(\mathbf{y})\,d\mathbf{y} = \int_{\Omega} w(\mathbf{y}-\mathbf{x})f(\mathbf{y})\,d\mathbf{y}$$

$$A\mathbf{u} = \mathbf{f}.$$

$$\mathbf{f}_i = \sum_{n=1}^{N} w(\mathbf{y}_i - \mathbf{x}_n)f(\mathbf{y}_n)\Delta V_n$$

$$A_{ij} = \sum_{n=1}^{N} \nabla_{\mathbf{y}} w(\mathbf{y}_i - \mathbf{x}_n)\cdot\mathbf{D}_{j,\mathbf{y}_n}\Delta V_n$$

$$u(\mathbf{x}) =$$

$$\sum_{n=1}^{N_n} w(\mathbf{y}_n-\mathbf{x})u(\mathbf{y}_n)\Delta V_n - \alpha\sum_i \frac{\partial u}{\partial x_i}\sum_{n=1}^{N_n} w(\mathbf{y}_n-\mathbf{x})\Delta V_n(y^0_{n,i}-x_i)$$

$$-\frac{\alpha^2}{2}\sum_{i,j}\frac{\partial u}{\partial x_i x_j}\sum_{n=1}^{N_n} w(\mathbf{y}_n-\mathbf{x})\Delta V_n(y^0_{n,i}-x_i)(y^0_{n,j}-x_j) + O(\alpha^3)$$

Quadrature & Solution Error

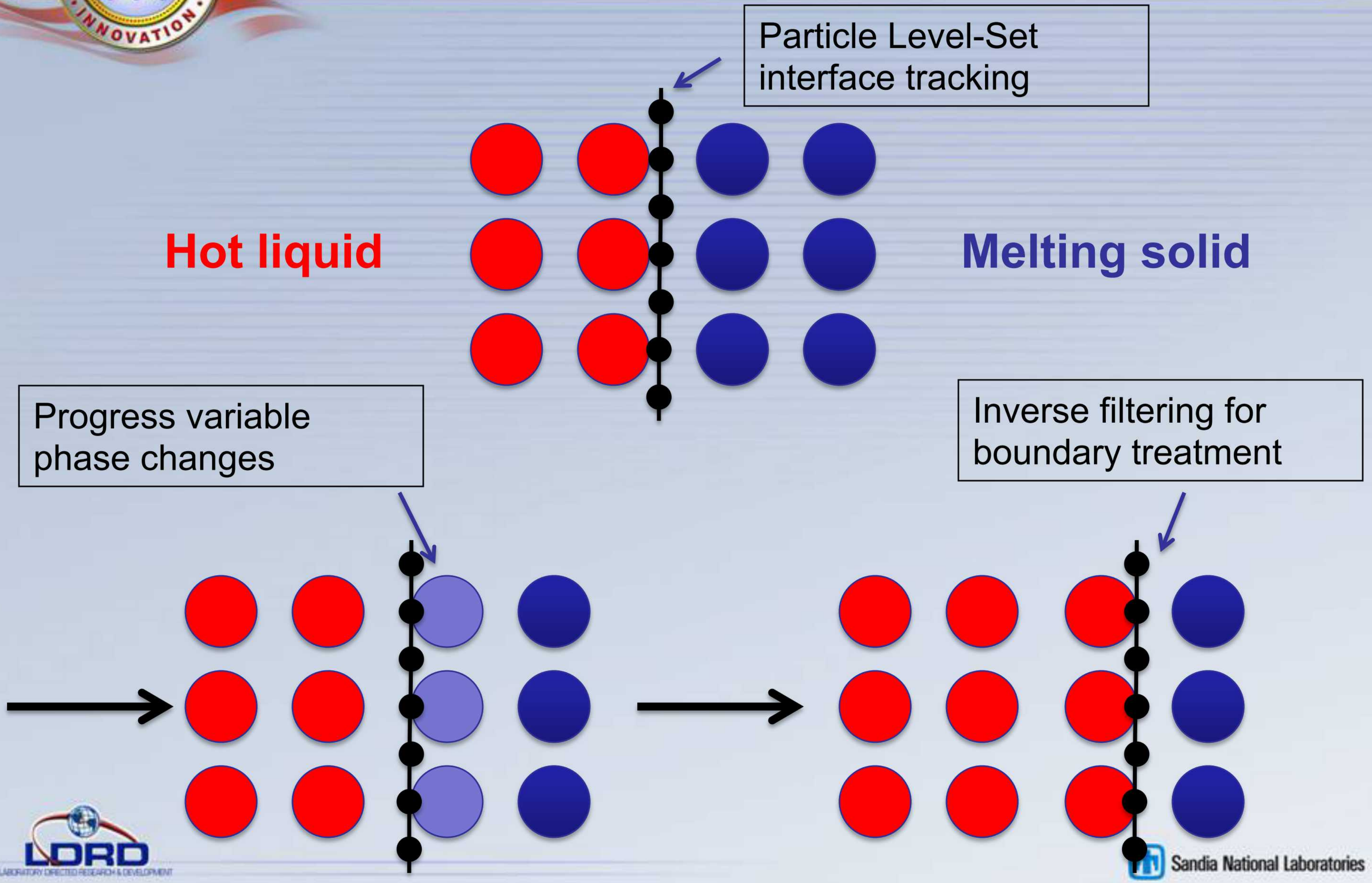
- **Holistic analysis, solution error terms and conditions**

$$\int_\Omega w(y-x)g(y)dy = \int_\Omega w(y-x)\left(g(x) + g'(x)(y-x) + \frac{g''(x)}{2}(y-x)^2 + O((y-x)^3)\right) dy$$
$$= g(x)\int_\Omega w(y-x)dy + g'(x)\int_\Omega w(y-x)(y-x)dy + \frac{g''(x)}{2}\int_\Omega w(y-x)(y-x)^2 dy + \dots$$

$$\int_\Omega \nabla_y w(y-x)u'(y)dy = \int_\Omega \nabla_y w(y-x)\left(u'(x) + u''(x)(y-x) + \frac{u'''}{2}(y-x)^2 + O((y-x)^3)\right) dy$$
$$= u'(x)\int_\Omega \nabla_y w(y-x)dy + u''(x)\int_\Omega \nabla_y w(y-x)(y-x)dy + \frac{u'''(x)}{2}\int_\Omega \nabla_y w(y-x)(y-x)^2 dy + \dots$$

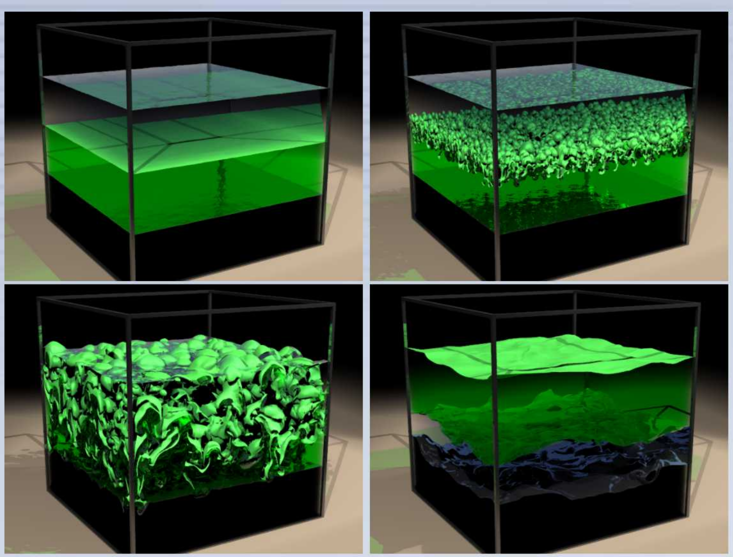
$$\int_\Omega \nabla_y w(y-x)dy = w(y_{\max}-x) - w(y_{\min}-x) \equiv 0$$
$$\int_\Omega \nabla_y w(y-x)(y-x)dy = \int_\Omega w(y-x)dy$$
$$\int_\Omega \nabla_y w(y-x)(y-x)^2 dy = \int_\Omega w(y-x)(y-x)dy$$

Interfacial Melting Dynamics



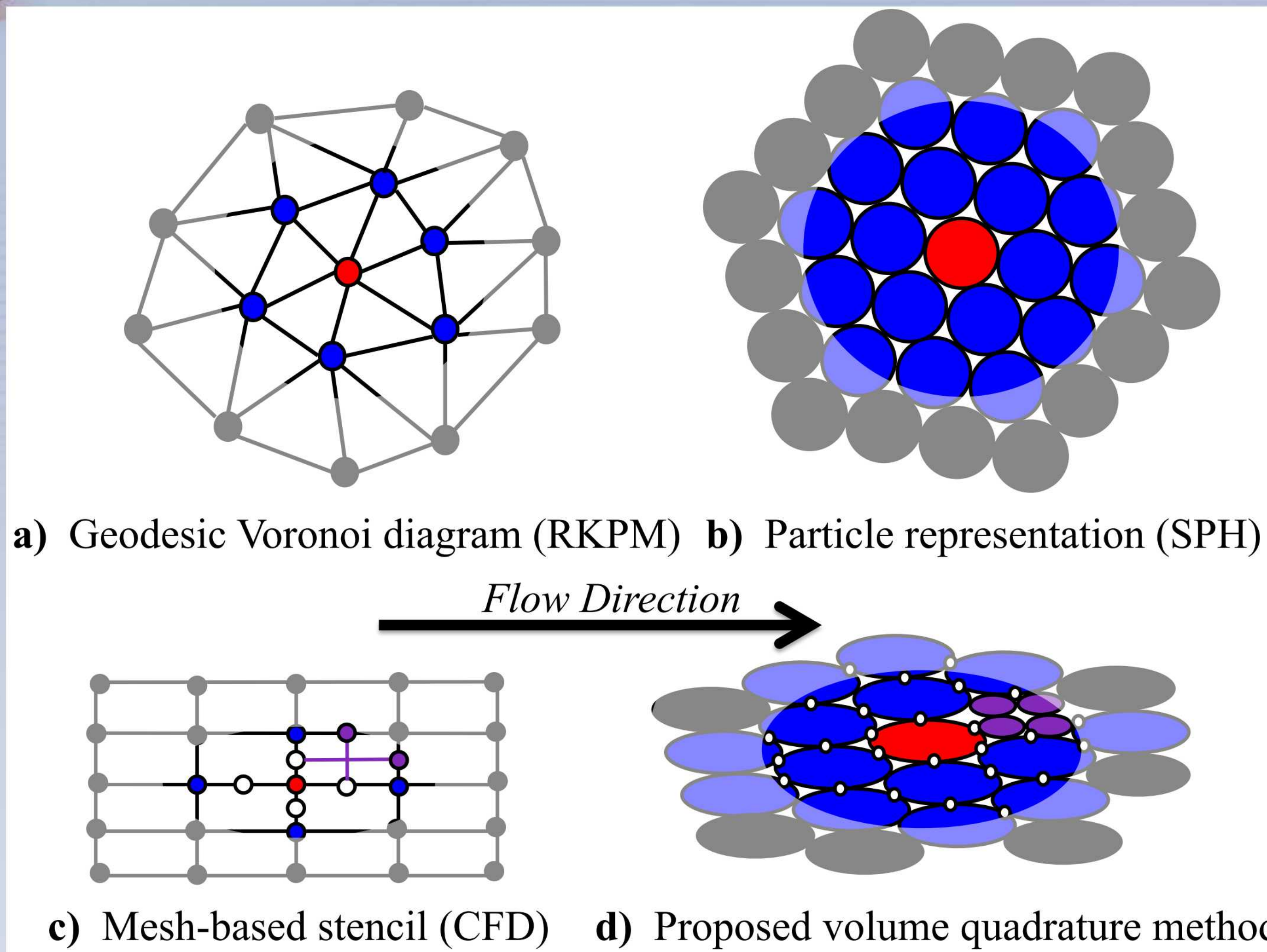
Key Objectives

- **Demonstrate a verifiable mesh-free method**
  - Quadrature error estimates
  - Adaptive quadrature
  - Verification demonstration
- **Free surface effects**
  - Nearest neighbor identification
  - Error estimates and adaptivity
  - Oxidation model
- **Solid/Fluid phase change**
  - Particle level-set method
  - Mesh-free solid model
  - Progress-variable melting model
  - Interfacial kernel adaptivity



SPH Simulation of the Rayleigh-Taylor Instability
Losasso *et al.* 2007

So What's New Here?

