Multiscale Models for Microstructure Evolution and Response

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Recent progress

- Modeling Solidification Microstructures
  - Cryopreservation of biological materials
  - 2D - 3D transition in directional solidification
- Spacetime Discontinuous Galerkin Methods
  - Adaptive $O(N)$ method for hyperbolic PDEs
  - Visualization & parallel implementation
  - Fracture and dewetting under shock loading
- Additional topics
  - Shape and topology optimization of microstructure
  - Phase field crystals
  - Atomistic / continuum coupling strategy

Modeling Solidification Microstructures

J. Dantzig, B. Athreya, A. Chang, L. Kale and K. Wang

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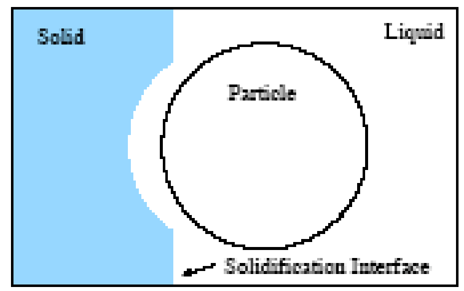
Cryopreservation Procedure



- Typical cryopreservation procedure
  - § Cool from 0°C$^+$ to $\mathcal{O}$(-15°C)
    - Formation of extracellular ice
    - Express H_2O from cell
  - § Cool to -196°C (LN_2)
- Major issues for consideration
  - § Lethal solute concentrations
  - § Intracellular ice formation(ICF)
  - § Mechanical deformation of cell

Freezing algae (Asymptote Ltd.)

Freezing protozoa (Asymptote Ltd.)

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Research goals

- Improvement of cryopreservation procedures
  - § Closer examination of freezing damage mechanisms
    - Concentration field surrounding cell
    - Mechanical deformation caused by solidifying interfaces
    - Simulation of intracellular ice formation
  - § Effects of macrosegregation on the survival of cells
  - § Changes in interface morphology caused by cryoprotectants
  - § Methods to induce favorable interface morphology for cell capture
- Current work
  - § Directional solidification simulations for the freezing of ice
  - § Level set method used to track particle/interface interaction
  - § Moving boundary fluid flow calculations to compute particle drag
  - § Code parallelization to decrease simulation time
  - § Correlation of local cellular environment to cell survival

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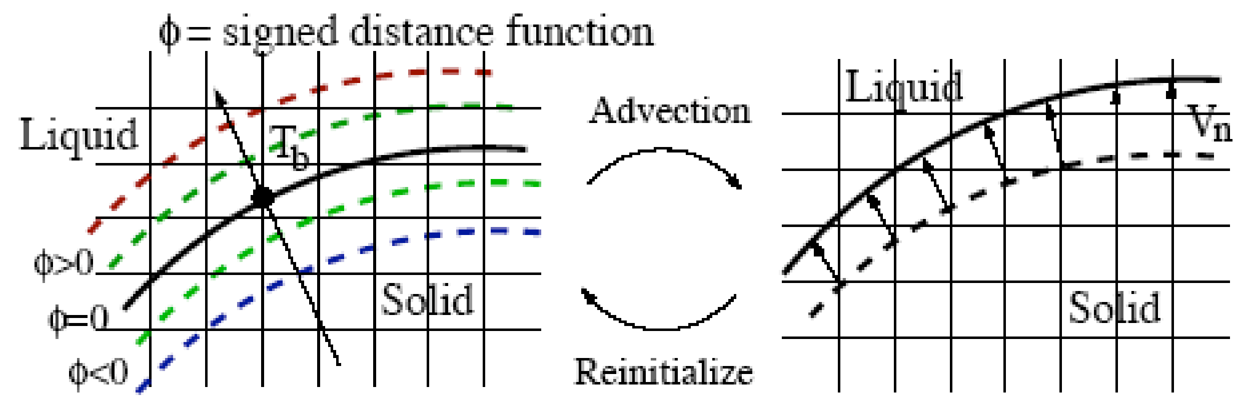
Level set method



- Solve for interface velocity using interface solute balance:

$$-D_\ell \partial_z C_\ell = V_n(1-k_\circ)C_\ell$$

- Advect ϕ:

$$\partial_t \phi + V_n \mathbf{n} \cdot \nabla \phi = 0$$

- Solve for concentration with Gibbs-Thompson equation at interface:

$$T_i = T_m - m_\ell C_\ell + \Gamma \kappa$$

- Reinitialize distance function:

$$\partial_\tau \phi + S(\phi_\circ)(|\nabla \phi| - 1) = 0$$

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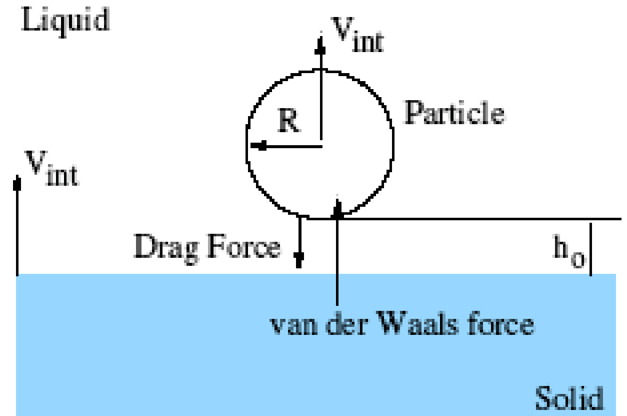
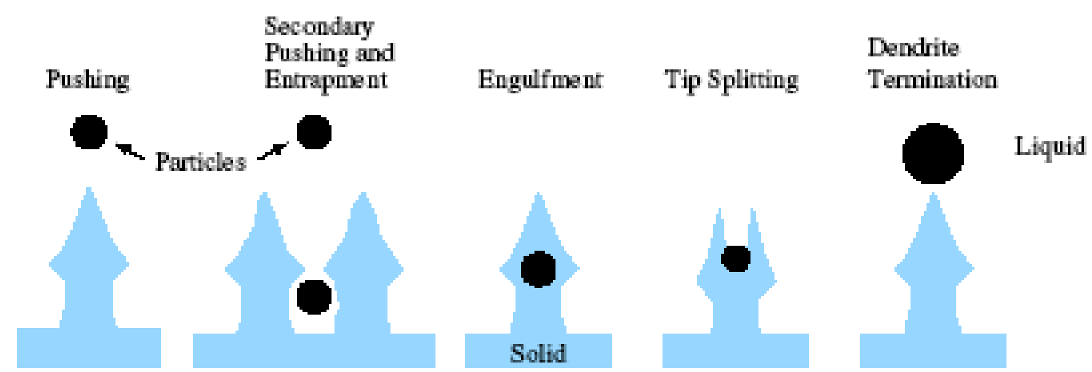
Particle pushing



- Force balance on particles
  - van der Waals repulsion
  - Drag force from flow between solid and particle
- Analytical solution exists for flat interface interaction
  - Dendritic interface interaction is significantly more complex
- Several types of particle interaction can occur



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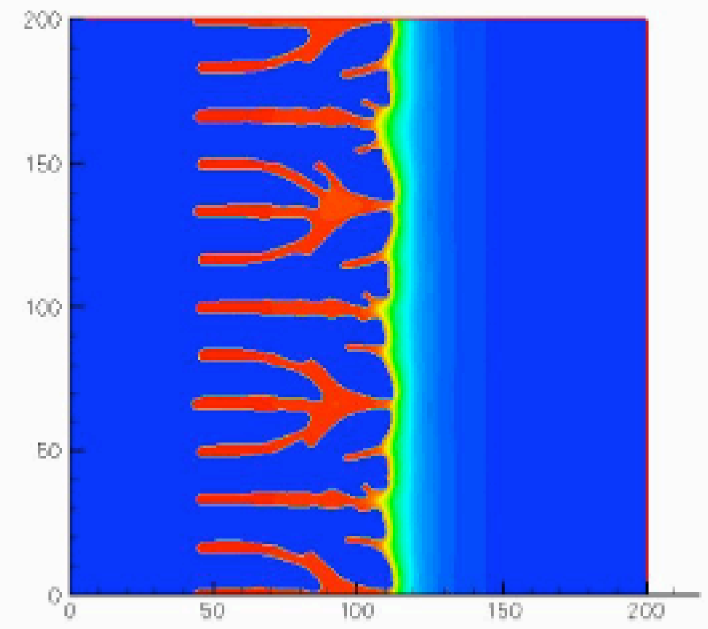
Example

- Set principal anisotropy at 45° to growth direction
- Drop in particles after pattern is established
- Capture depends on placement, size, parameters...



