MULTISCALE METHODS, MOVING BOUNDARIES AND INVERSE PROBLEMS

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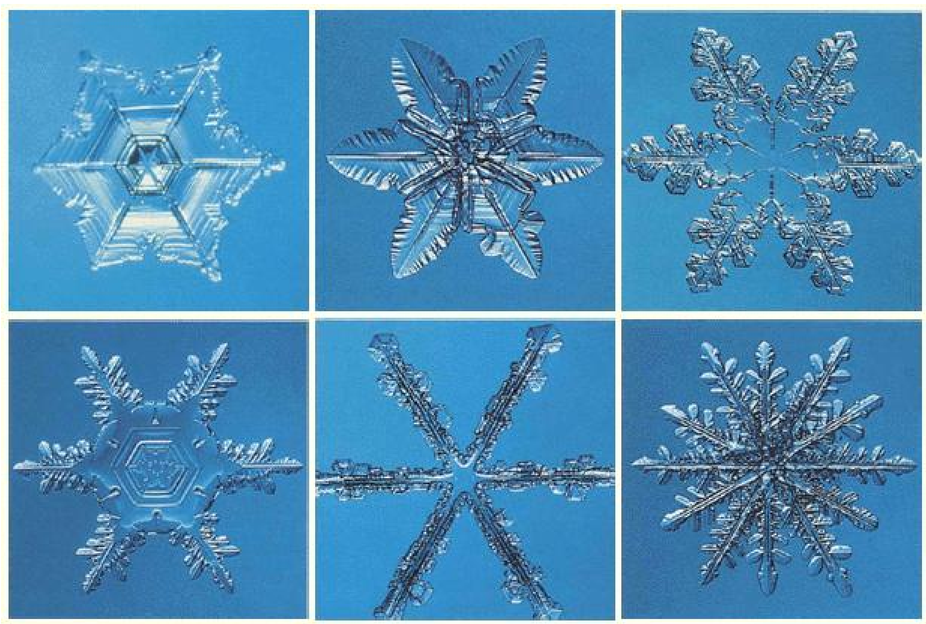
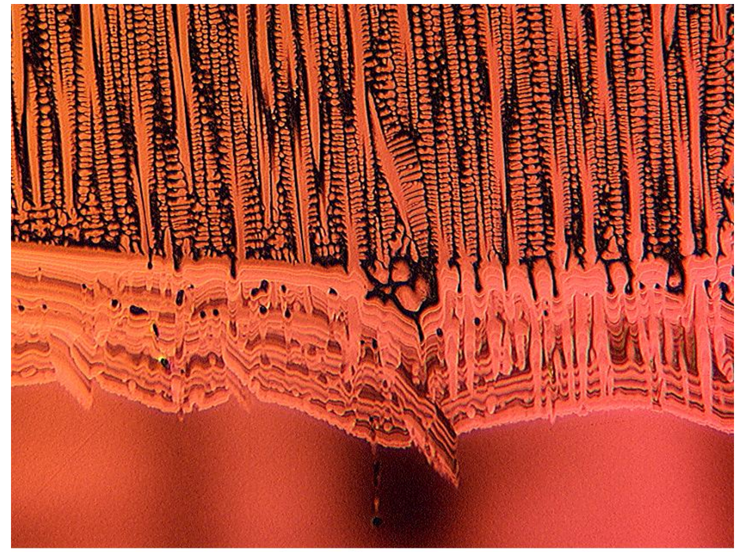
Presentation outline

- Multiscale and moving boundary problems
  - § Multiple length and time scales
  - § Formulation of mathematical problem
  - § Moving boundary problems
  - § Adaptive methods for resolving length scales
  - § Solidification problems as a context
- Inverse methods for design and parameter identification
  - § Design as a complement to analysis
  - § Mathematical methods for inverse problems
  - § Examples: shape and topology optimization
- Summary and conclusions