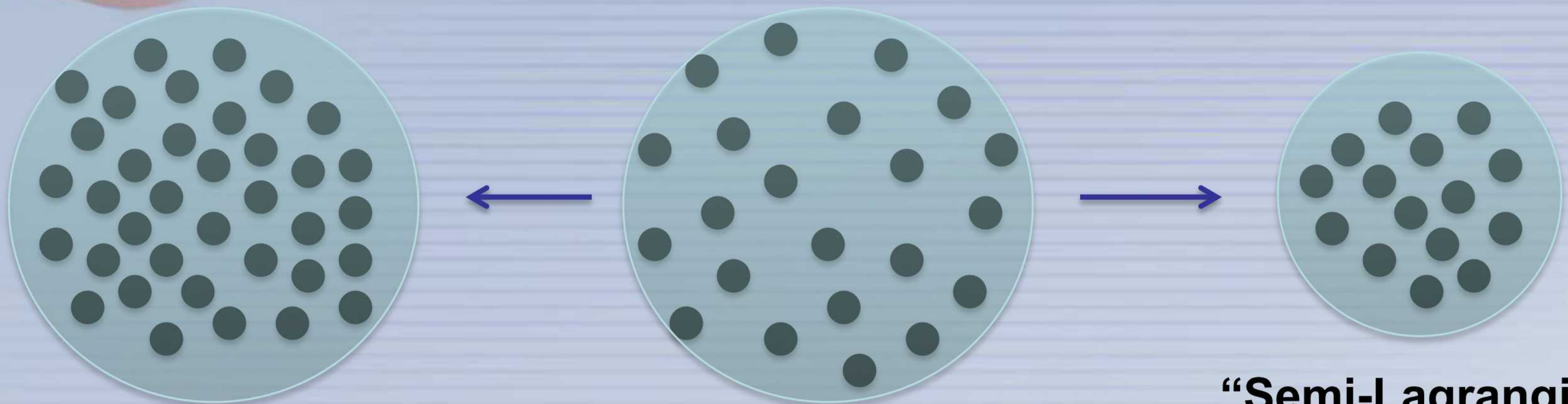


a) Geodesic Voronoi diagram (RKPM) **b)** Particle representation (SPH)

c) Mesh-based stencil (CFD) **d)** Proposed volume quadrature method

Verification & Validation

Support of kernel function *G*



Increased quadrature point density

Original

"Semi-Lagrangian" Dilation parameter refinement

Fictitious pressure from Prakash *et al.*

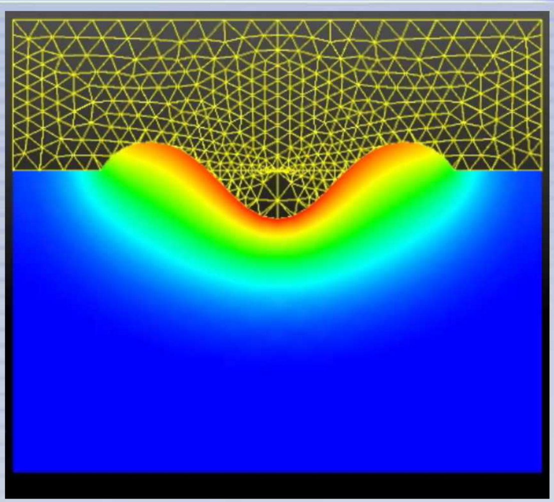
$$P = P_0\left[\left(\frac{\rho}{\rho_0}\right)^{\gamma} - 1\right] \qquad \frac{\gamma P_0}{\rho_0} = 100\mathrm{V}^2 \qquad \gamma = 7\text{, not 1.4 for ideal gas law}$$

Our proposed consistent pressure

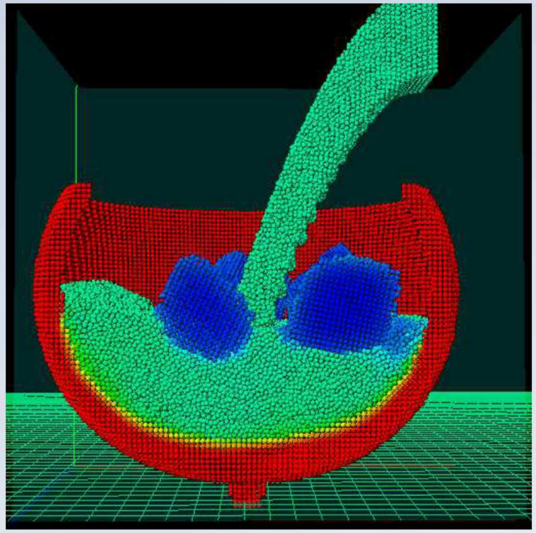
$$\int_Z P(z)\left(\int_Y \left(\nabla G(z,y)\right)^T \left(\nabla G(y,x)\right)\,dy\right)dz = \int_Z \mathbf{v}(z)\cdot\nabla G(z,x)\,dz$$

Computational Approaches

- **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
    - Multiphysics code coupling necessitates cross-package interaction
- **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
    - Phase transitions relatively unexplored



CDFEM of Laser Weld, D. Noble



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

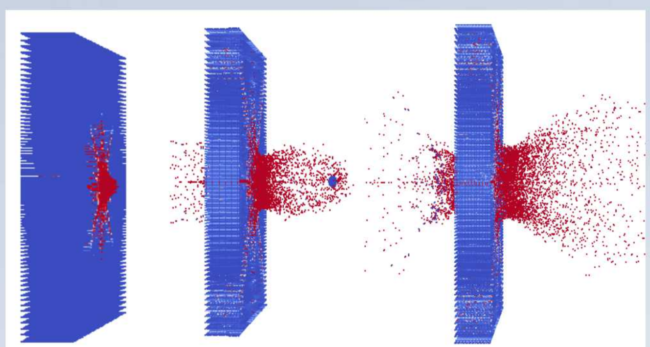
Existing Mesh-Free Methods

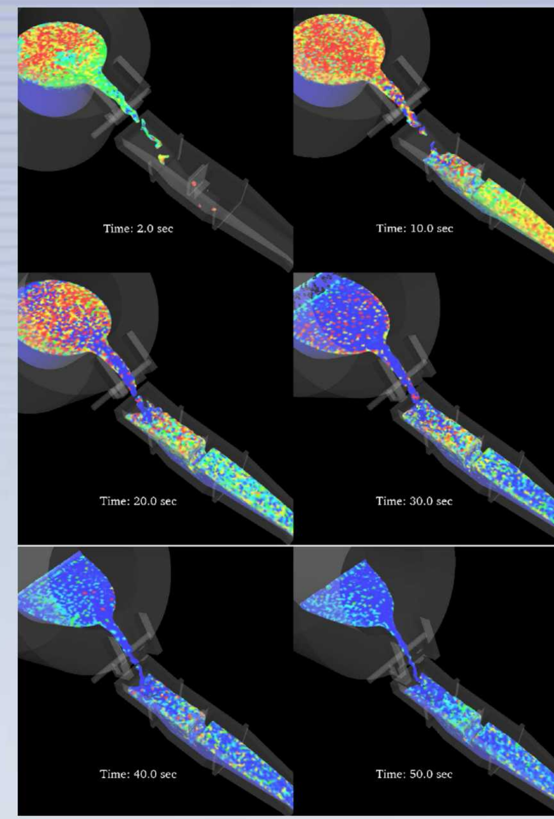
Motivating problem: Al melt, relocation, & oxidation

Particle methods (SPH, DPD, etc.) have had more impact on fluids, but tend to be less rigorous

Integral-based methods (RKPM, PD, etc.) are more rigorous, but have been more successfully used for solids

Particle Penetration using RKPM, Chen (2013)

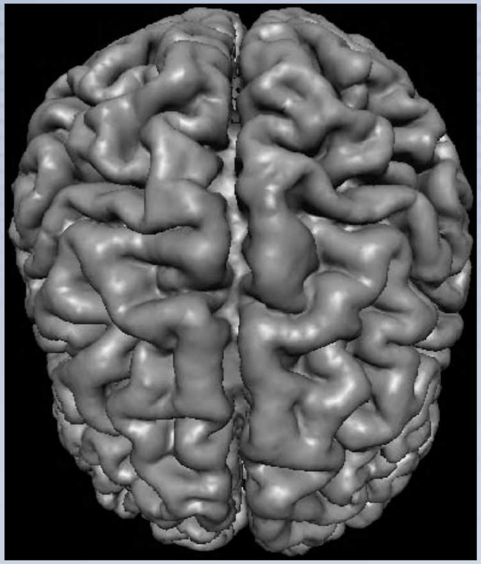




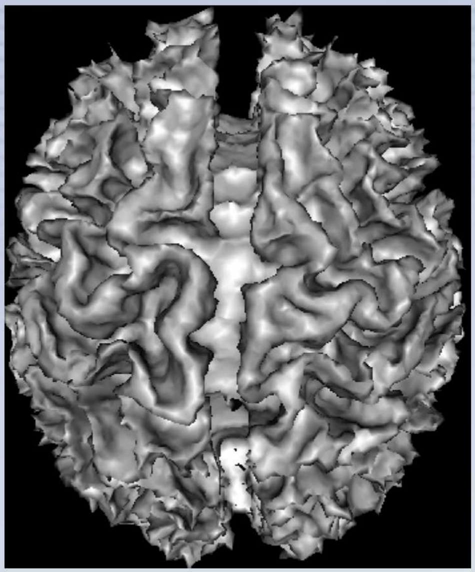
Cast house molten aluminum flow and oxidation sing SPH, Prakash *et al.* (2009)