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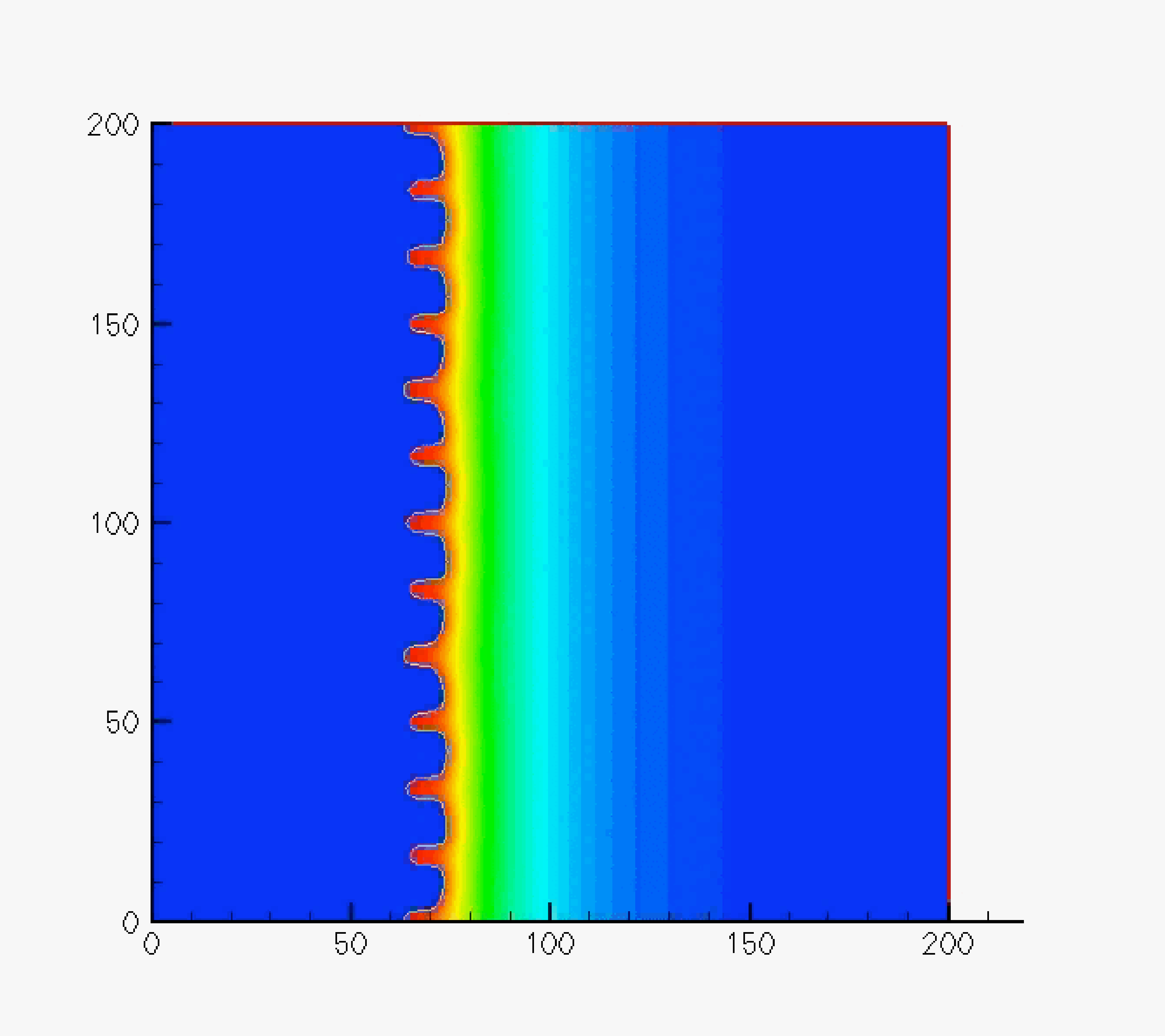

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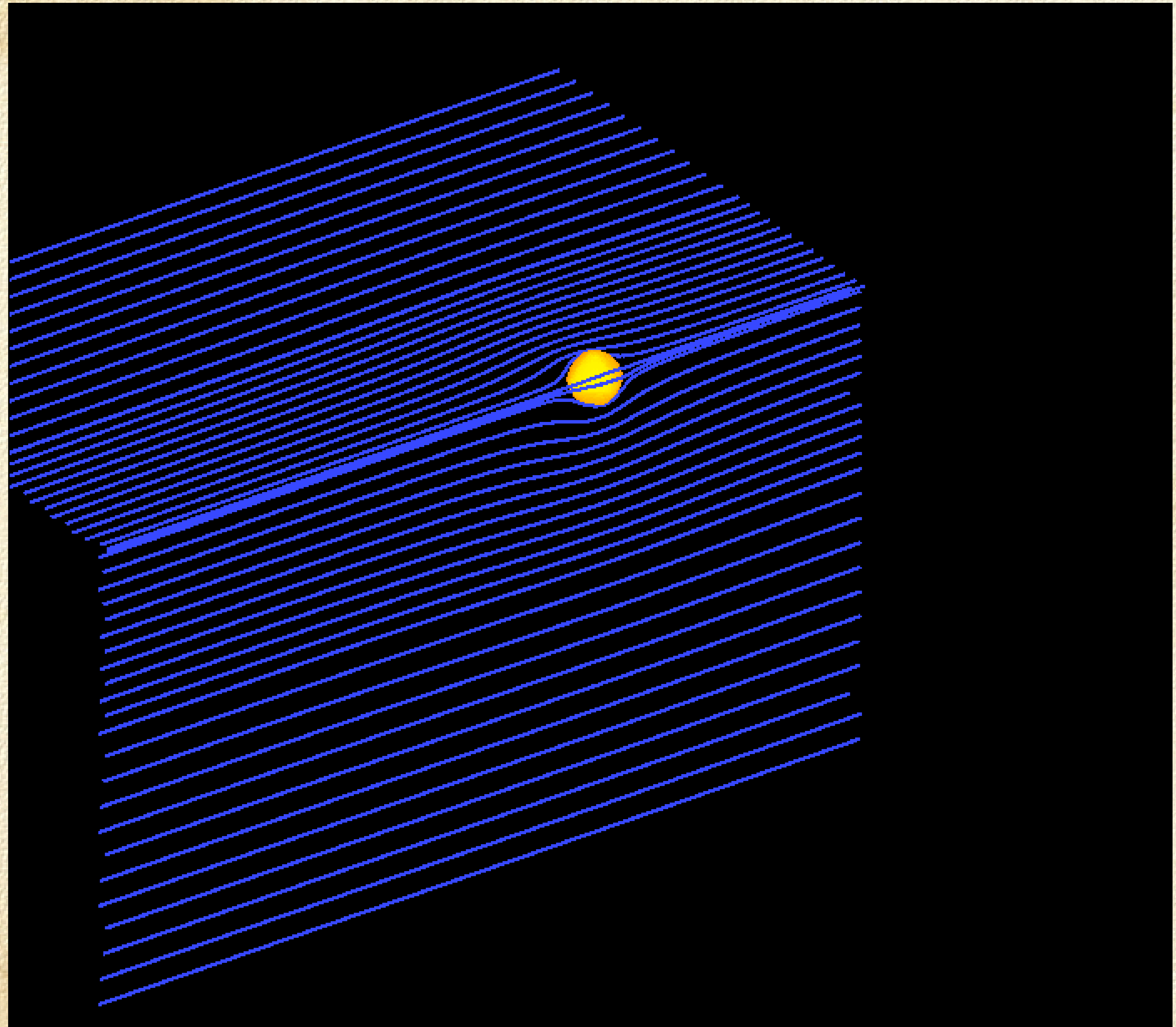

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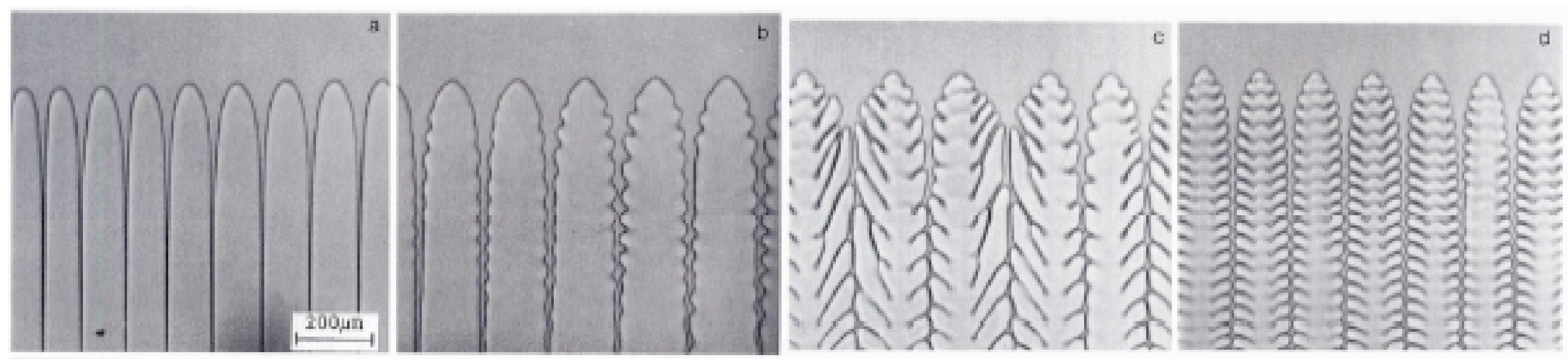
Spatial constraint

- Alloy solidification: SCN-Salol experiments (Liu and Kirkaldy, JCG, 1994)
  - § $L_z = 55\ \mu\text{m},\ G = 4.5\ \text{K/mm},\ V = 4.2,\ 5.7,\ 7.6,\ 10.8\ \mu/\text{s}$



- Observe 3-D to 2-D transition for different V
- Get different growth morphology as L_z varies (Liu et al., TMS, 2004)
- Models assume free 3-D growth
- Presence of boundaries can affect results

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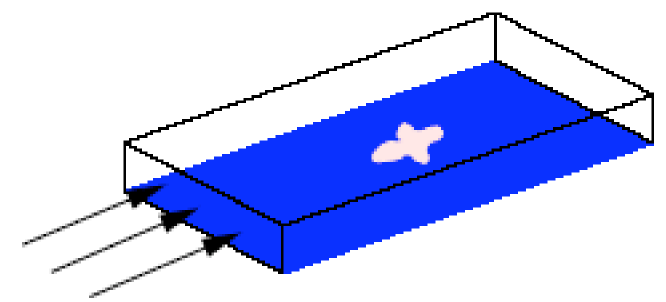
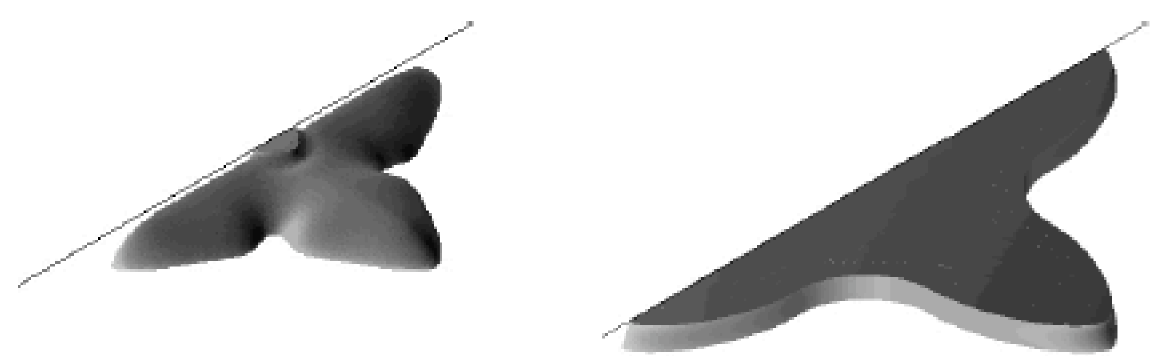
Spatially constrained growth: pure materials