Crystal pattern selection

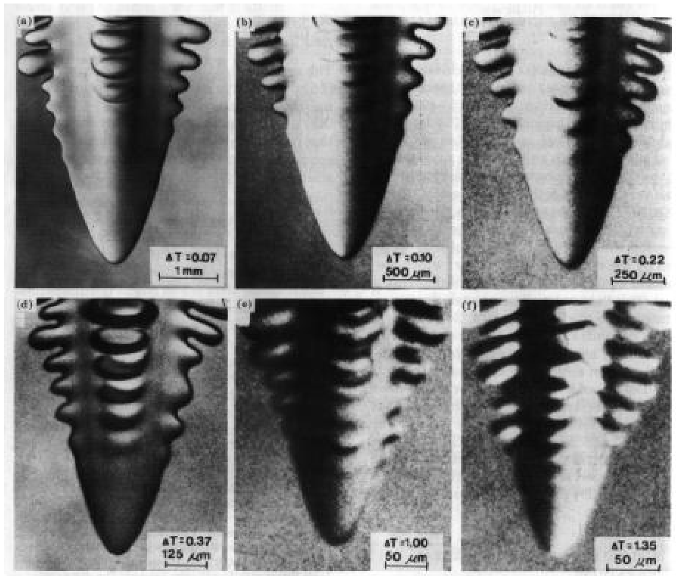


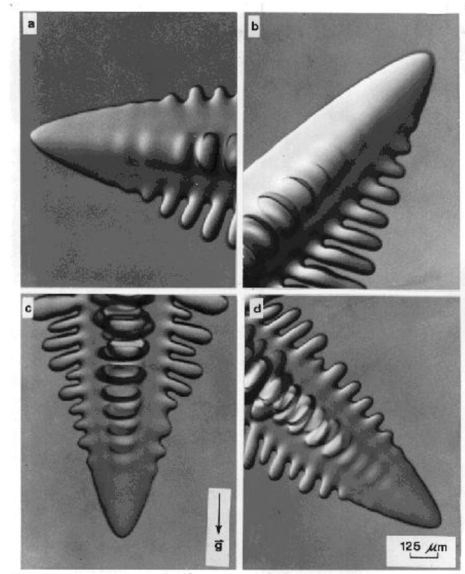


01-2993-11c #1 (TMS75-No slope-L) 200X 20μm
Glyceregia

- "Every snowflake is different"
  - § Pattern set by environment during growth (Furukawa)
- Dendrite also canonical microstructural form in metals and alloys
  - § Spot weld in Ni-based superalloy (Babu and David, ORNL)
- Processing conditions determine microstructure and properties