Free Surface Effects

Adaptive RKPM for Extraction of the Cortical Surface,
Xu *et al.* 2006

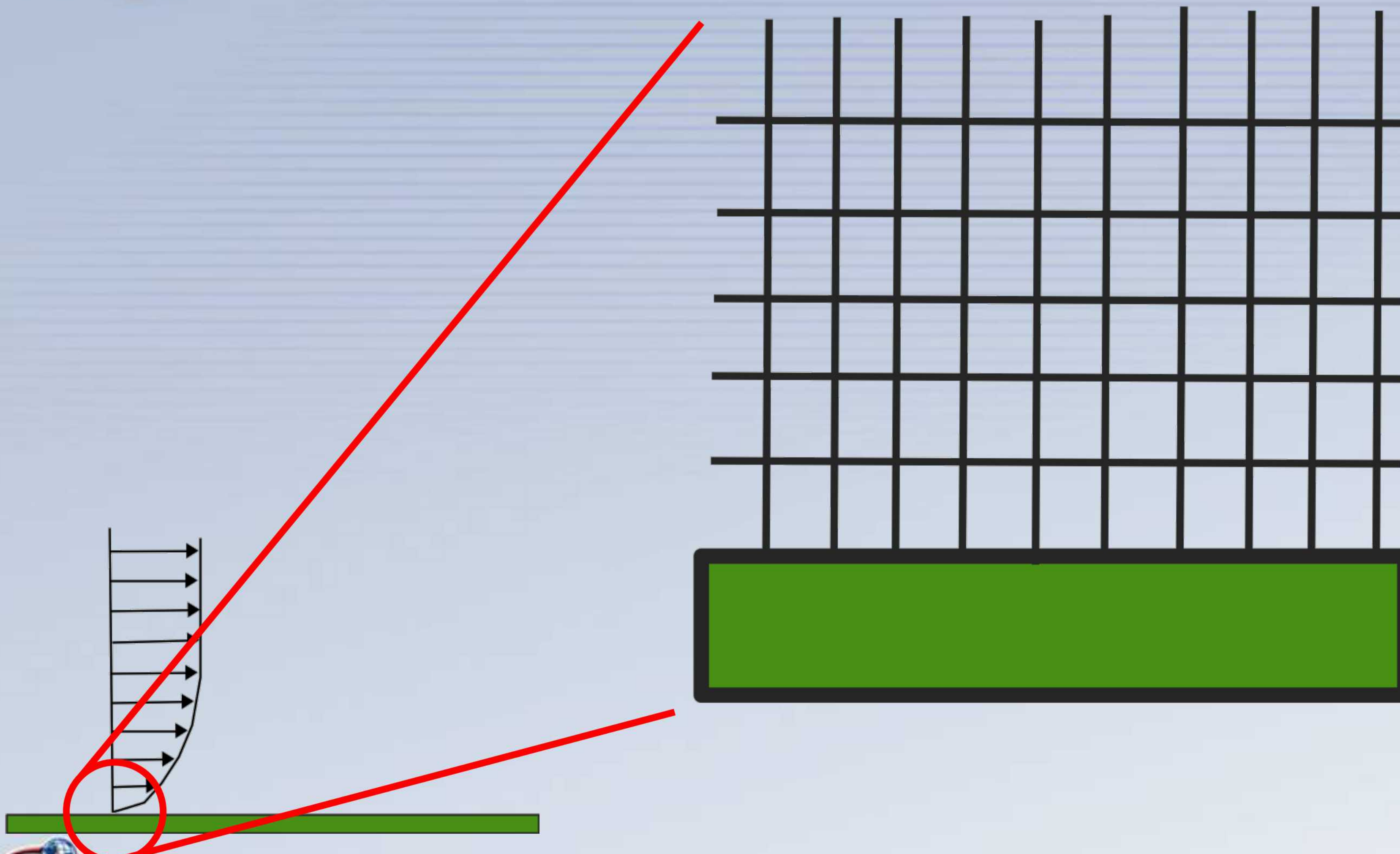


Cortical surface

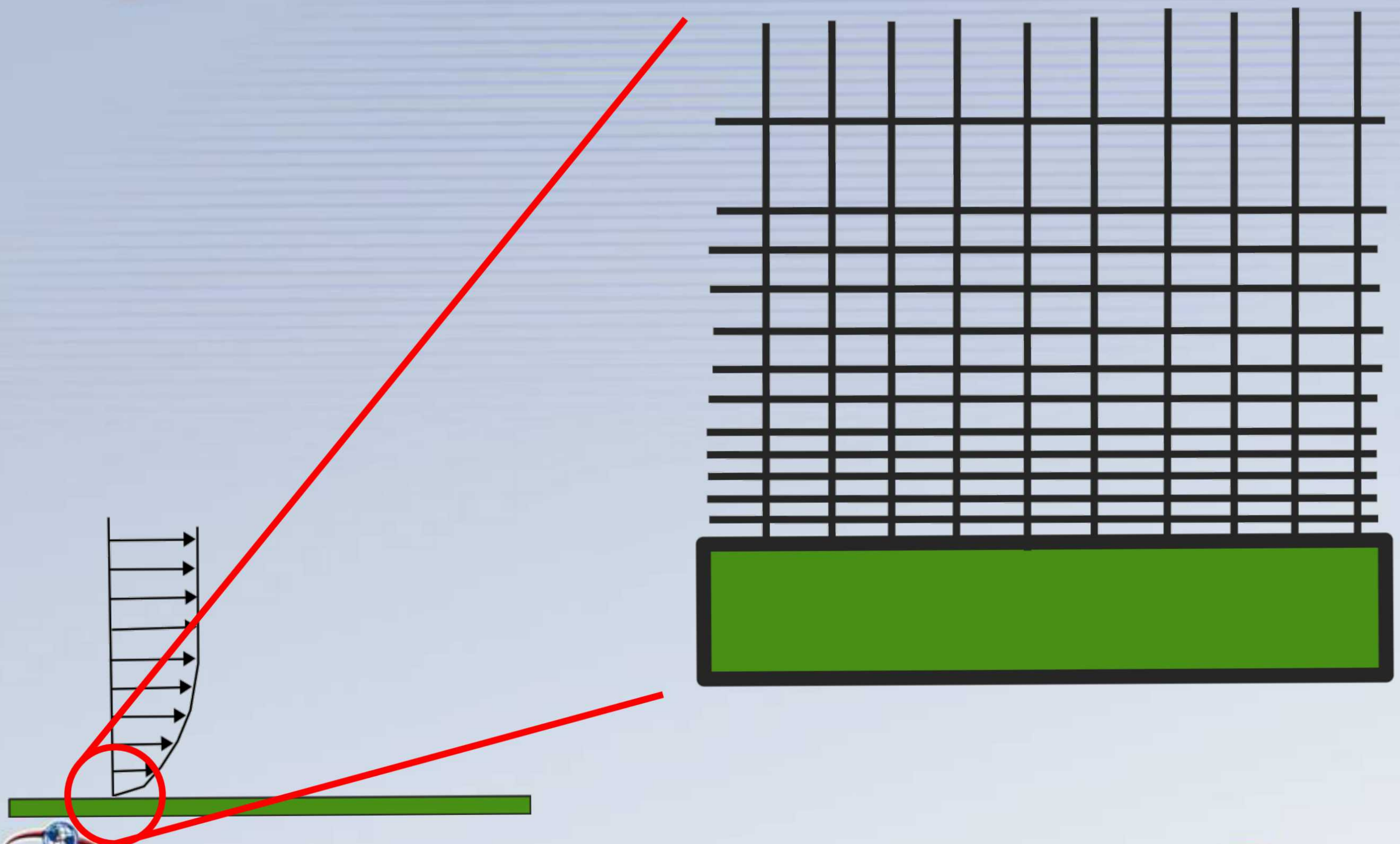


Extracted gray-white matter surface

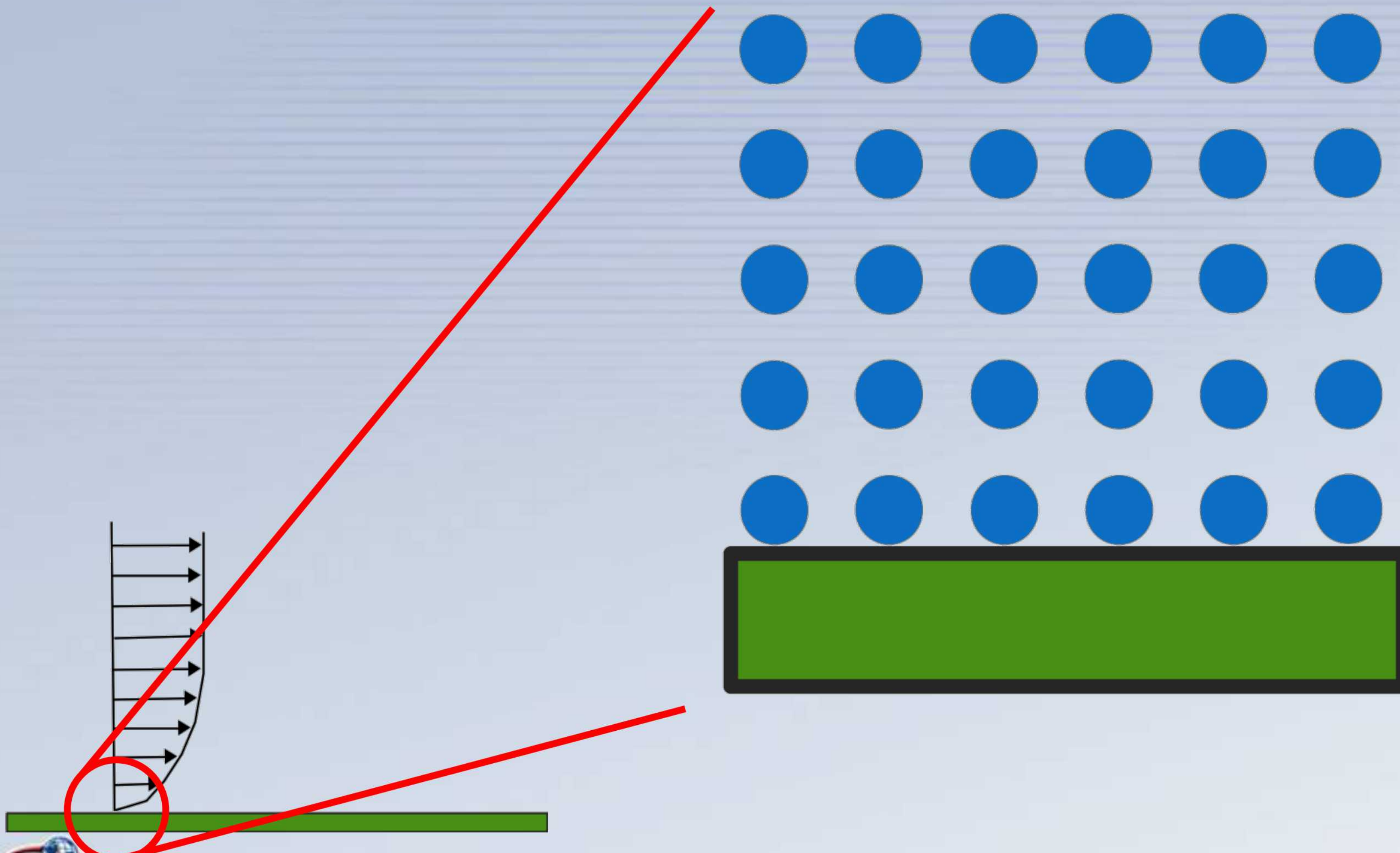
Maintaining High-Order Quadrature



Maintaining High-Order Quadrature



Maintaining High-Order Quadrature



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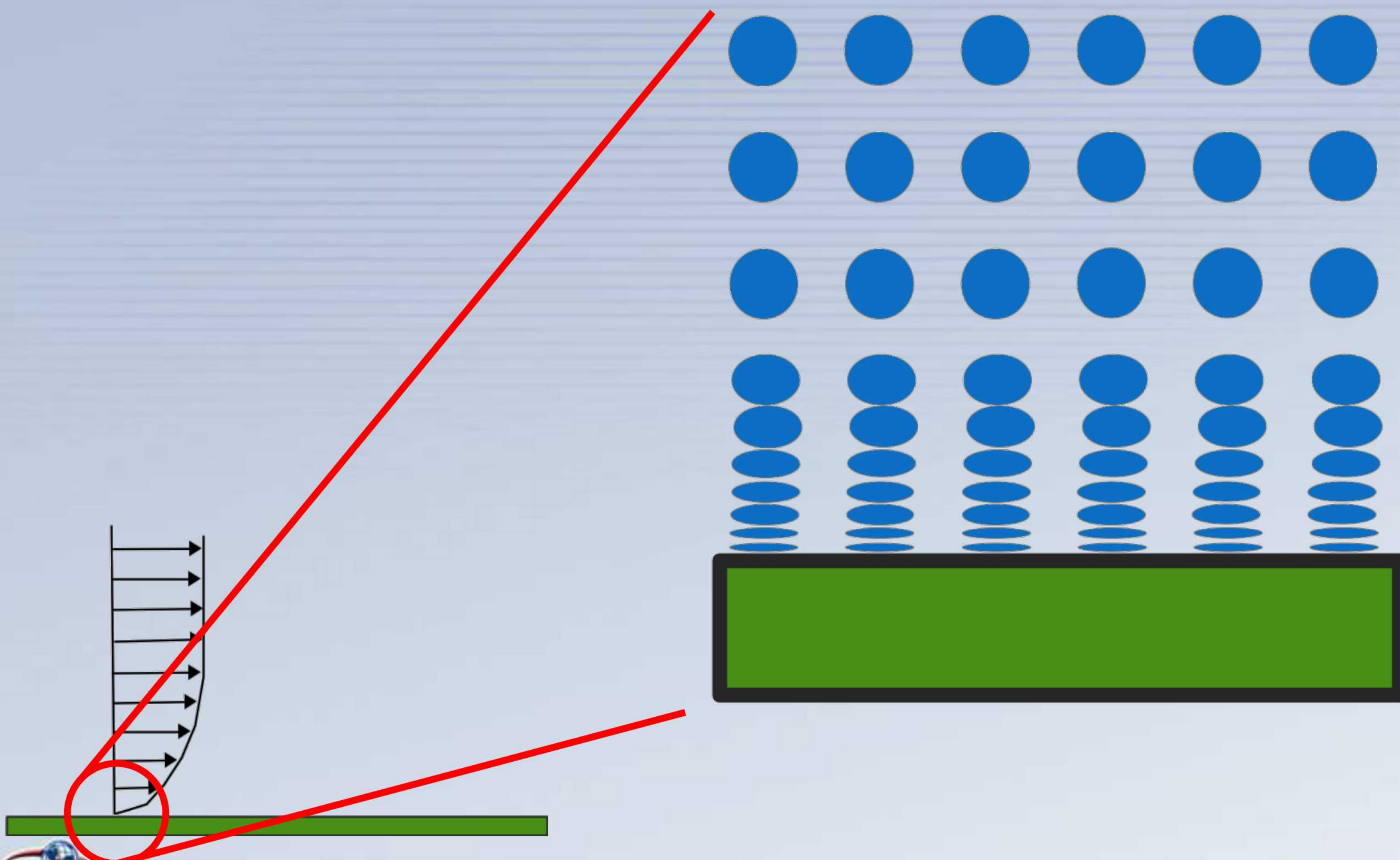
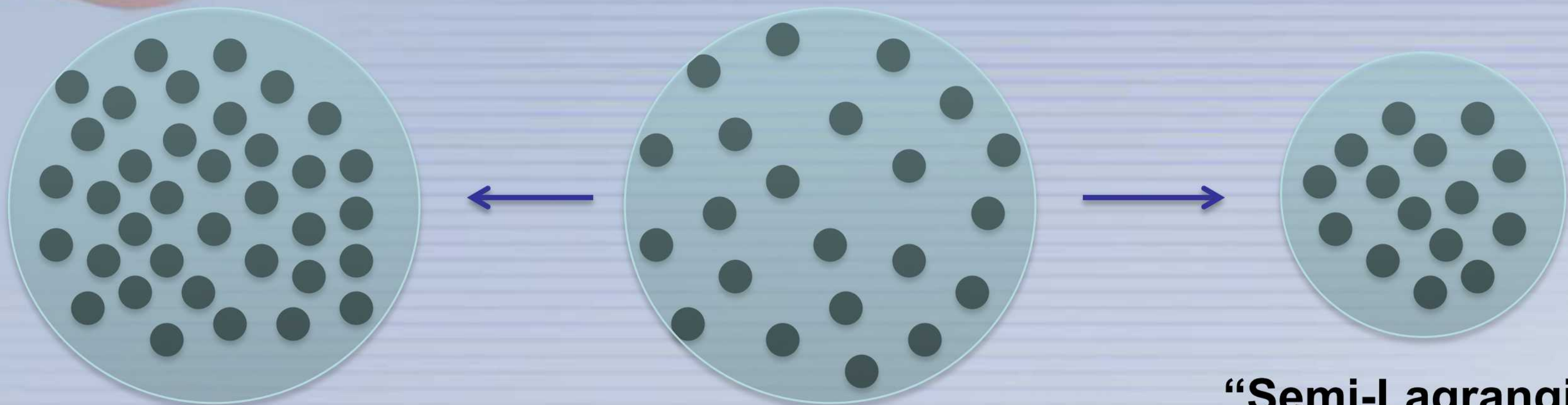