- Example: $\Delta = 0.55,\ U_\infty = 0,\ L_z = 16,\ 4,\ \epsilon_4 = 0.05$
- Find 3-D to 2-D transition for small enough slide spacing



Free　　Confined

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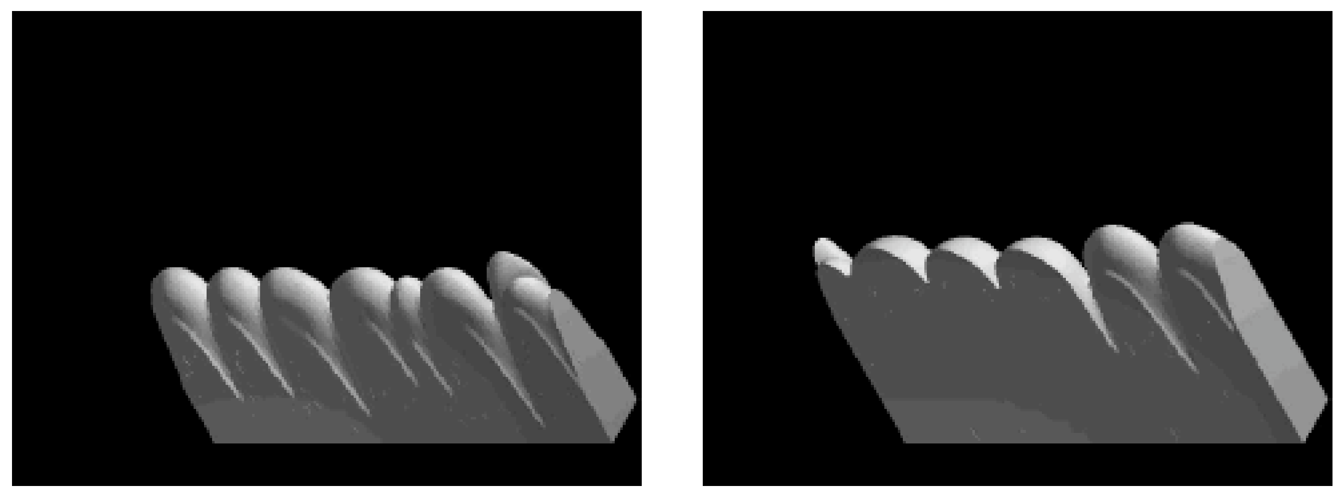
3D alloy directional solidification

- Follow phase-field model by Karma for different D_S and D_L (Karma, PRE, 2002)
- Use "Frozen temperature" approximation



- Find 3-D to 2-D transition
- Determine correlation for transition
- Comparison with experiments by Trivedi, Kirkaldy

Austenite-Martensite phase transition in shocked shape-memory alloys

"Standard numerical methods, such as shock capturing schemes and finite element methods, cannot be applied directly to the sharp interface model. Undercompressive waves such as phase interfaces turn out to be very sensitive to numerical dissipation, regularization, mesh refinements, etc. ..." – LeFloch

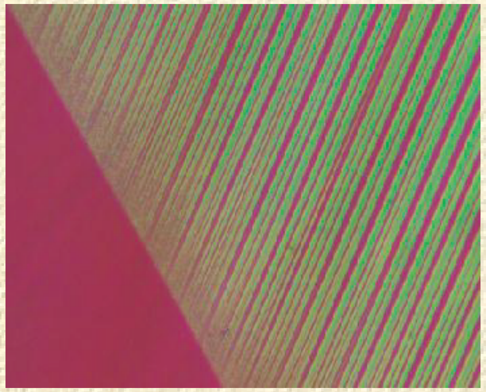
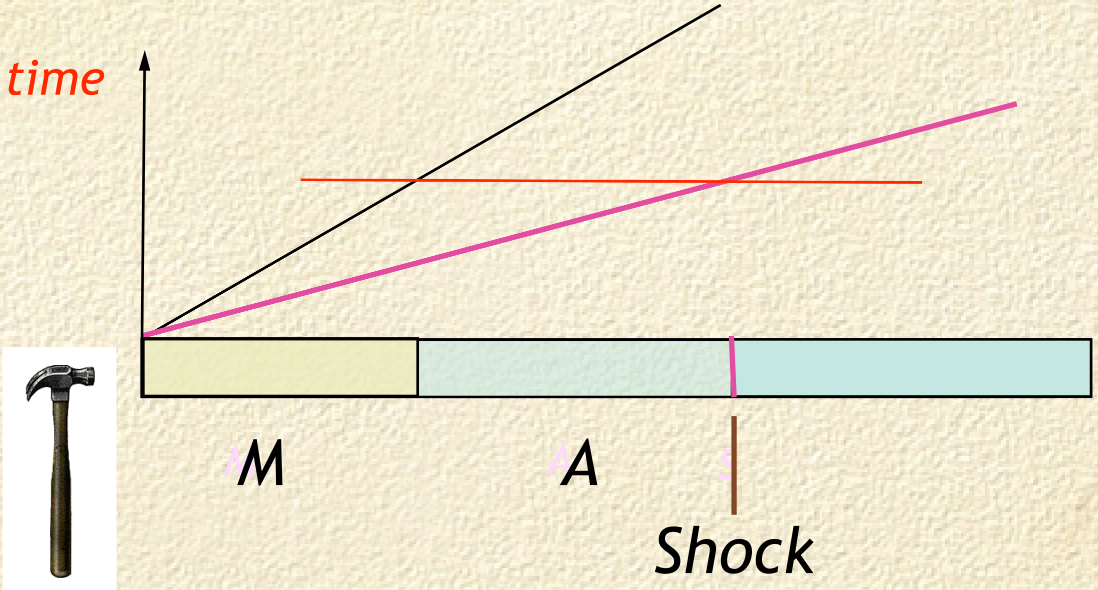
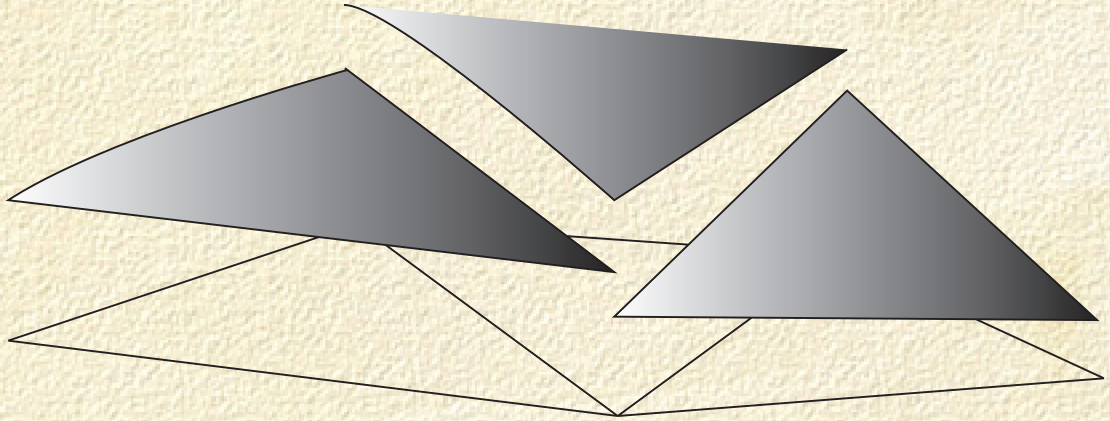


Fig. 1 Martensite–Austenite phase boundary (Credit: Thomas Shield, University of Minnesota)

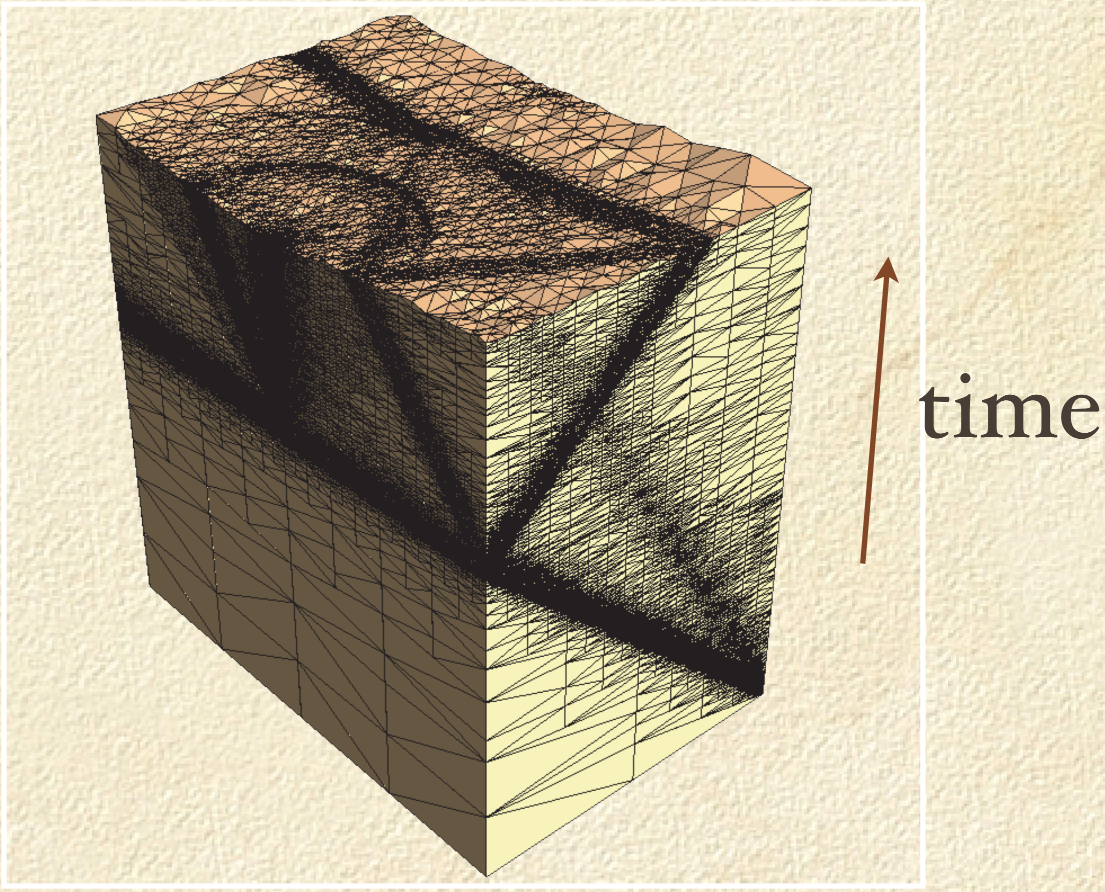


- Discontinuous fields play central role
  - shocks --- use SDG method for elastodynamics
  - phase boundary kinetics --- use SDG method for Hamilton–Jacobi equations