Observations in succinonitrile

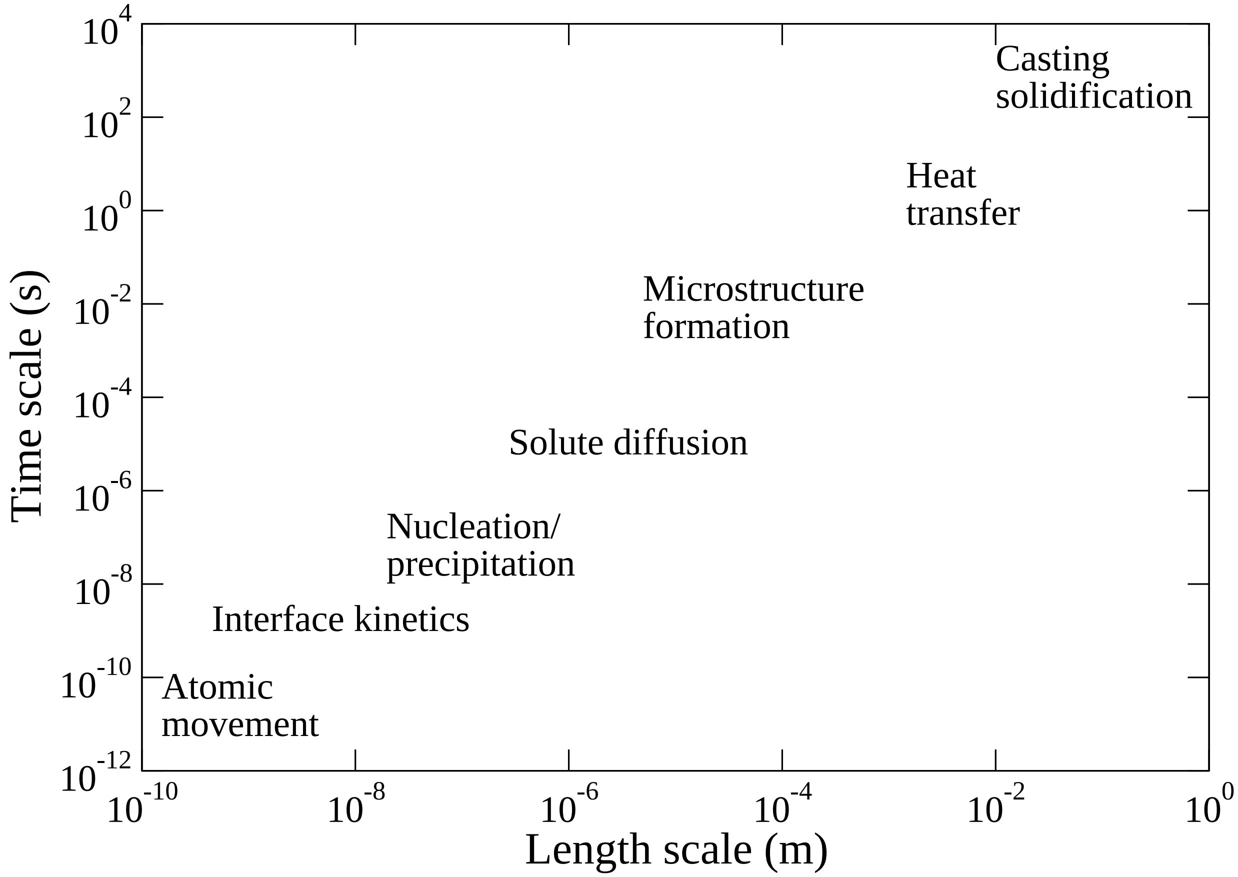




- Succinonitrile (SCN) is transparent organic analog for metals
- High purity SCN growing into undercooled melt
- Experiments by Glicksman, et al., $0.02 < \Delta T/(L_f/c_p) < 0.06$
- Left-hand photographs scaled on ΔT
- Right-hand photos at different orientations wrt gravity

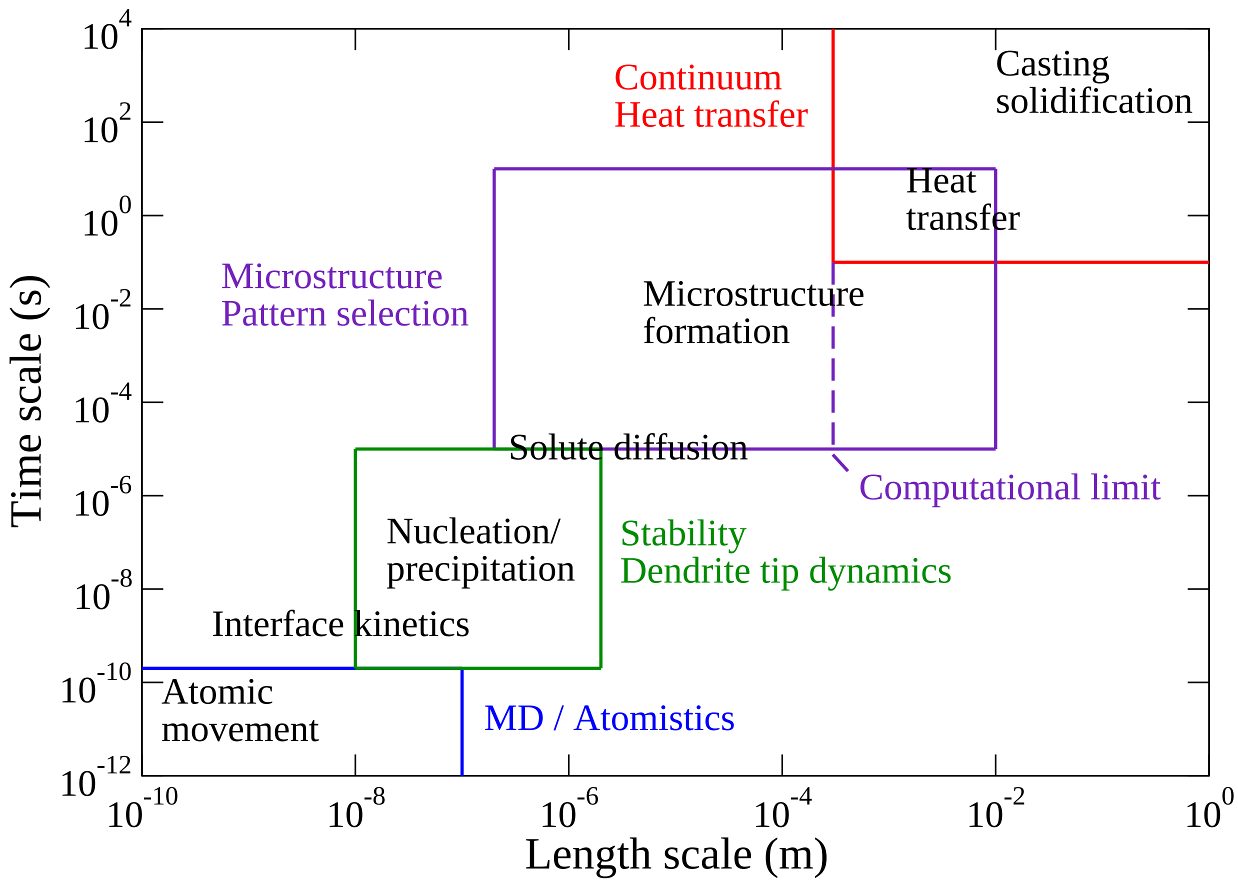
Solidification phenomena

- Vast range of length and time scales
- Slope of 1 cm/s typical interface speed



Computational models and limits

- 2D: $10^3 \times 10^3$ in space, 10^3 in time, 8 bytes/datum = 8Gb
- 3D: $10^2 \times 10^2 \times 10^2$ in space, 10^3 in time, 8 bytes/datum = 8Gb