Verification & Validation

Support of kernel function *G*



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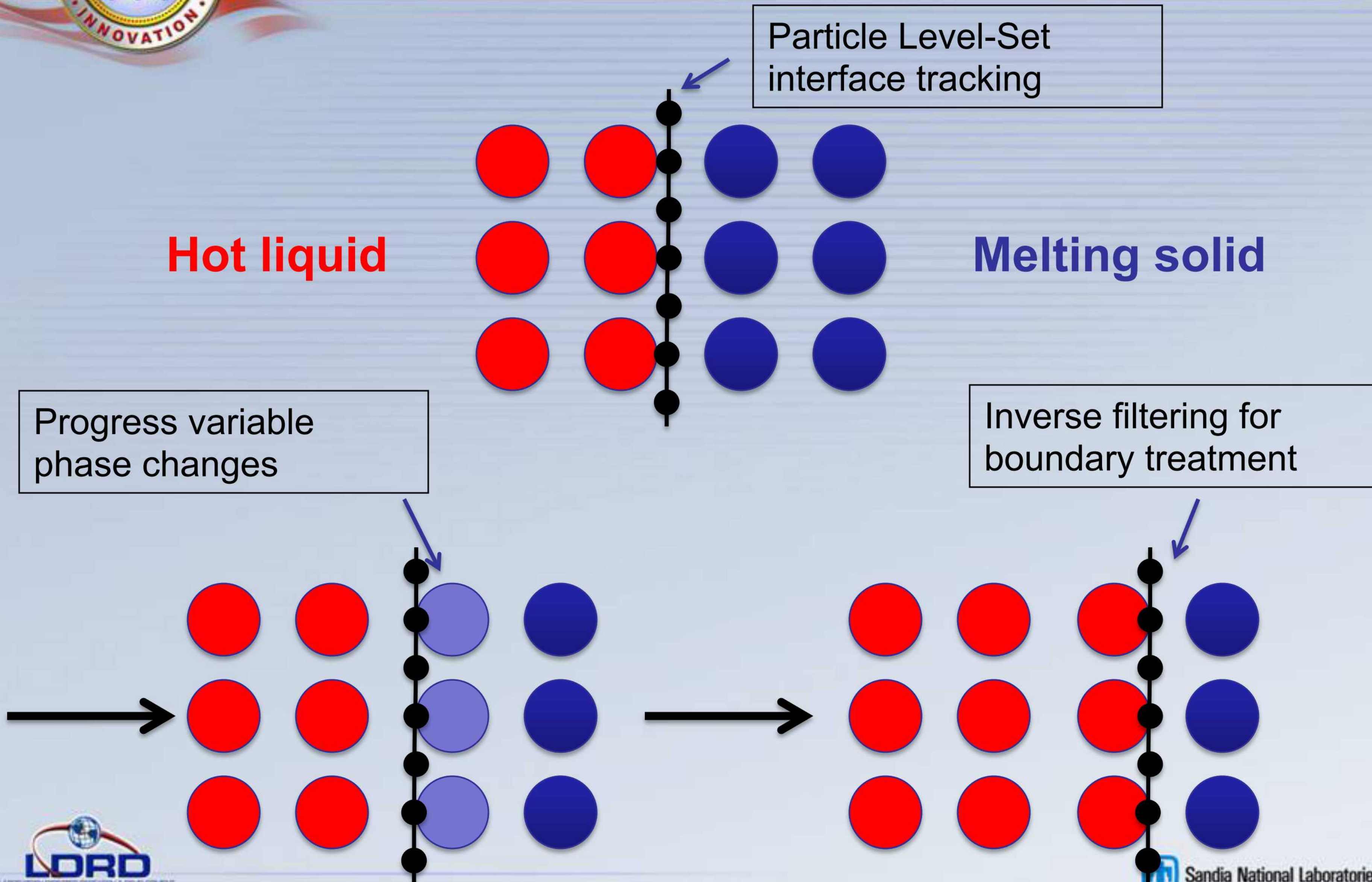
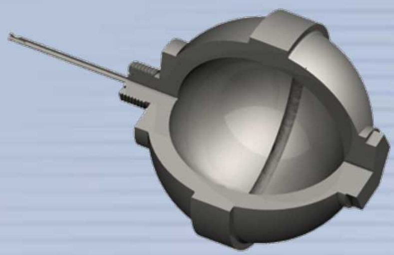
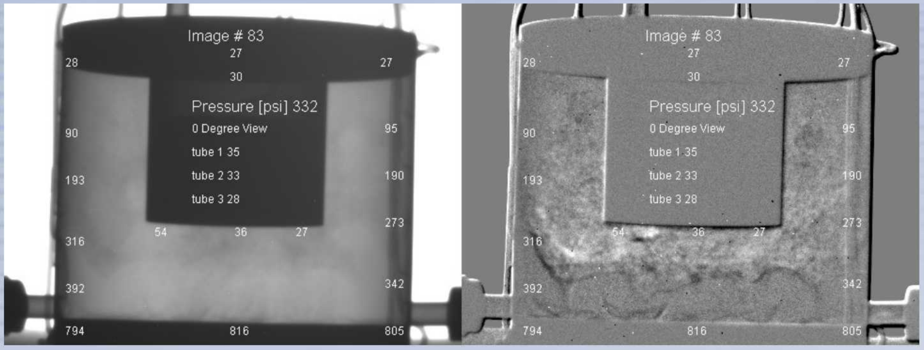
Interfacial Melting Dynamics



Impact and Future

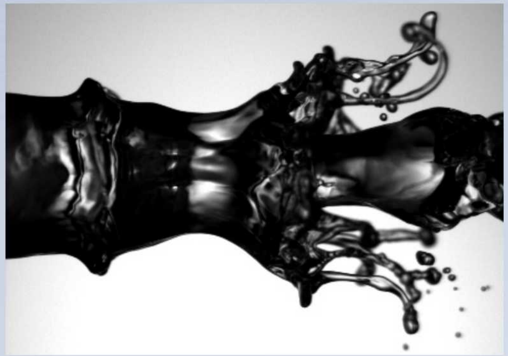


Welding/Manufacturing



Foam decomposition

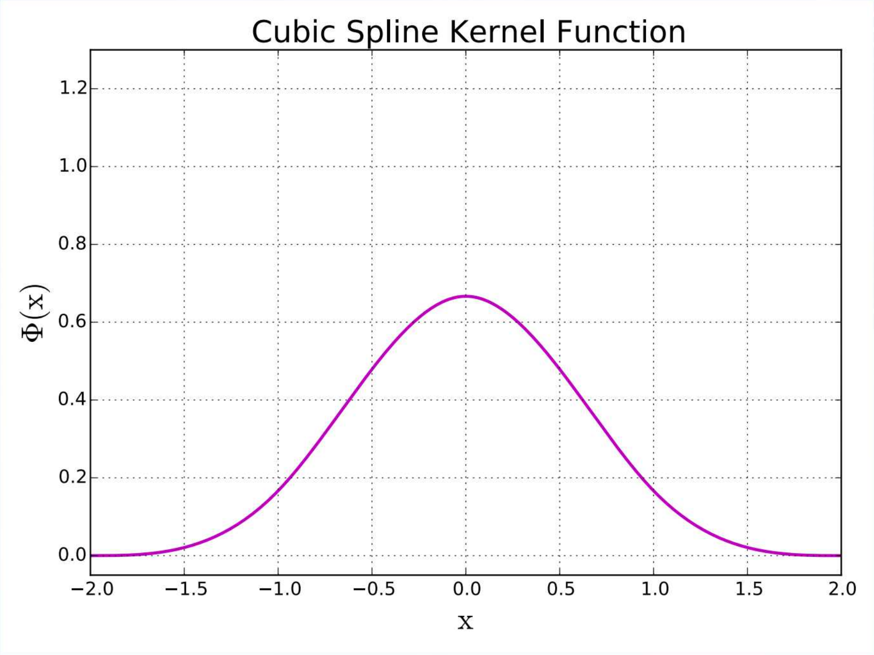
NW safety assessments



Liquid fuel spray break-up

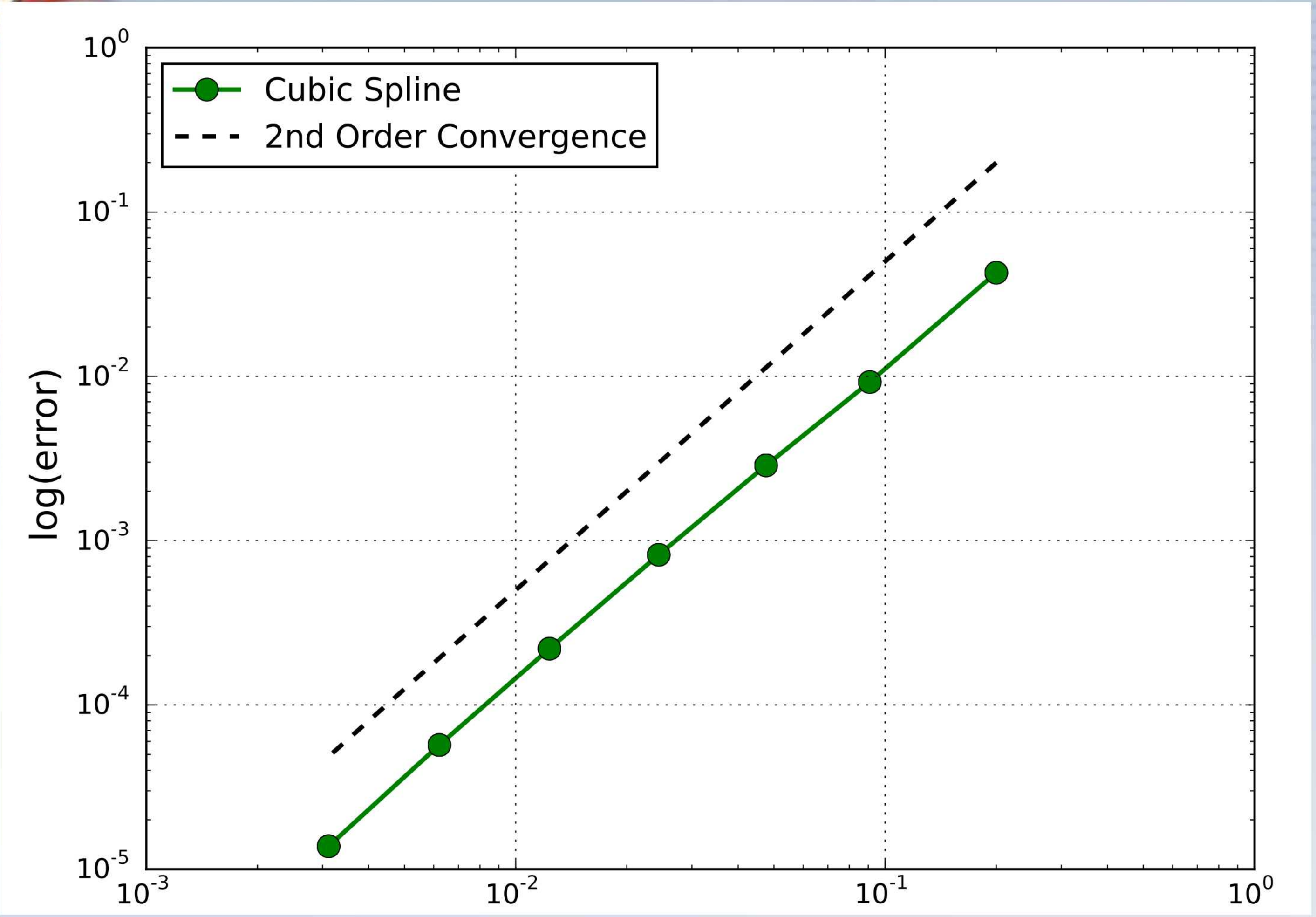
Splash modeling

Quadrature Error for Kernel Functions



- Most widely used smoothing kernel function.
- Resembles a Gaussian functions while having a compact support
- Second derivative is a piecewise linear, which reduces stability properties

Convergence for 2nd Order PDE



$$\frac{\partial^2 u}{\partial x^2} = \frac{105}{2}x^2 - \frac{15}{2}, \quad u(x=0) = 3/8, \quad u(x=1) = 17/2 \quad u = \frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}$$