Spacetime discontinuous Galerkin finite element method

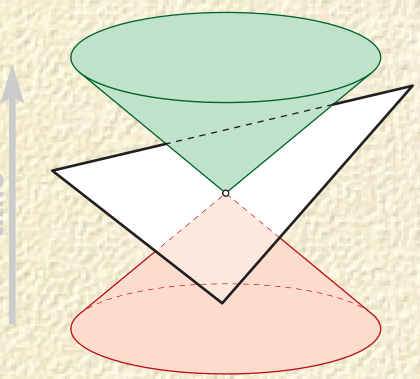


- Distinguishing features of SDG method
  - discontinuous basis functions
  - spacetime interpolation

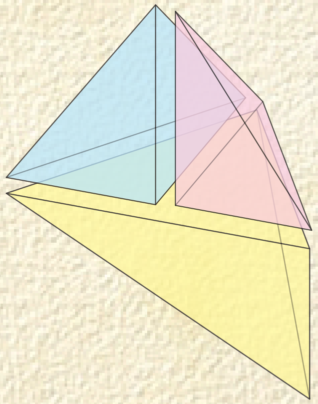


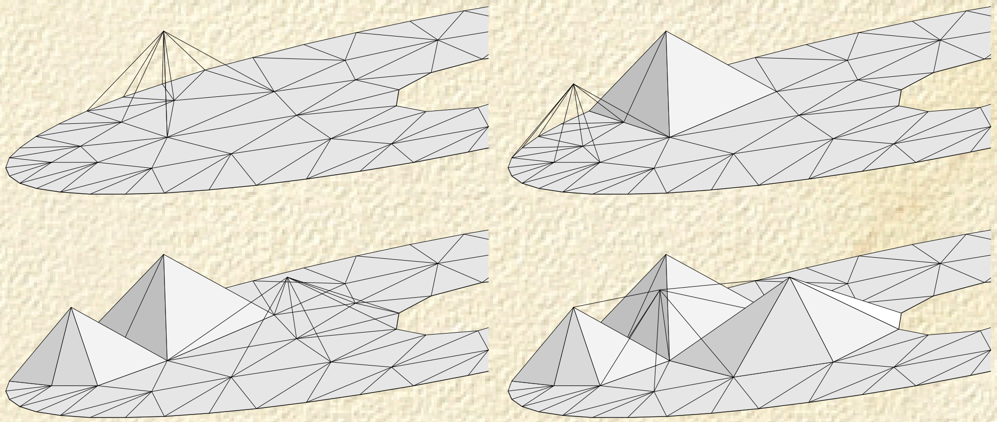
Tent Pitcher
Adaptive spacetime meshing

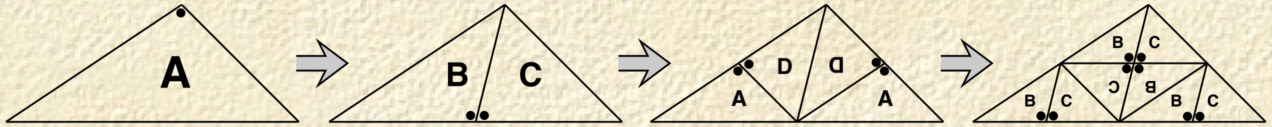
- Given a space mesh, Tent Pitcher constructs a spacetime mesh such that the slope of every facet is bounded to satisfy causality
- Patches ("tents") of tetrahedra are created and solved one at a time to yield an O(*N*) method with rich parallel structure
- Individual patches are refined by a *newest vertex method* on the space mesh to produce a nonconforming spacetime grid