Solidification of a pure material in an undercooled melt

- Dendritic growth as a generalized Stefan problem

$$\frac{\partial T}{dt} = \frac{k}{\rho c_p}\nabla^2 T = \alpha \nabla^2 T$$

  § Interface conditions:

$$\begin{aligned} \rho L_f V_n &= k\left(\nabla T \cdot \vec{n}|_S - \nabla T \cdot \vec{n}|_L\right) \\ T &= T_m - \Gamma[(a + a_{\theta\theta})\kappa_\theta + (a + a_{\phi\phi})\kappa_\phi)] - \beta(\boldsymbol{n})V_n \end{aligned}$$

  § Anisotropy: $a(\boldsymbol{n}) = 1 - 3\epsilon_4 + 4\epsilon_4\left(n_x^4 + n_y^4 + n_z^4\right)$

  § Far-field condition: $T(\infty) = T_\infty$

- Scaling temperature $\theta = \frac{T - T_m}{L_f / c_p}$ gives

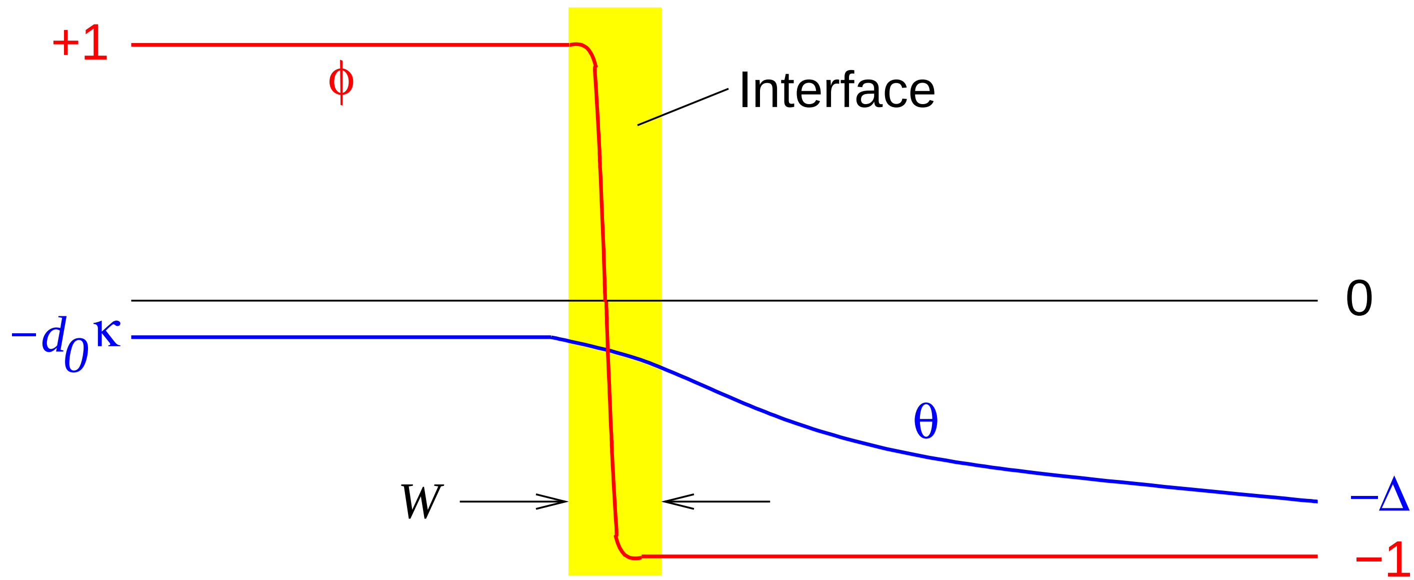
$$\begin{aligned} \frac{\partial \theta}{\partial t} &= \alpha \nabla^2 \theta \\ V_n &= \alpha\left(\nabla\theta \cdot \vec{n}|_S - \nabla\theta \cdot \vec{n}|_L\right) \\ \theta &= -d_0[(a + a_{\theta\theta})\kappa_\theta + (a + a_{\phi\phi})\kappa_\phi)] - \beta' V_n \\ \theta(\infty) &= -\Delta \end{aligned}$$