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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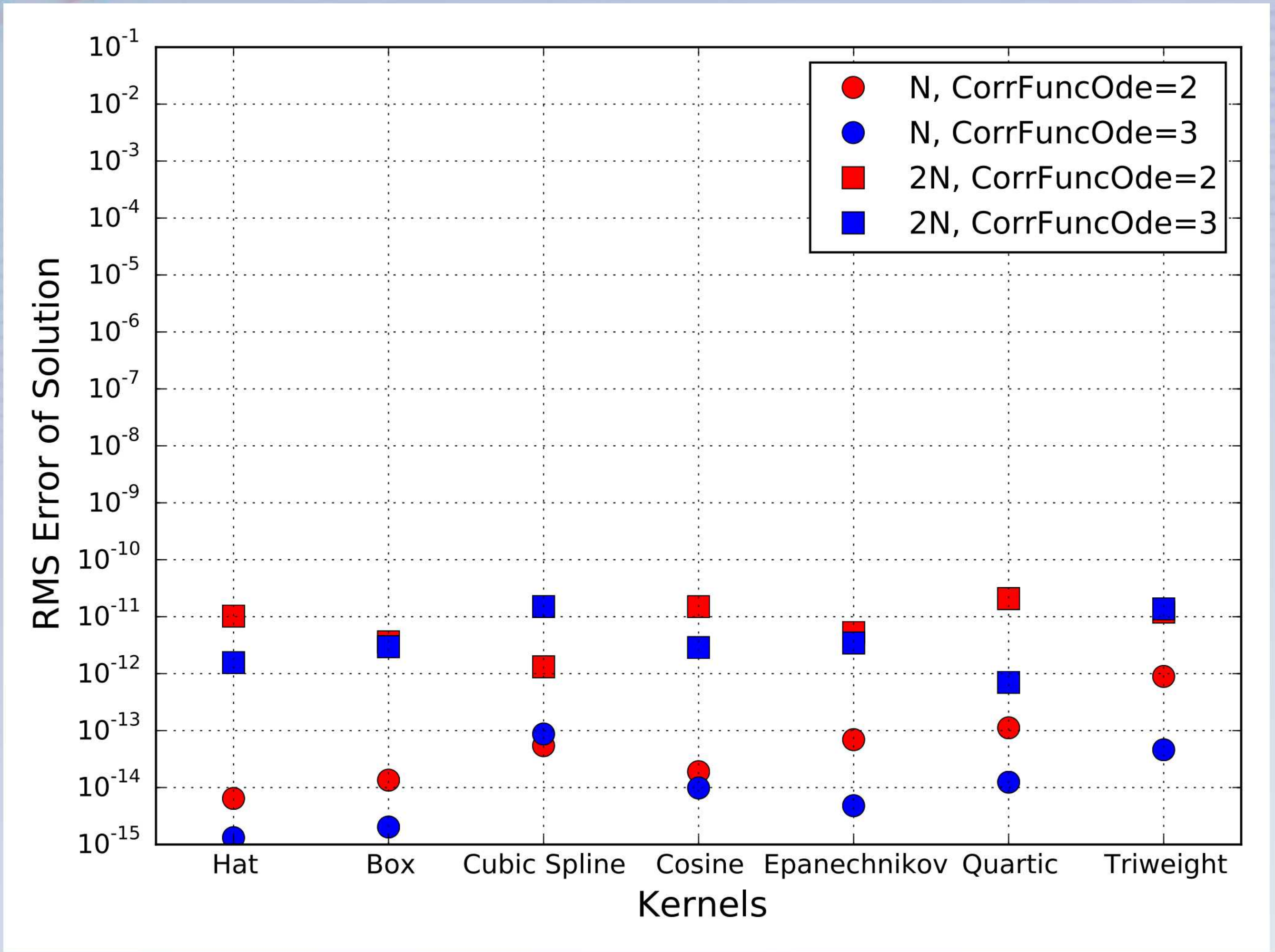
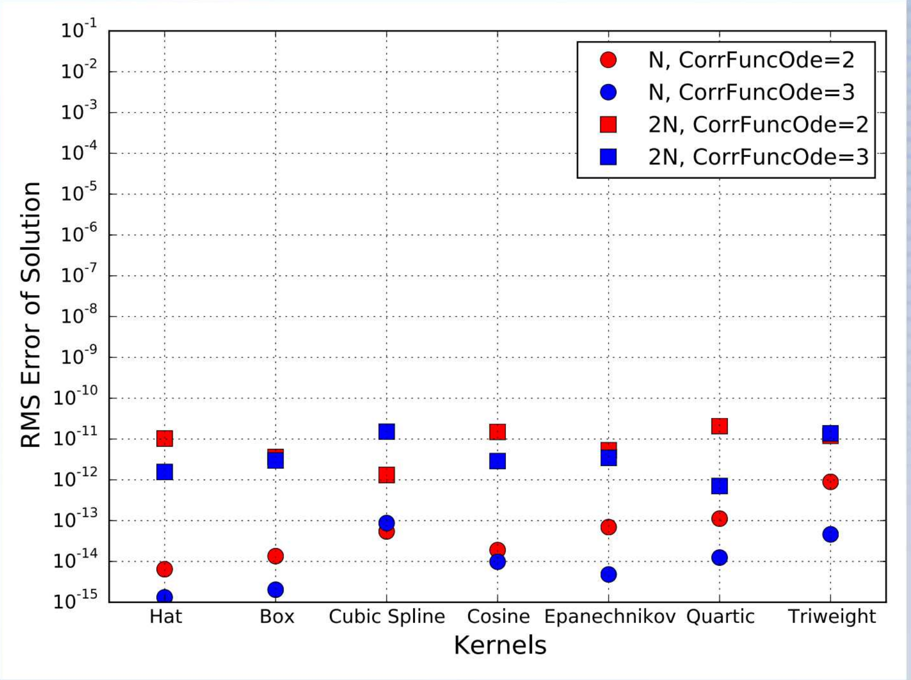
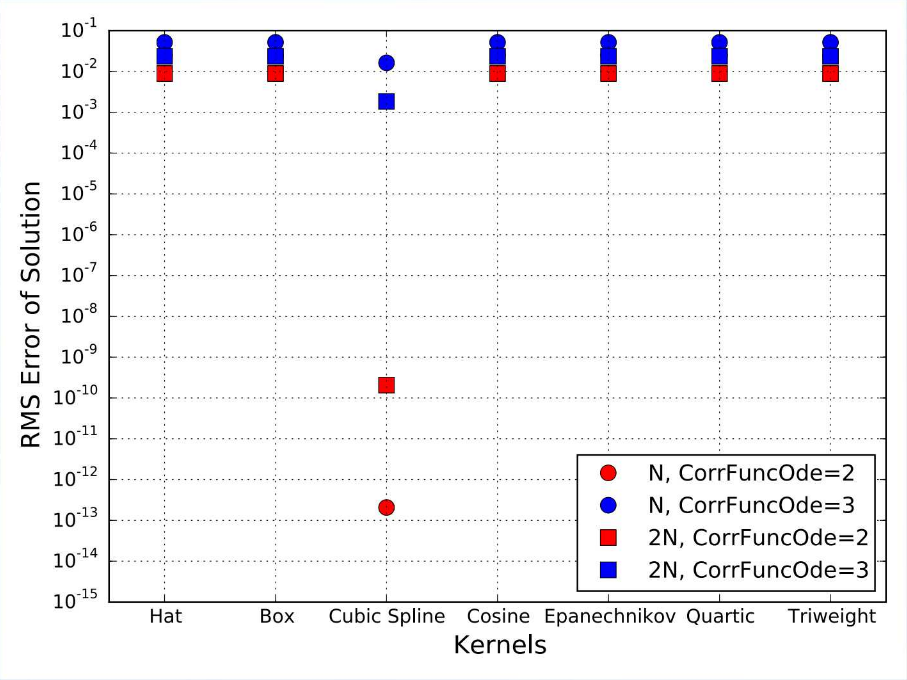
2^{nd} Order PDE: Solution RMS Error



$$\frac{\partial^2 u}{\partial x^2} = 2, u(x=0) = 0, u(x=1) = 1$$

Parameters Effects on PDE Solution RMS Error





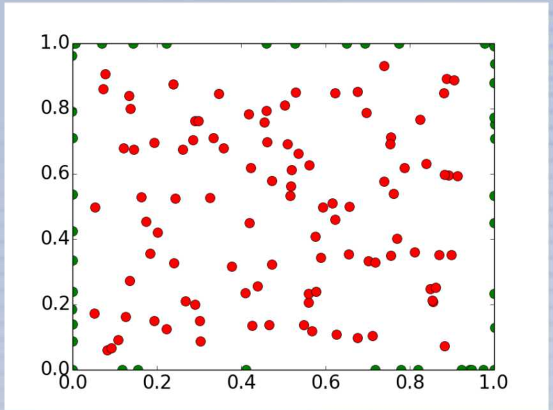
$$\frac{\partial^2 u}{\partial x^2} = 2, u(x=0) = 0, u(x=1) = 1$$

$$\frac{\partial^2 u}{\partial x^2} = 2, u(x=0) = 0, \frac{\partial u}{\partial x}(x=1) = 1$$

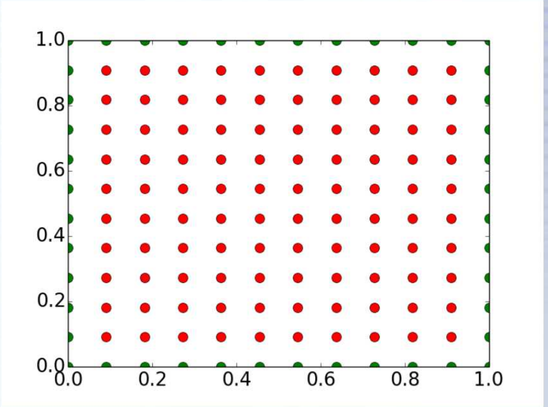
- Lost accuracy for Neumann Boundary Conditions
- Similar behavior for 1st order PDE

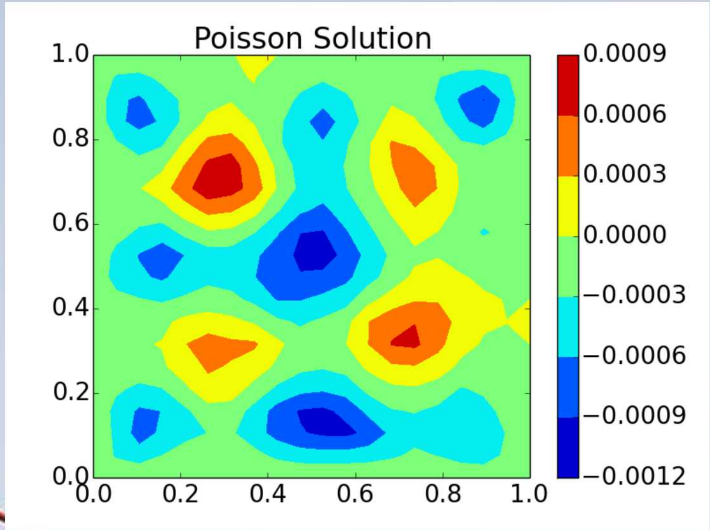
Adaptive Particle Motion

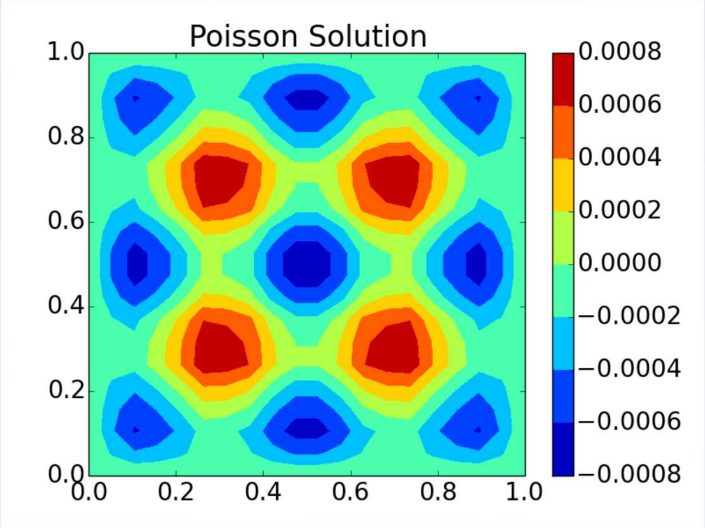
Fully Random



Fully Ordered







LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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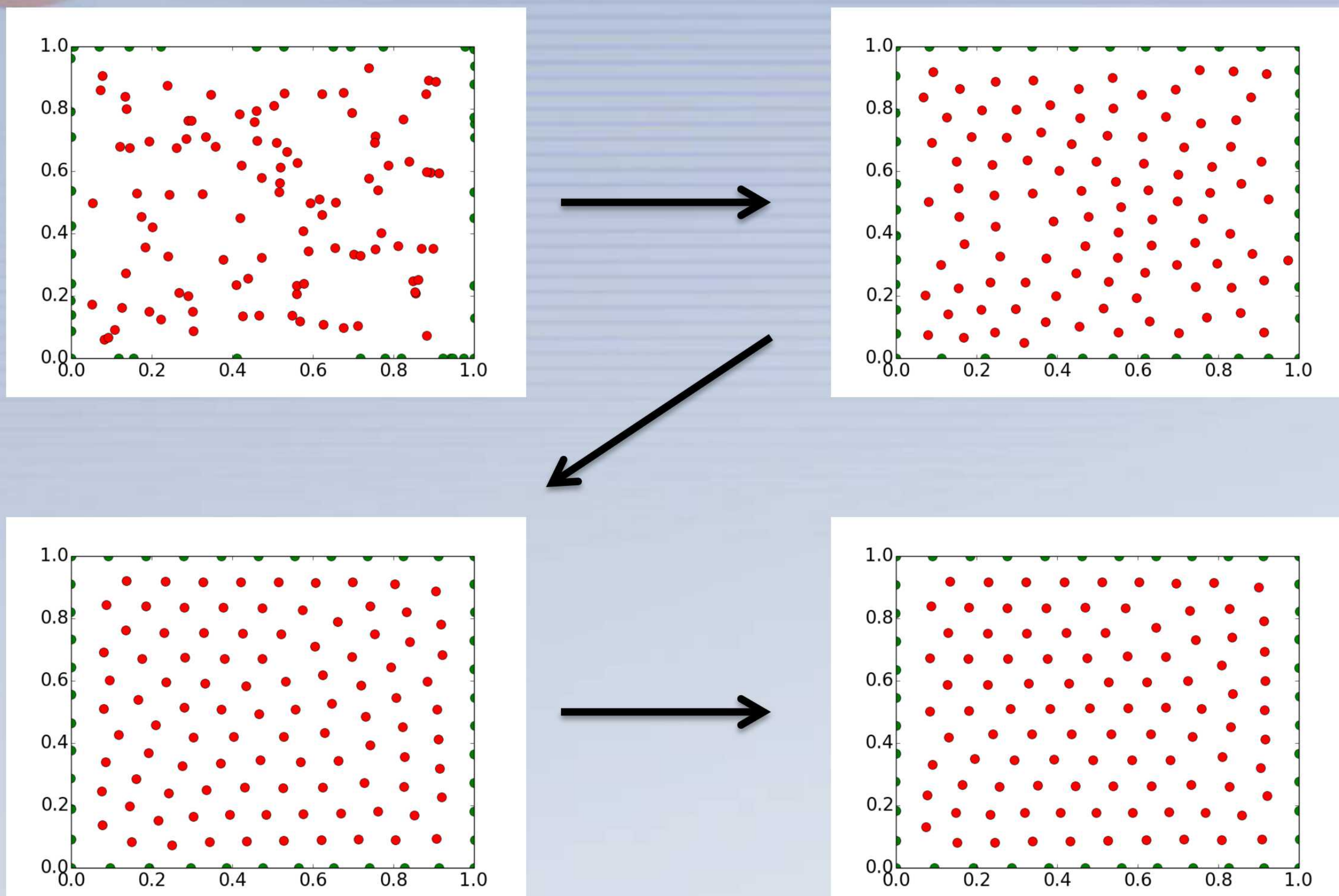
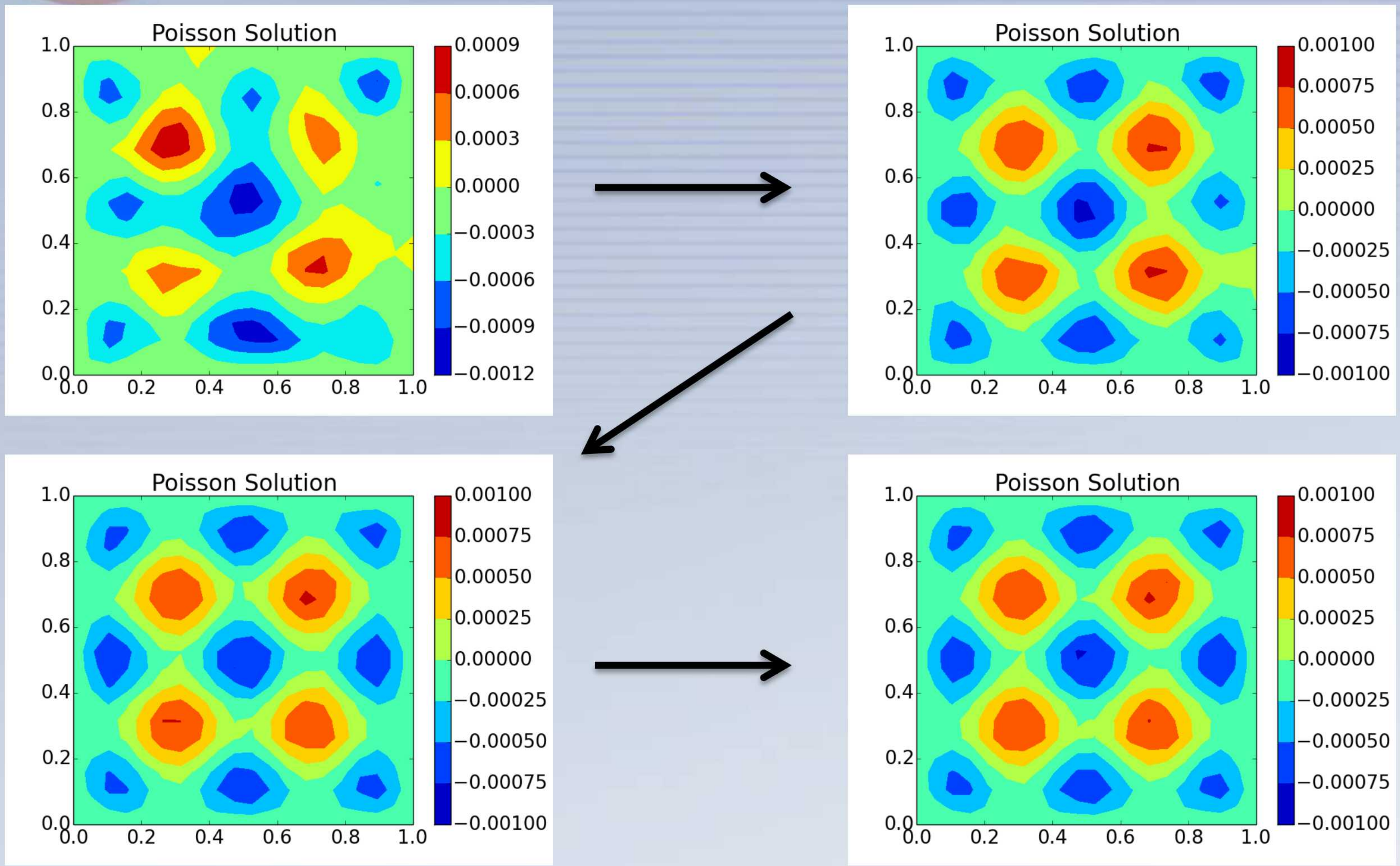
Molecular Dynamics Energy Minimization