causality constraint


nonconforming mesh

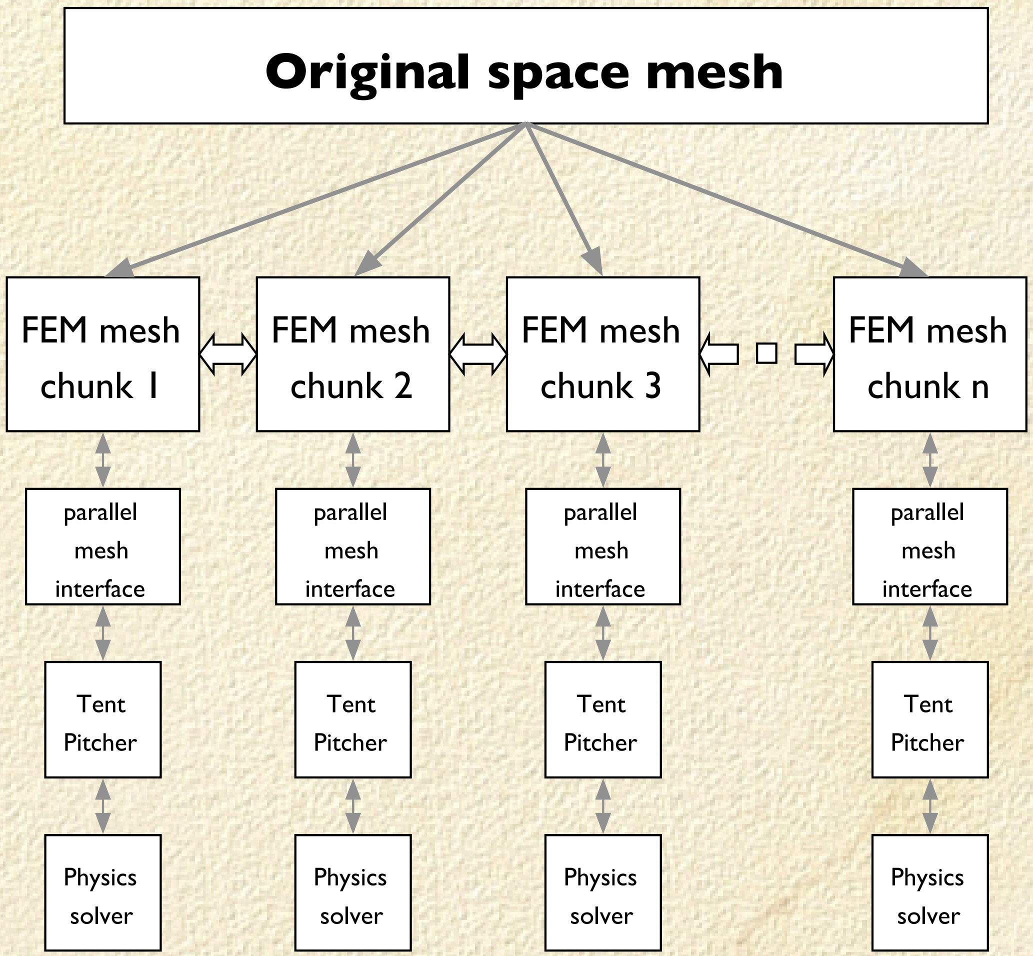

tent-pitching sequence

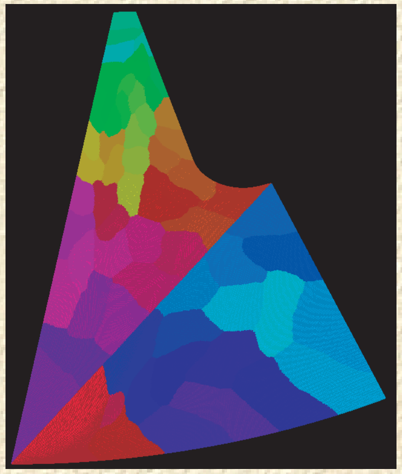


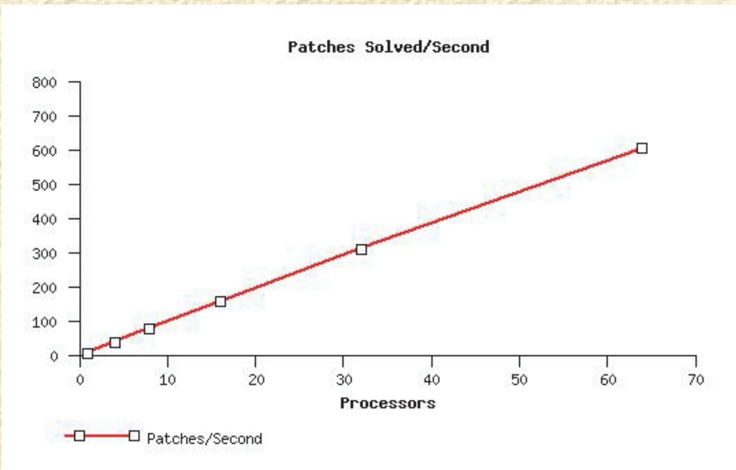
newest-vertex refinement strategy

Parallel Solution Strategy

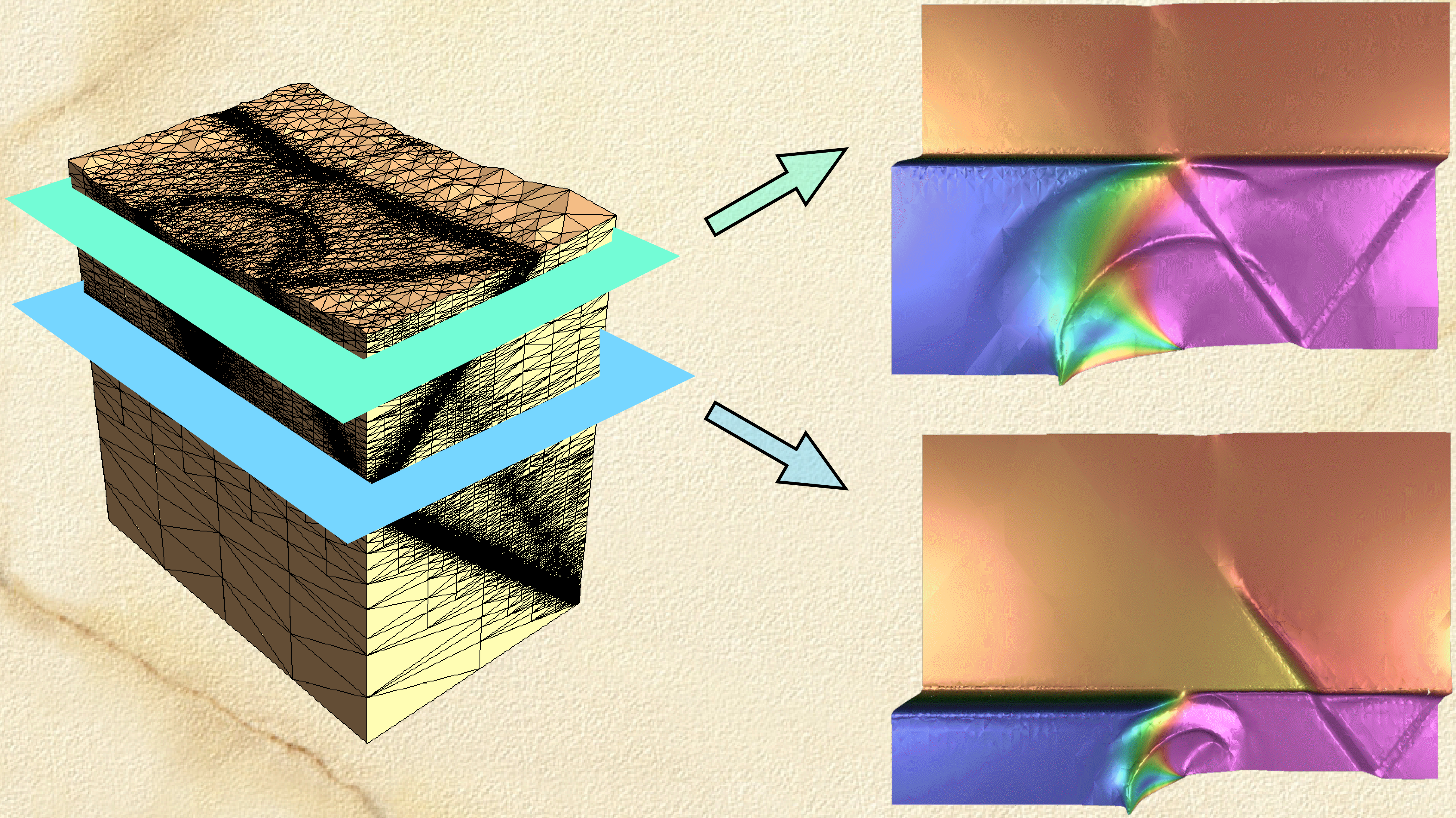
- Built on top of *Finite Element Framework* within the Charm++ parallel programming environment
- Provides domain decomposition into "chunks", transparent message passing, and dynamic load balancing
- Chunks run Tent Pitcher in parallel; physics code "thinks" it is serial
- Good scaling and processor utilization