Moving boundary problems

- Must apply boundary conditions on interface whose location is unknown
- Deforming mesh methods (UNGAR AND BROWN, PRB, 1985)
  - § Adjust grid to align with interface
  - § Works in 2D, when mesh deformation is not large
  - § Satisfy one BC (Gibbs-Thomson), advance interface with other
  - § Cannot accommodate topology changes
- Fixed grid methods
  - § Grid remains fixed and interface moves through it
  - § Level set method (OSHER AND SETHIAN, JCP, 1988)
  - § Other hybrid methods (JURIC AND TRYGVASSON, JCP, 1996)
  - § Phase field method (LANGER, REV. MOD. PHYS., 1980)

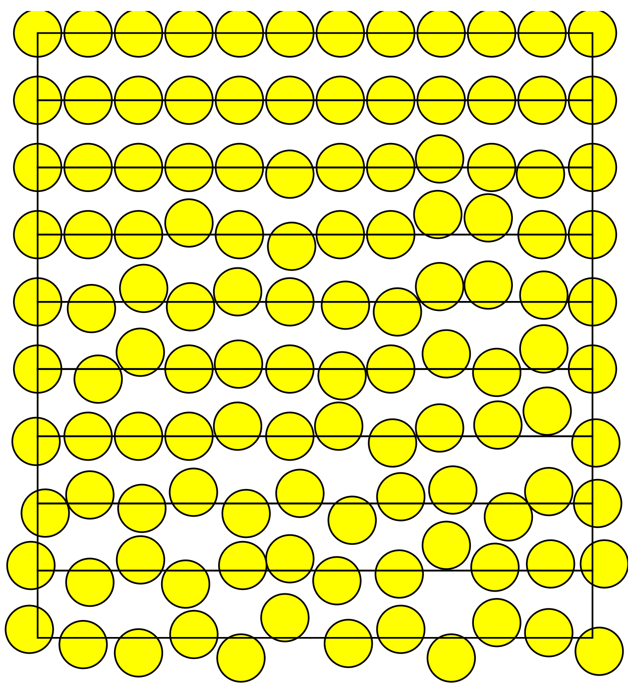
Phase-field method for solidification

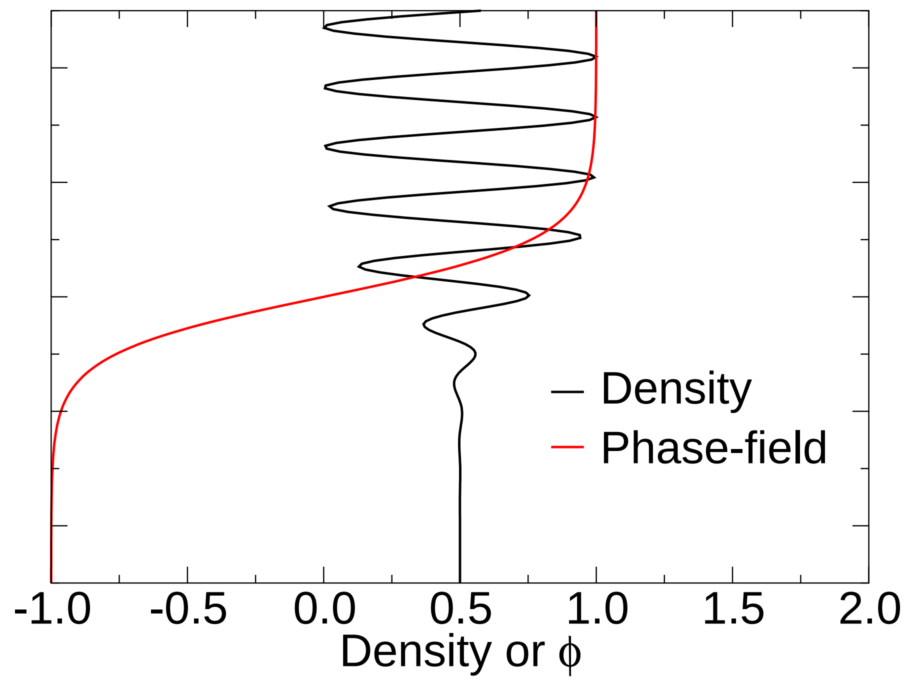
- Introduce *phase-field* on a fixed grid
  - § Define a continuous order parameter $-1 < \phi < 1$
  - § $\phi = -1$ corresponds to liquid, $\phi = +1$ to solid
  - § Define interface position as $\phi = 0$
- Interface is now a diffuse region, finite width W



Physical interpretation of the phase-field

- Consider a rough interface (WARREN AND BOETTINGER)
- Plot atomic density near interface