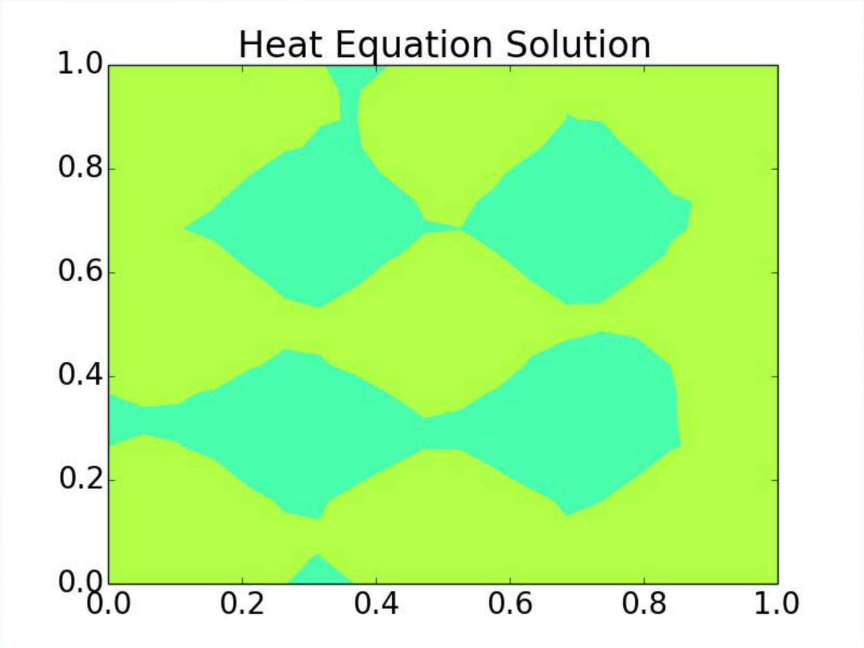


Molecular Dynamics Energy Minimization

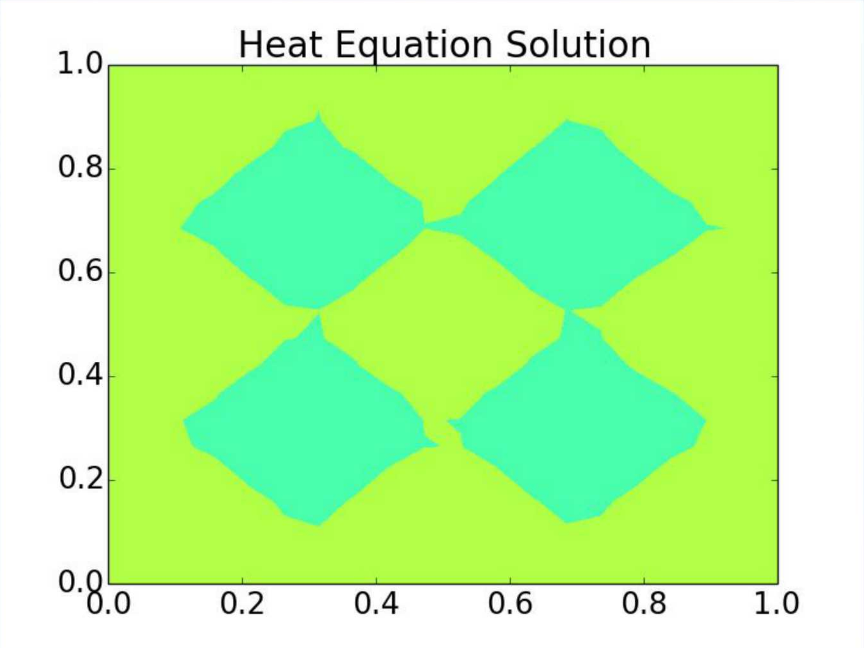


Similar Behavior for Transient Systems

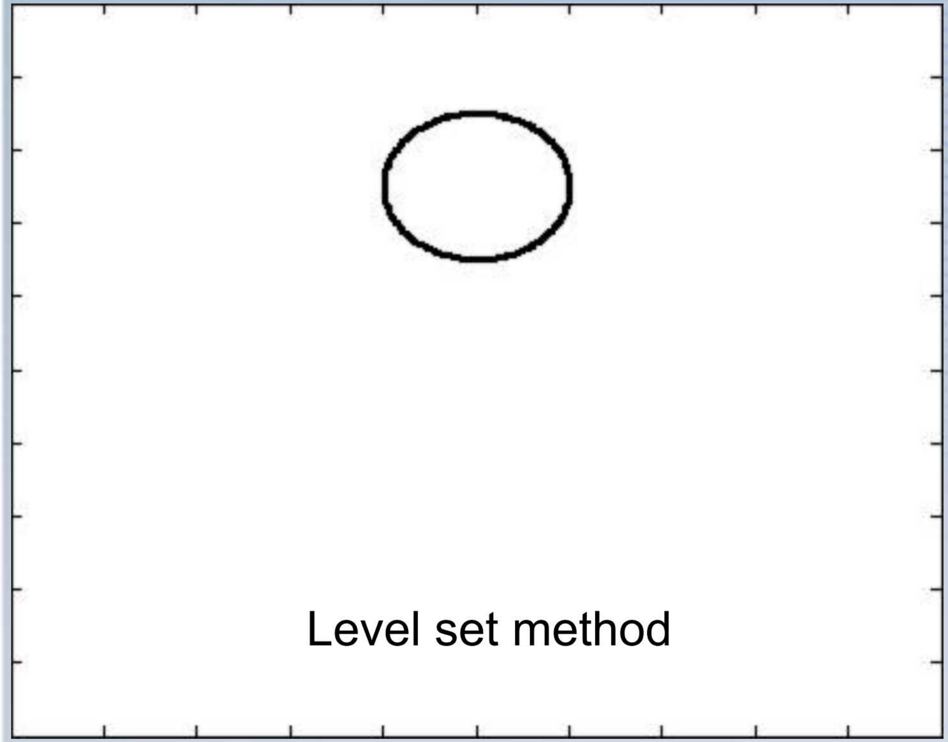
Heat Equation: Initial Configuration

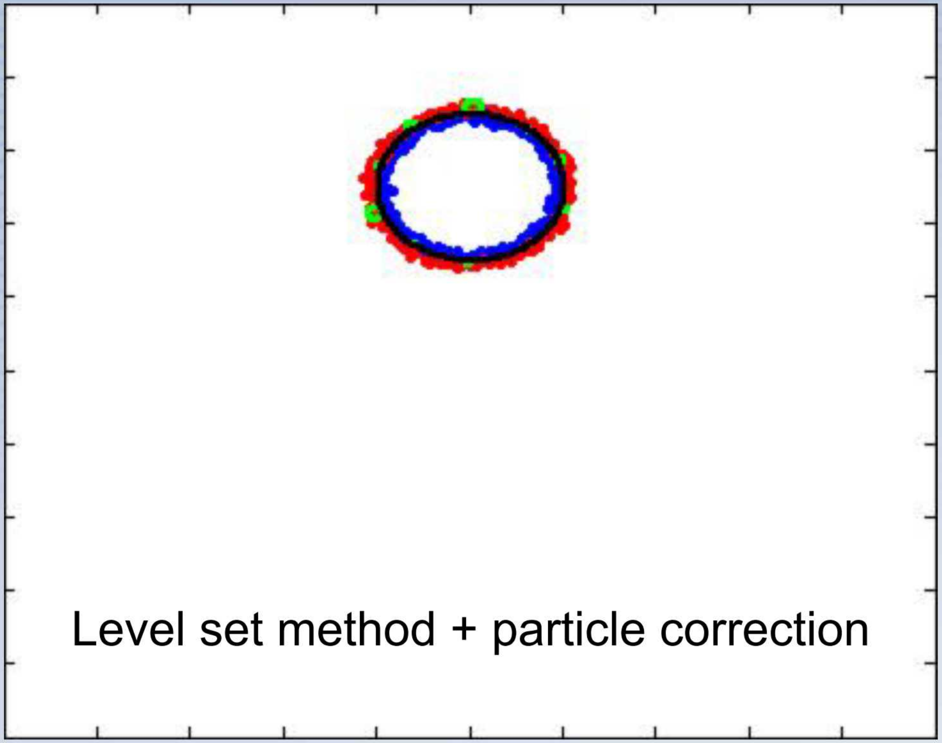


Heat Equation: Minimized Configuration



Particle level set method reduces the numerical diffusion of the level set method



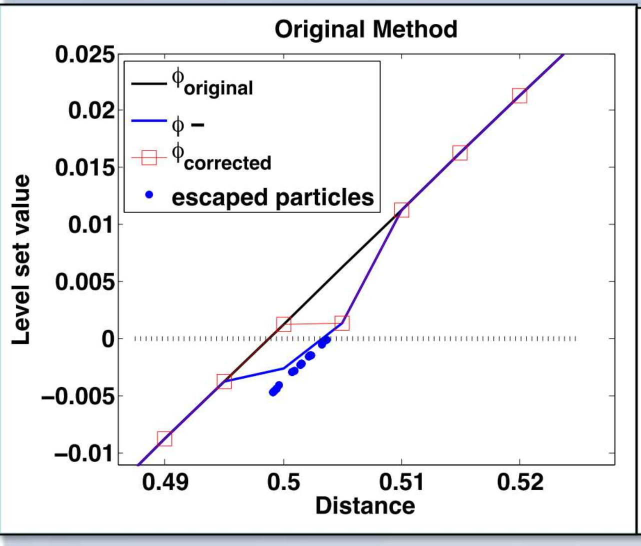


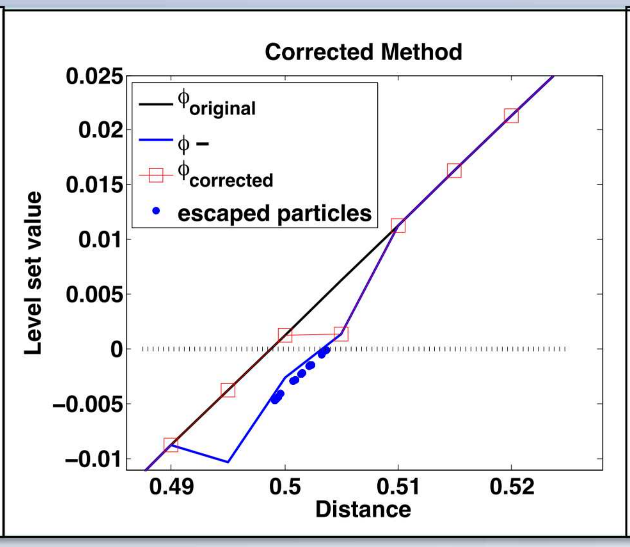
- PLS beats traditional level set method when tested on a single vortex problem
  - Limits numerical diffusion
  - Resolves thin filaments on the mesh scale