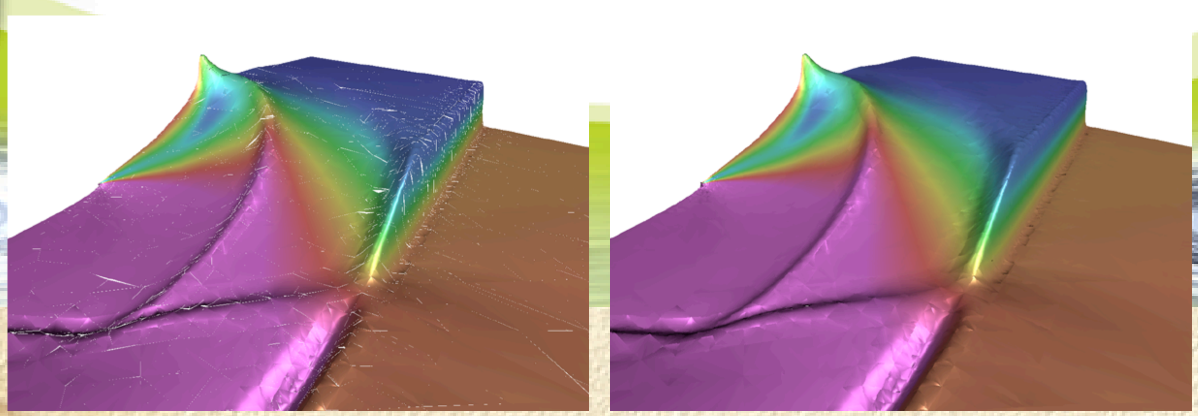


Pixel-Exact Rendering of Spacetime Data Sets

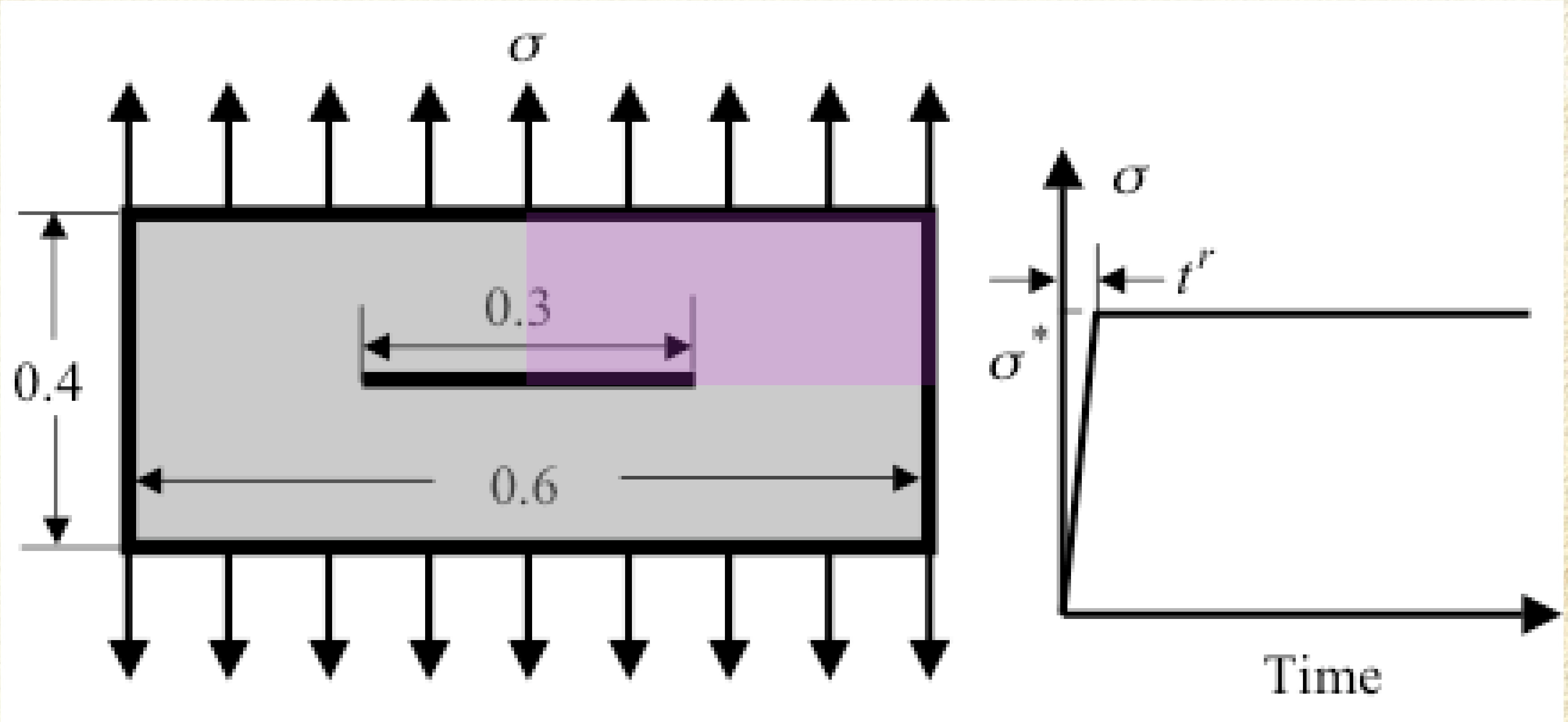


High-Performance and Hi-Fidelity Rendering Techniques

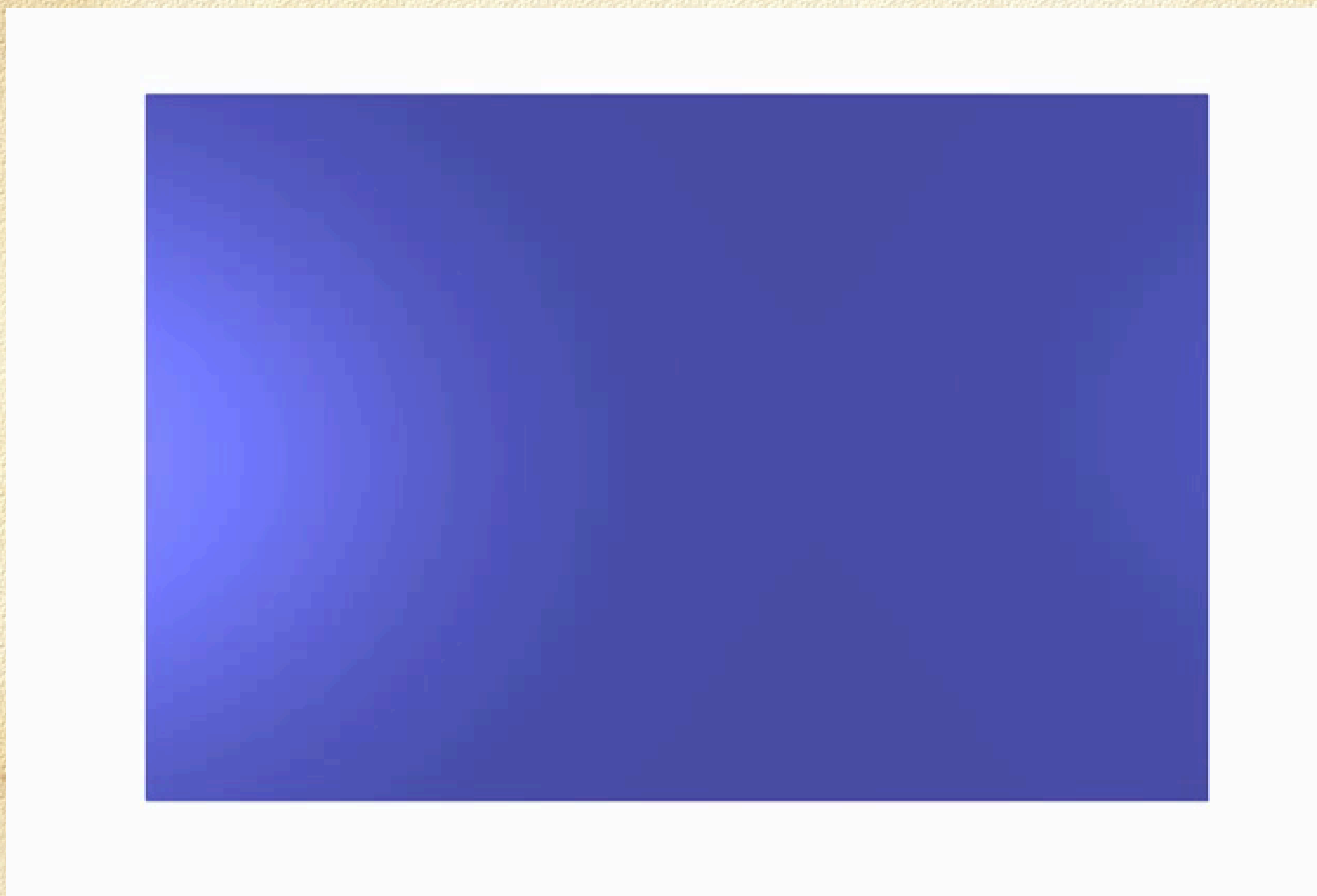
- Programmable GPUs post-process physics data at pixel level
- Heavily pipelined and 16 x parallel
- Discontinuity anti-aliasing