Phase-field model for a pure material

- Coupled equations for temperature and ϕ

$$\frac{\partial\theta}{\partial t} = \nabla\cdot(\alpha\nabla\theta) + \frac{1}{2}\frac{\partial\phi}{\partial t}$$
$$\tau\frac{\partial\phi}{\partial t} = -\frac{\delta\mathcal{F}}{\delta\phi}$$

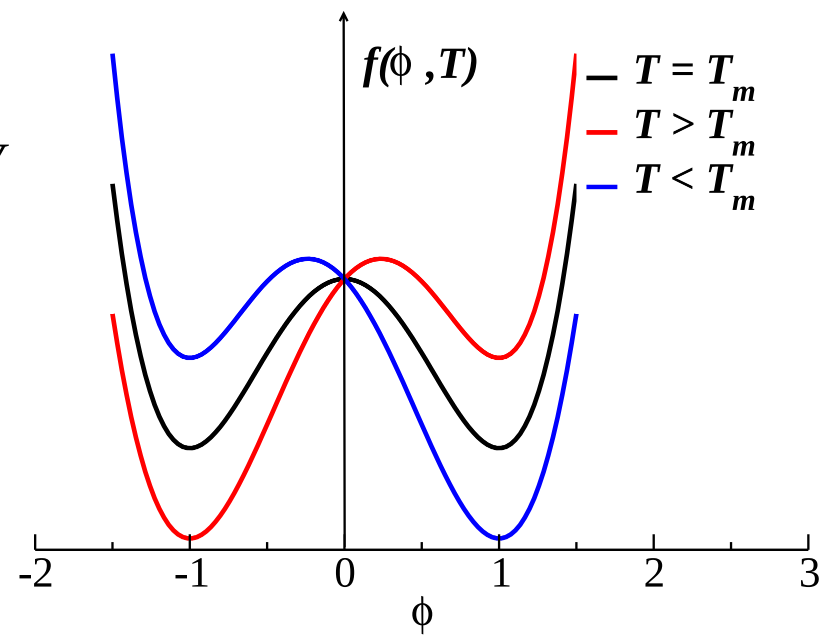
- Attributes: thin interface, $\phi = \pm 1$ as stable states

$$\mathcal{F} = \int_V \left(\frac{1}{2}|w(\vec{n})\nabla\phi|^2 + f(\phi, T)\right) dV$$

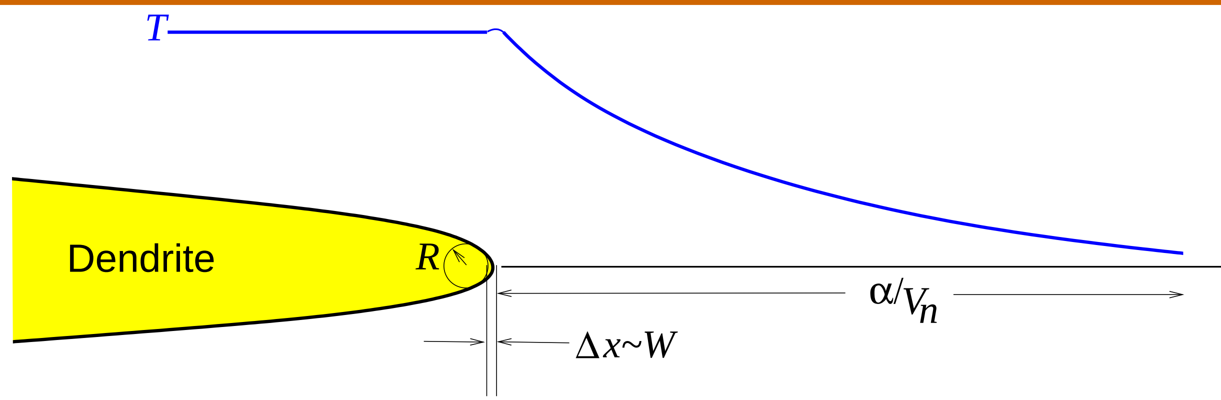
$$f(\phi, T) = \phi(1-\phi^2)+\lambda\theta(1-\phi^2)^2$$