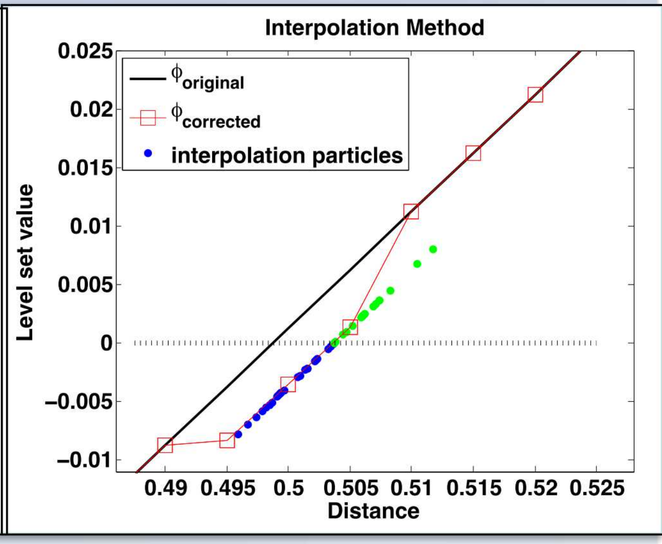
Particle Level Set Method Comparison

- Particle Level Set (PLS) Method[1]
- Corrected PLS[2]
- Interpolative PLS[3] **Most advanced in literature**

New Method

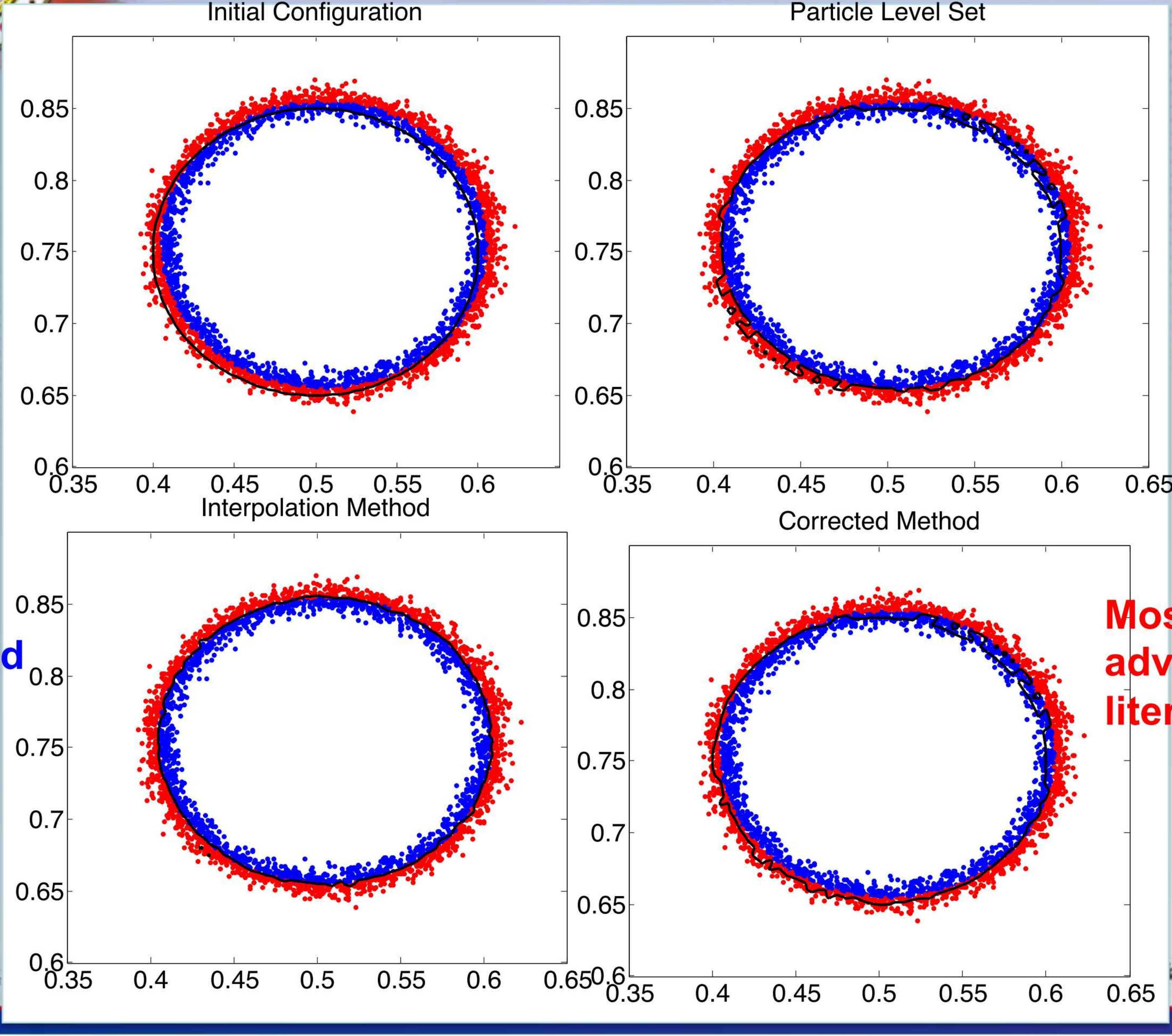






[1] Enright, Fedkiw, Ferziger, Mitchell, "A hybrid particle level set method for improved interface capturing," J. Comp. Phys. (2002).
[2] Wang, Yang, Stern, "An improved particle correction procedure for the particle level set method," J. Comp. Phys. (2009).
[3] **Erickson, Morris, Poliakoff, Templeton, "An interpolative particle level set method," in preparation.**

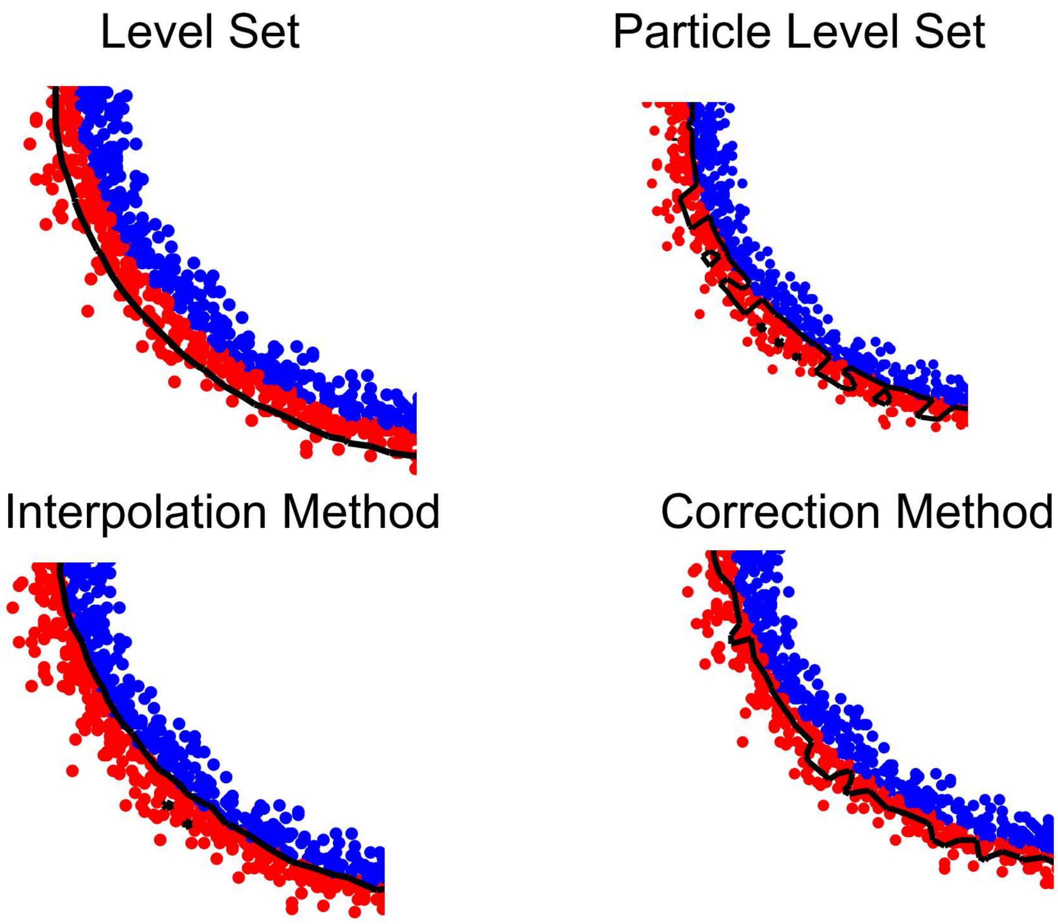
Interpolation method outperforms other methods for 2D circle test



New Method

Most advanced in literature

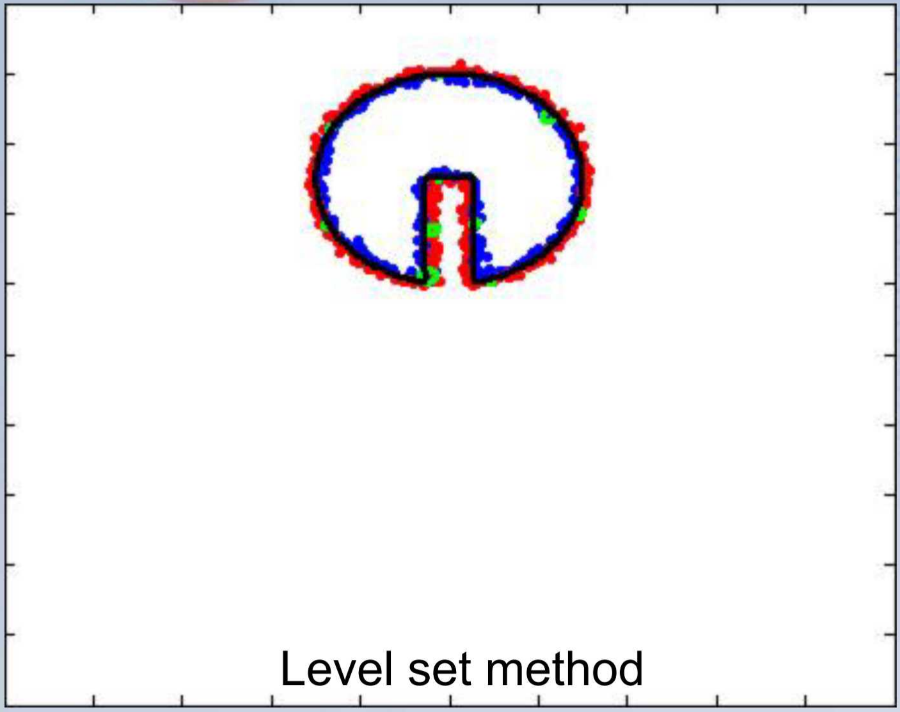
Interpolation method outperforms other methods for 2D circle test

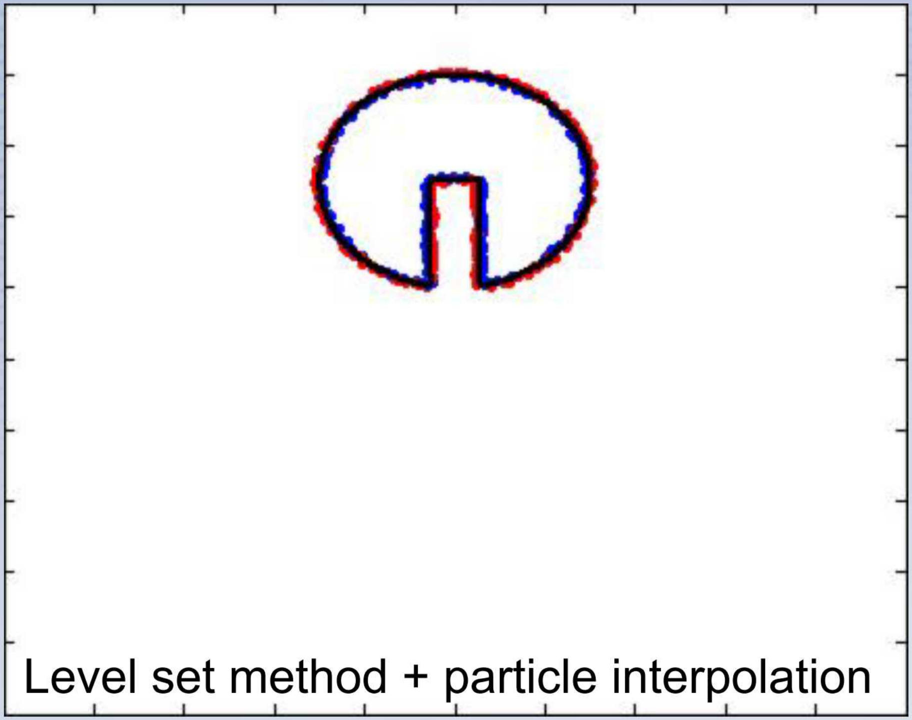


New Method

Most advanced in literature

Rotating Zalesak's disk test

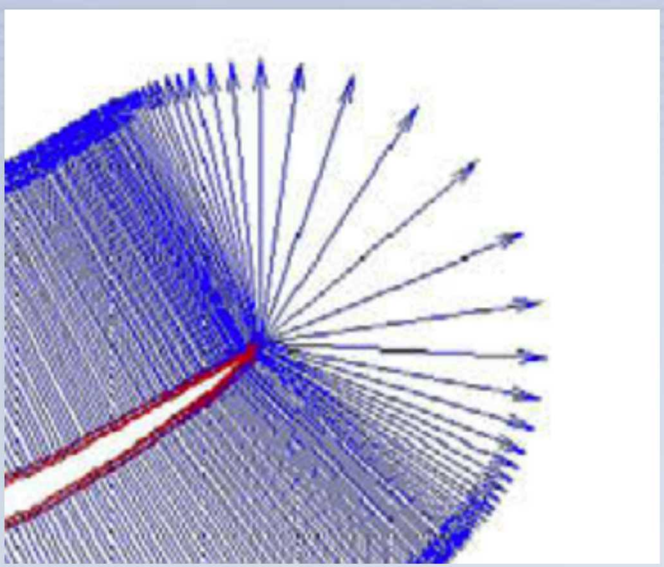




- Comparing numerical diffusion between traditional level set method and one using our particle interpolation procedure
  - Numerical diffusion taken care of
  - Errors away from boundary start developing

Oriented particle level set approach

- Alternatively, we could use an oriented particle approach[1]
  - Particles lie exactly on interface
  - Separate governing equations for normal vector and curvature
  - No need for level set equation to evolve the interface



[1] Ianniello, Mascio, "A self-adaptive particles Level-Set method for tracking interfaces," J. Comp. Phys., 2010.