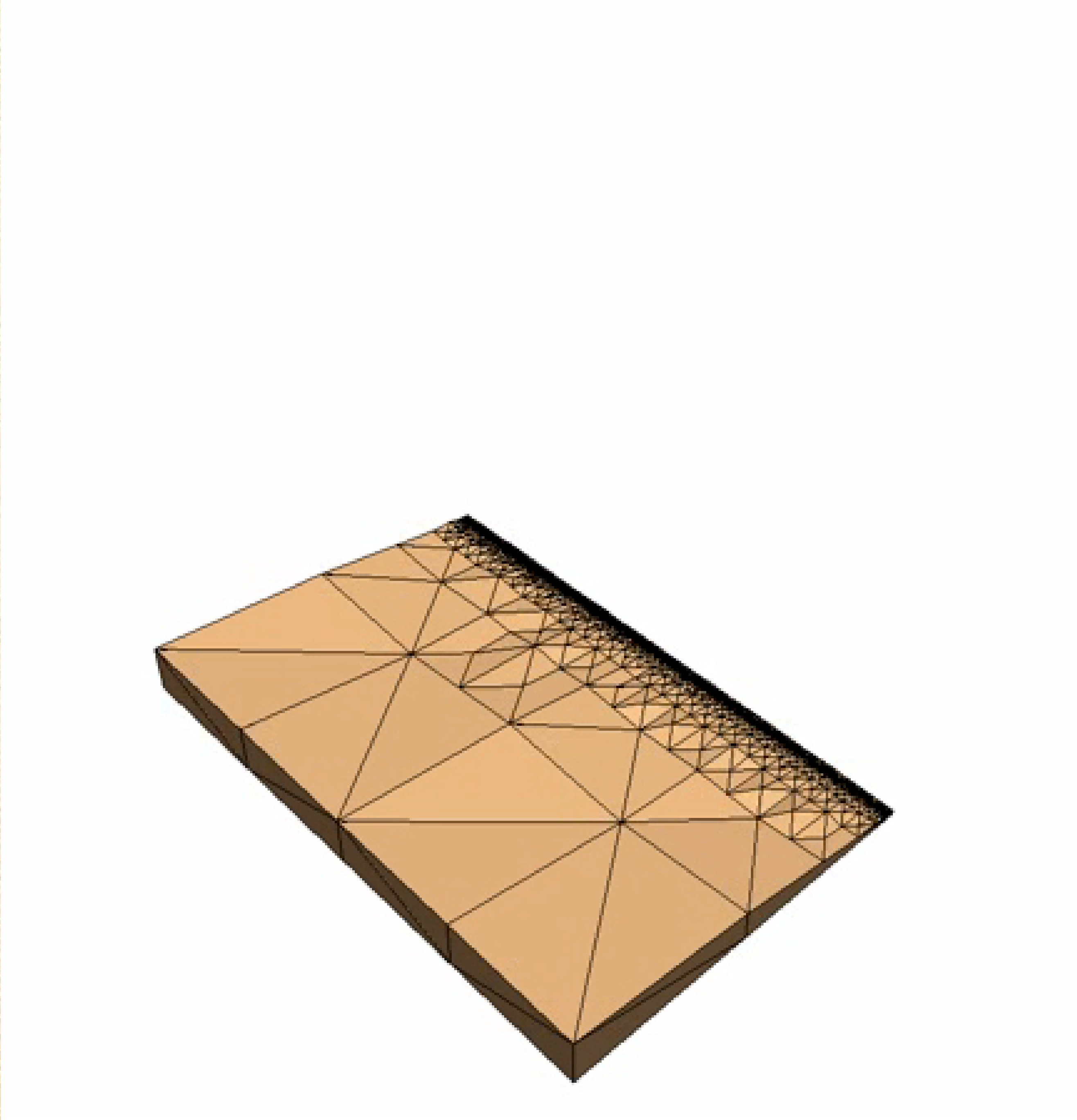
Crack-tip Wave Scattering Example



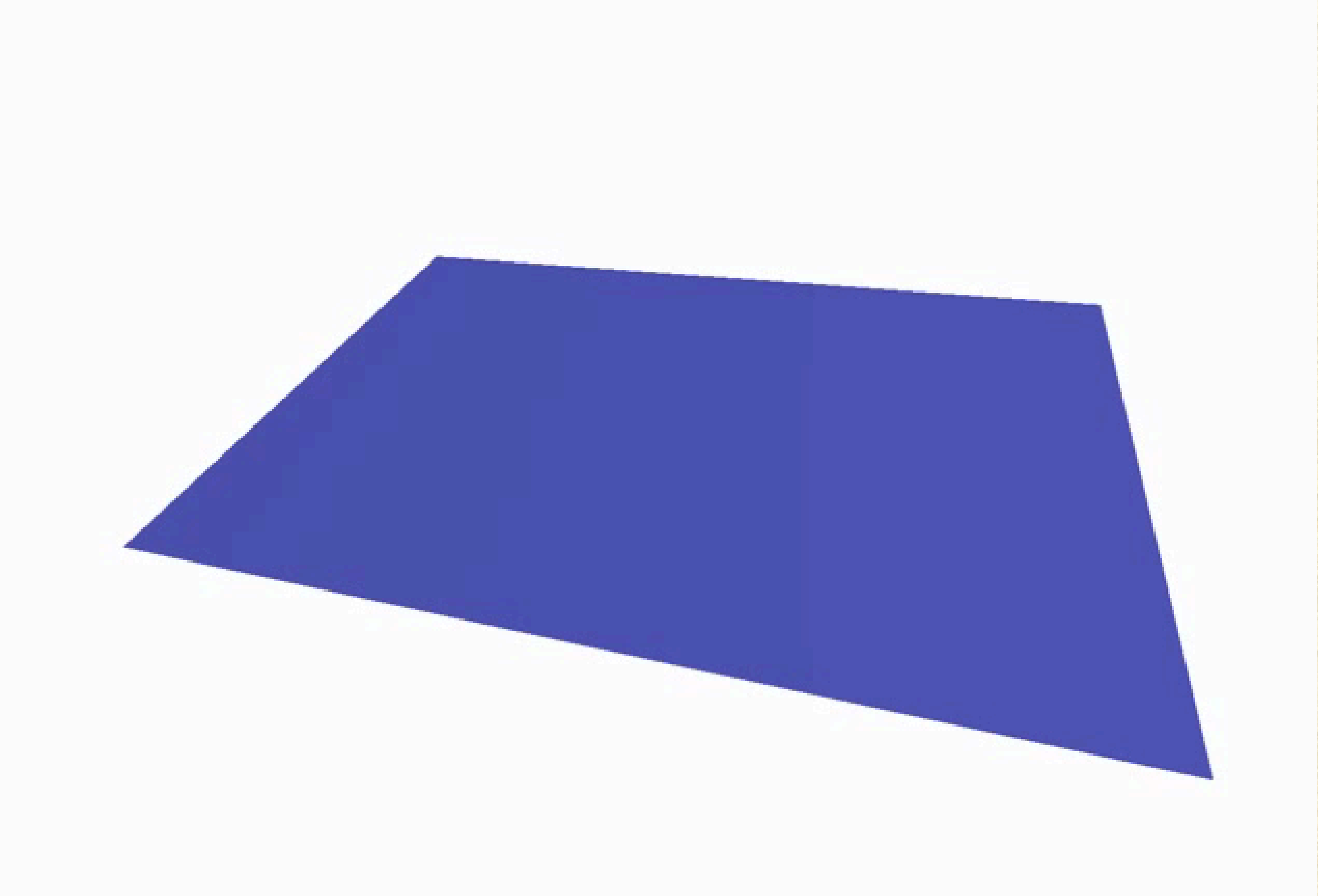
Crack-tip Wave Scattering Example



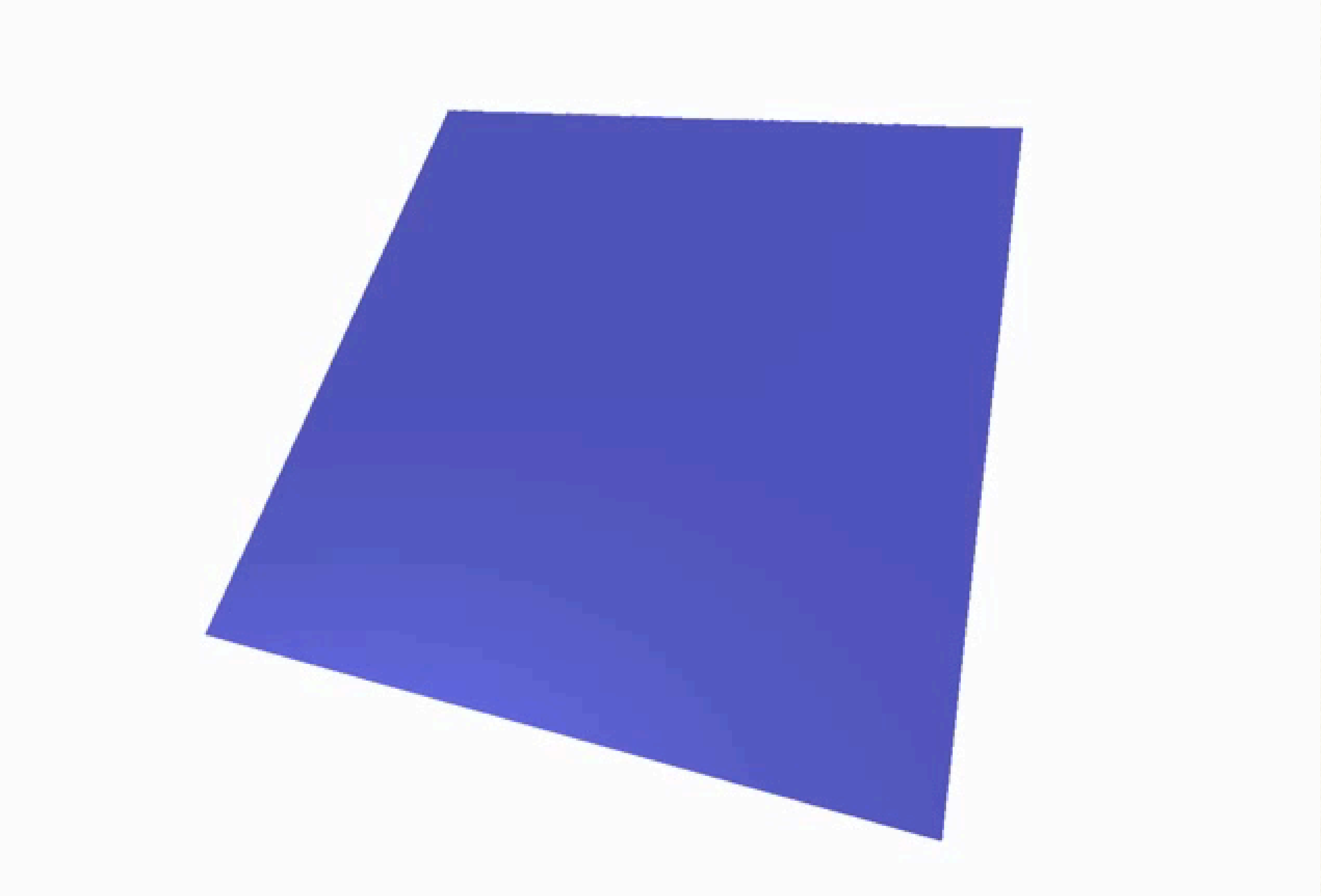
Crack-tip Wave Scattering Example



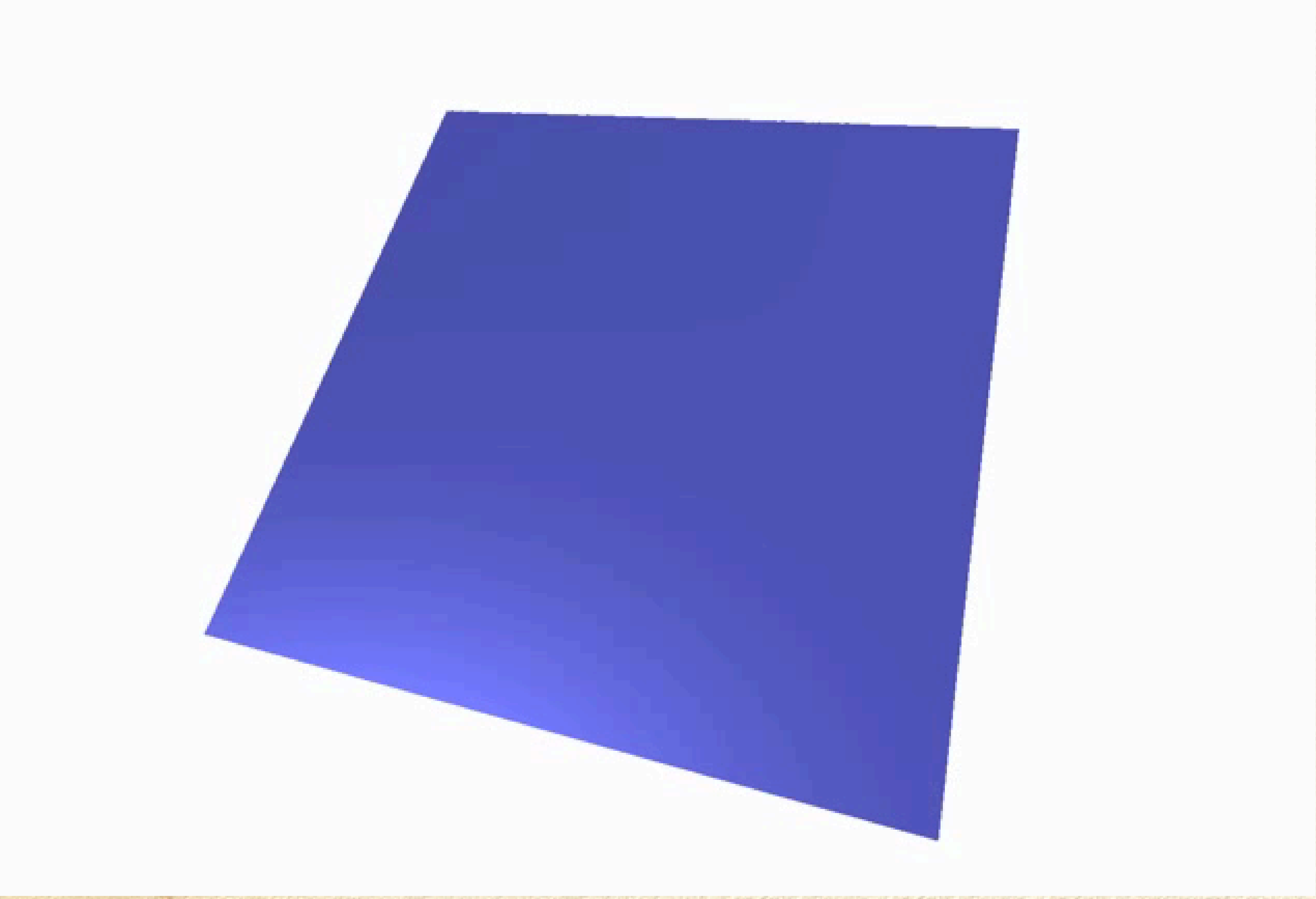
Crack Propagation Example with Cohesive Interface



Shock Scattering by Stiff Circular Inclusions in a Composite Material



Particle Dewetting in a Shocked Composite



Continuing Work on SDG Methods

- Code optimizations, combine parallel and adaptive (near term)
- Inclined tent poles to track moving interfaces (and shocks?)
- Extend SDG method to three dimensions
- Combine elastodynamics with conservation laws solver to address shocked SMAs
- Model dislocation density evolution in thin films (new proposal with Acharya et al.)
- Applications to Schrödinger equation

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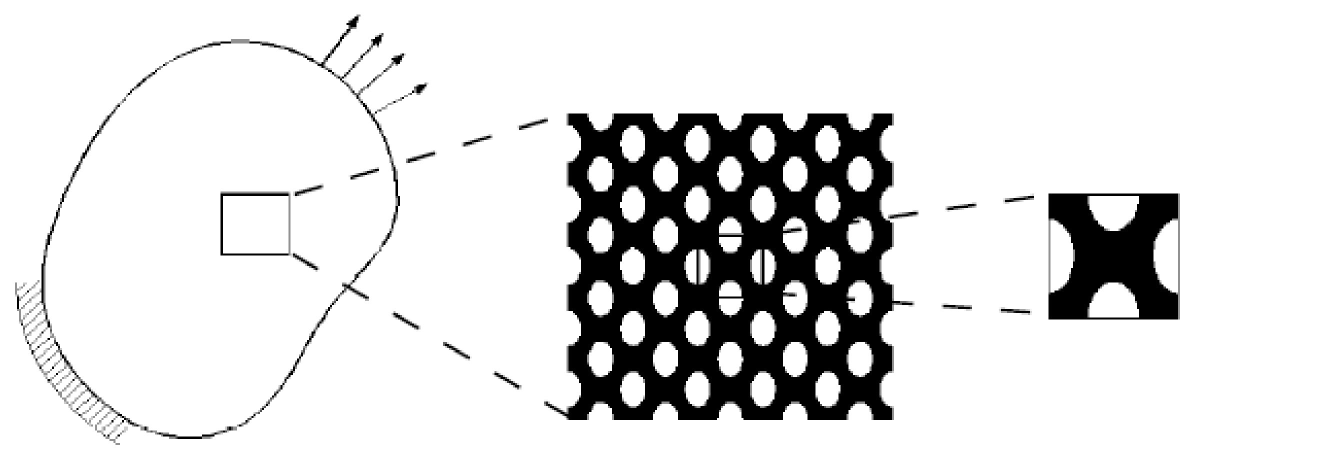
Shape and Topology Optimization of Material Microstructures