§ λ controls double well tilt

§ $f(\phi, T)$ form *not* crucial



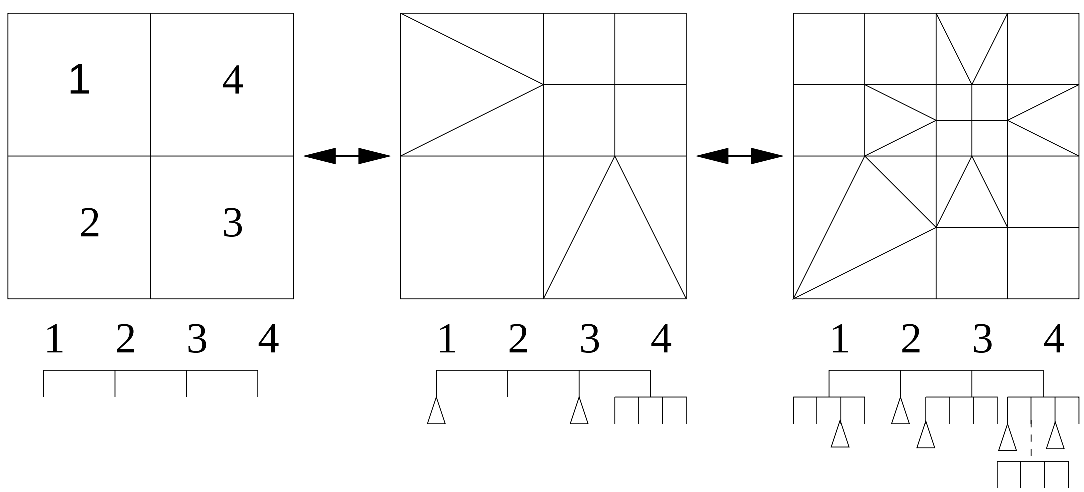
Hierarchy of length scales



- Length scales: $d_0 (10^{-9}\text{m})$, $R(10^{-5}\text{m})$, $\alpha / V_n (10^{-4}\text{m})$, W_0, Δx, L_B
  - § Grid convergence requires $\Delta x \sim \mathcal{O}(W)$
  - § Karma and Rappel, *PRE*, 1995: $W/(\alpha / V_n) \ll 1$ $(\sim 10^{-2})$
  - § Domain independence requires $L_B/(\alpha / V_n) \gg 1$ (~ 10)
  - § $L_B/W \sim L_B/\Delta x \sim 10^3$
  - § Uniform mesh requires $N_g = (L_B/\Delta x)^d$ (10^6 in 2-D, 10^9 in 3-D)
- Problem is even more acute at low Δ
  - § Slow approach to steady state $\Rightarrow L_B/(\alpha / V_n) \sim 100$
  - § Experiments at $\Delta < 0.1$