RKPM: Different Algorithms

- **Point Collocation Method**

$$u^{\mathrm{a}}(x,y)=\int_{\Omega}\mathscr{C}(x,y,x-s,y-t)\varphi(x-s,y-t)u(s,t)\,\mathrm{d}s\,\mathrm{d}t$$

- **Fixed Point Reproducing Kernel Method**

$$u^{\mathrm{a}}=\int_{\Omega}\mathscr{C}(x,y,s,t)\varphi(x_K-s,y_K-t)u(s,t)\,\mathrm{d}s\,\mathrm{d}t$$

- **Moving Reproducing Kernel Method**

$$u^{\mathrm{a}}(x,y)=\int_{\Omega}\mathscr{C}(x,y,s,t)\varphi(x-s,y-t)u(s,t)\,\mathrm{d}s\,\mathrm{d}t$$

- **Multiple Fixed Reproducing Kernel Method**

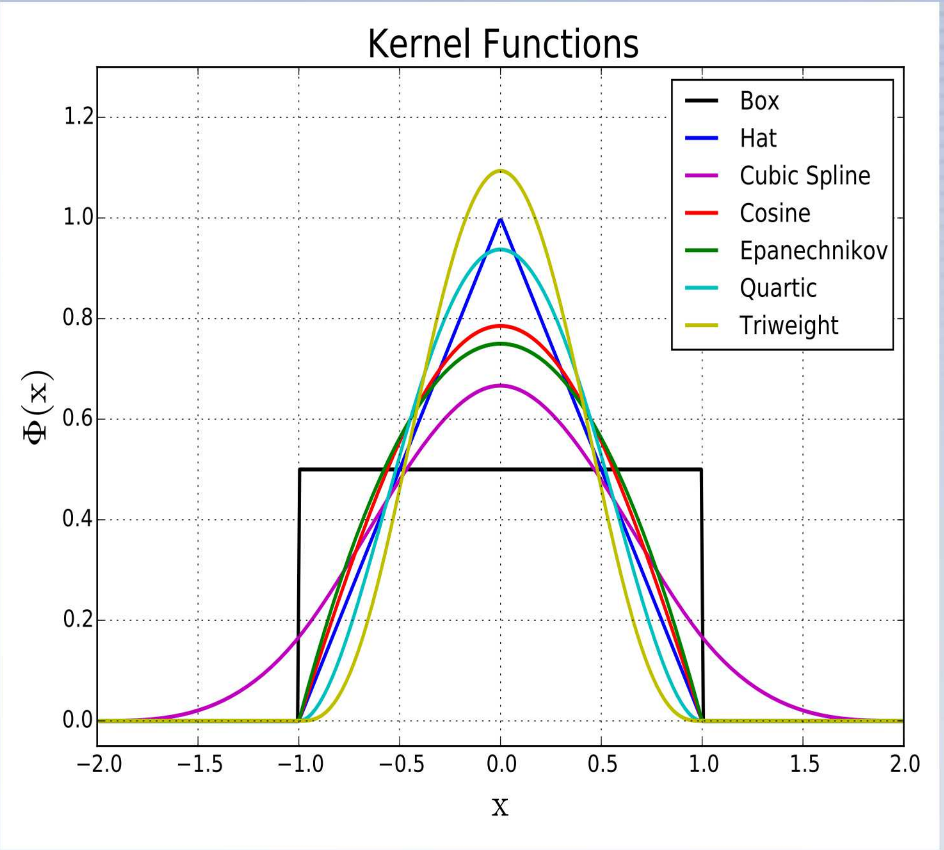
$$u^{\mathrm{a}}(x,y)=\int_{\Omega}\mathscr{C}(x,y,s,t)\varphi_{s,t}(s-x,t-y)u(s,t)\,\mathrm{d}s\,\mathrm{d}t$$

Correction Function: $\mathscr{C}(x,y,s,t)$

Kernel Function: φ

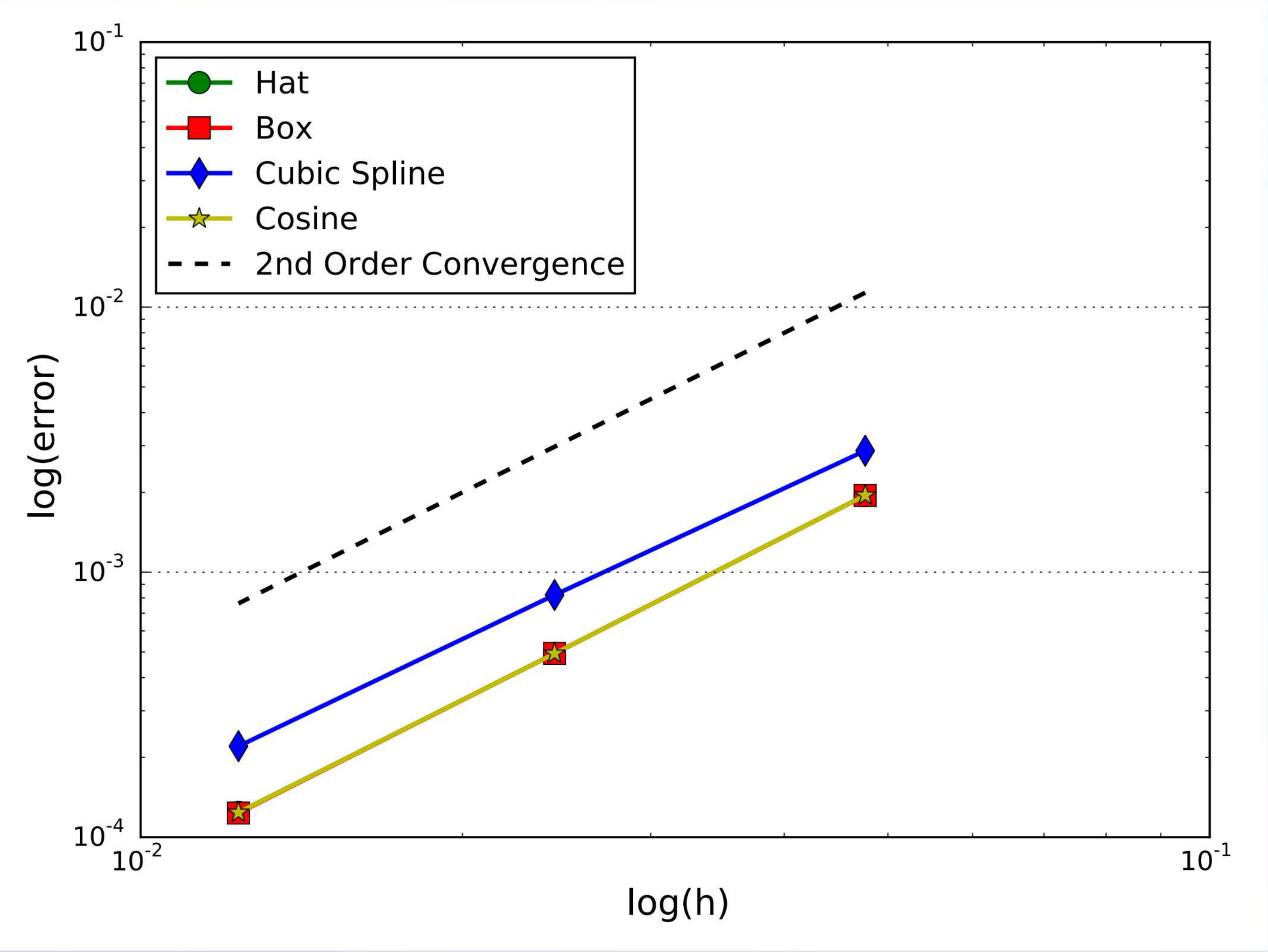
Unknown Function: $u(s,t)$

Implemented Kernel Functions



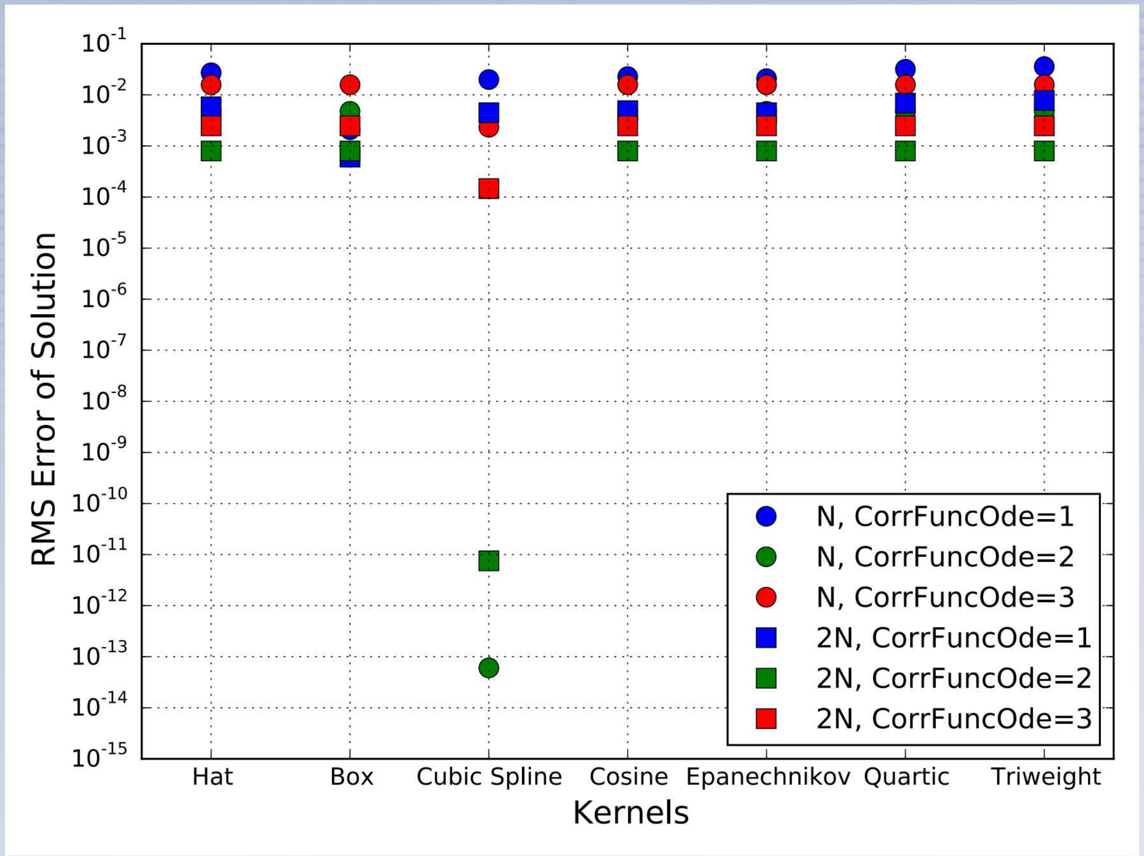
- Kernel Function Properties:
  - Normalized over its support domain
  - Compactly supported
  - Positive for any point within the support domain
  - Kernel value for a particle monotonically decreases with increasing distance away from the particle
  - Satisfies the dirac delta function condition as the smoothing length approaches zero.
  - Even and symmetric function
  - Smooth function

Convergence for 2nd Order PDE



$$\frac{\partial^2 u}{\partial x^2} = \frac{105}{2}x^2 - \frac{15}{2}, \qquad \begin{aligned} u(x=0) &= 3/8, \\ u(x=1) &= 17/2 \end{aligned} \qquad u = \frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}$$

First order ODE displays anomalous results



$$\frac{\partial u}{\partial x} = 2x, u(x=0) = 0, u(x=1) = 1$$

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

RKPM: Algorithms Properties

- **Point Collocation Method**
  - Computationally intensive due to additional system solve for moment matrix and its derivative
- **Fixed Point Reproducing Kernel Method**
  - Reduced computation and algorithm complexity by fixing the kernel evaluation
  - Shape function derivatives are independent of the kernel function
  - Requires dealing with multi-valued Shape functions
- **Moving Reproducing Kernel Method**
  - Shape functions are not multi-valued
  - Shape function derivatives are kernel function dependent
- **Multiple Fixed Reproducing Kernel Method**
  - Shape functions are not multi-valued they can be computed uniquely
  - Shape function derivatives are kernel function dependent
  - Different kernel functions can be used at each point.

Solving the Stefan problem for melting solids

- Solving the heat equation for a solidifying liquid
- The interface is defined at the melt temperature