M. Bendsøe, R. Haber, J. Norato and D. Tortorelli

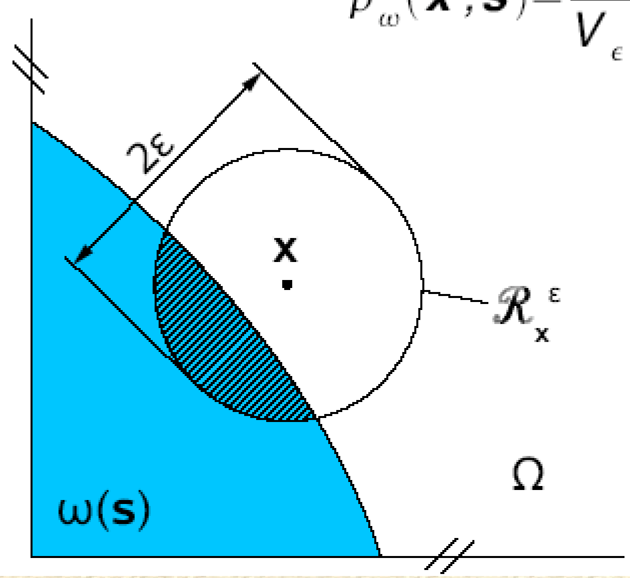


The geometry measure is defined as

$$\mu_{\omega}^{\alpha,\epsilon}(\boldsymbol{x},\boldsymbol{s})=\alpha+(1-\alpha)\,\rho_{\omega}^{\epsilon}(\boldsymbol{x};\boldsymbol{s}),\quad 0<\alpha\ll 1$$

where ρ_ω^ε is the volume fraction field defined as

$$\rho_{\omega}^{\epsilon}(\boldsymbol{x},\boldsymbol{s})=\frac{1}{V_{\epsilon}}\int_{\mathcal{R}_{\boldsymbol{x}}^{\epsilon}}\chi_{\omega}\,dv=\frac{1}{V_{\epsilon}}\int_{\mathcal{R}_{\boldsymbol{x}}^{\epsilon}\cap\omega}dv$$



- ρ_ω^ε is derived from the geometry model.
- $\rho_\omega^\varepsilon \rightarrow \chi_\omega$ as $\varepsilon \rightarrow 0^+$

Phase Field Crystals

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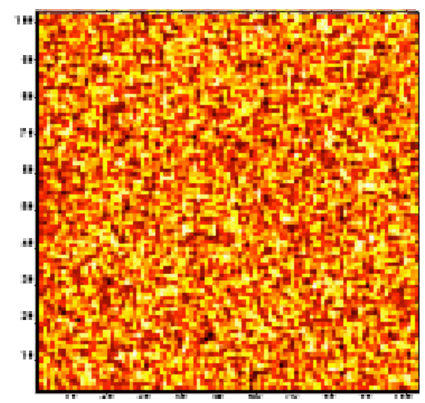
RG solution to S-H equation

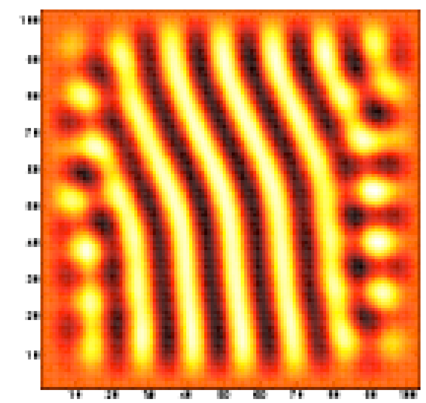
- E-G equation is conservative form of Swift-Hohenberg equation

$$\partial_t \psi = \epsilon \psi - \psi^3 - (\nabla^2 + 1)^2 \psi$$

- Studied in context of evolution of spatially periodic Rayleigh-Bénard cells (rolls)



t = 0

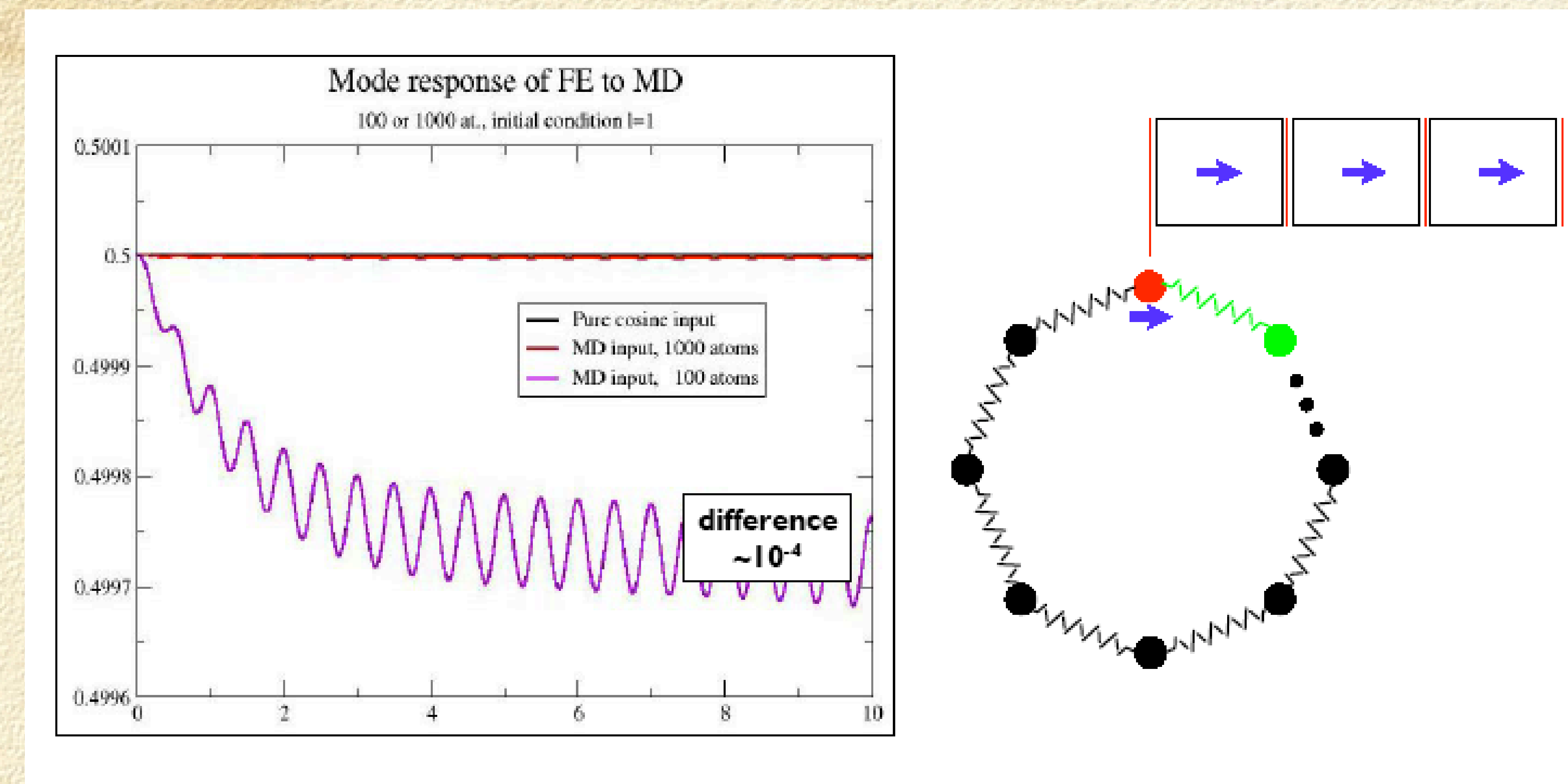


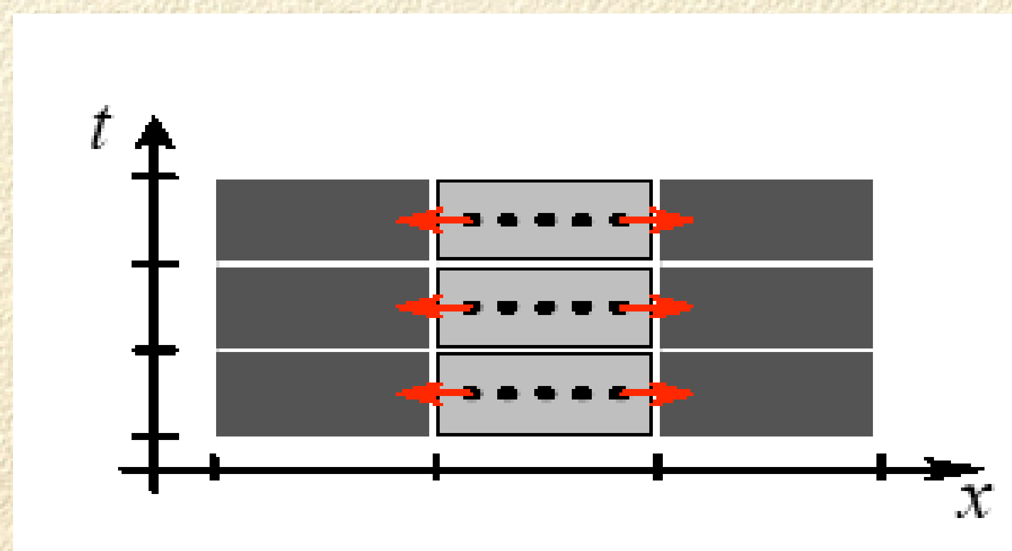
t = 500

- When $\epsilon \gg \epsilon_c$, rolls evolve slowly through wave-vector adjustment
- Treat $\partial_t \psi$ as multiplied by small parameter η

Atomistic / Continuum Coupling in Spacetime

R. Haber, D.Johnson, B. Kraczek, C. Xia





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- M&IE: Jon Dantzig, Dan Tortorelli, Julian Norato, B. Athreya, A. Chang
- MatSE/Physics: Duane Johnson, Brent Kraczek