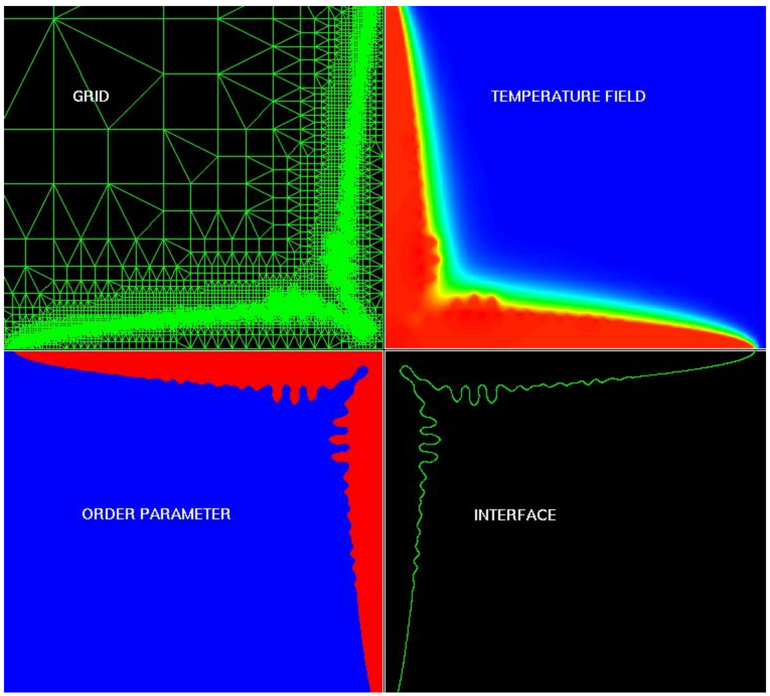
Finessing the length scale problem

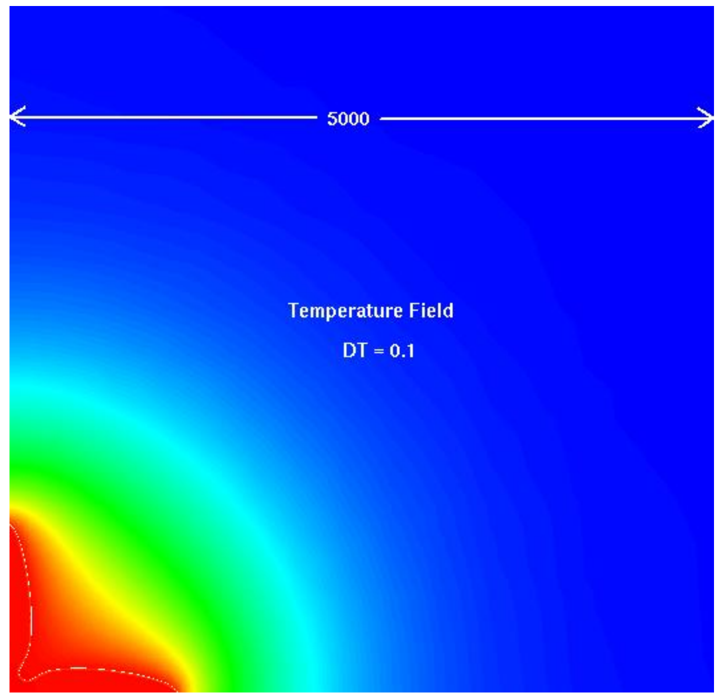
- Maximum resolution needed only near the interface
- Adaptive FEM grid (Provatas, Goldenfeld and Dantzig, PRL, JCP, 1998-2000)
- Initial mesh of 4-noded quadrilateral elements
- Refinement/fusion based on local error estimator $f(\nabla\phi, \nabla U)$
- Data structure
  - § Linked lists and quadtrees makes element traversal efficient
  - § Extra side nodes resolved with triangular elements (in 2D)



Dendritic growth at high and low undercooling

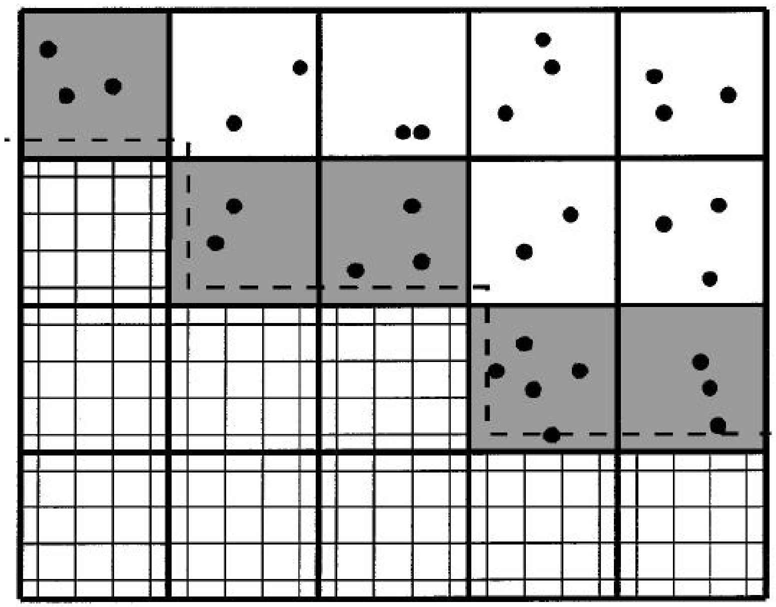
- Analytical theory for isolated arm in infinite medium
  - Tip speed and shape match theory at high Δ (left)
  - Both arms within thermal boundary layer at low Δ (right)

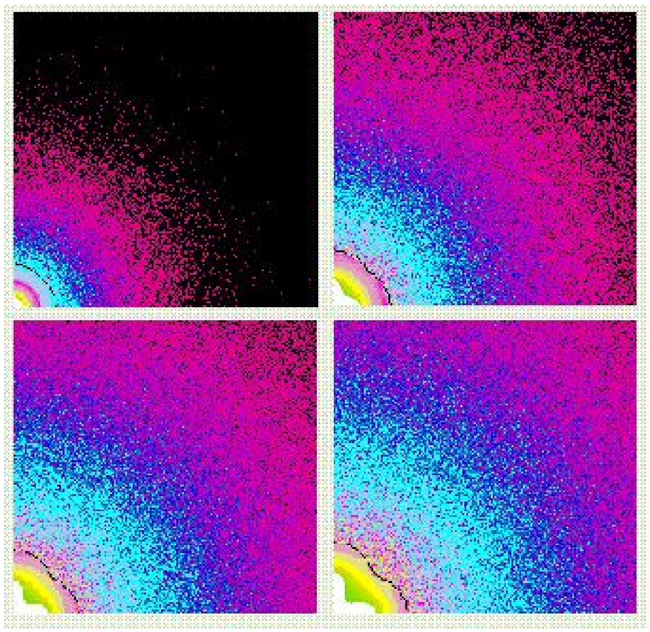




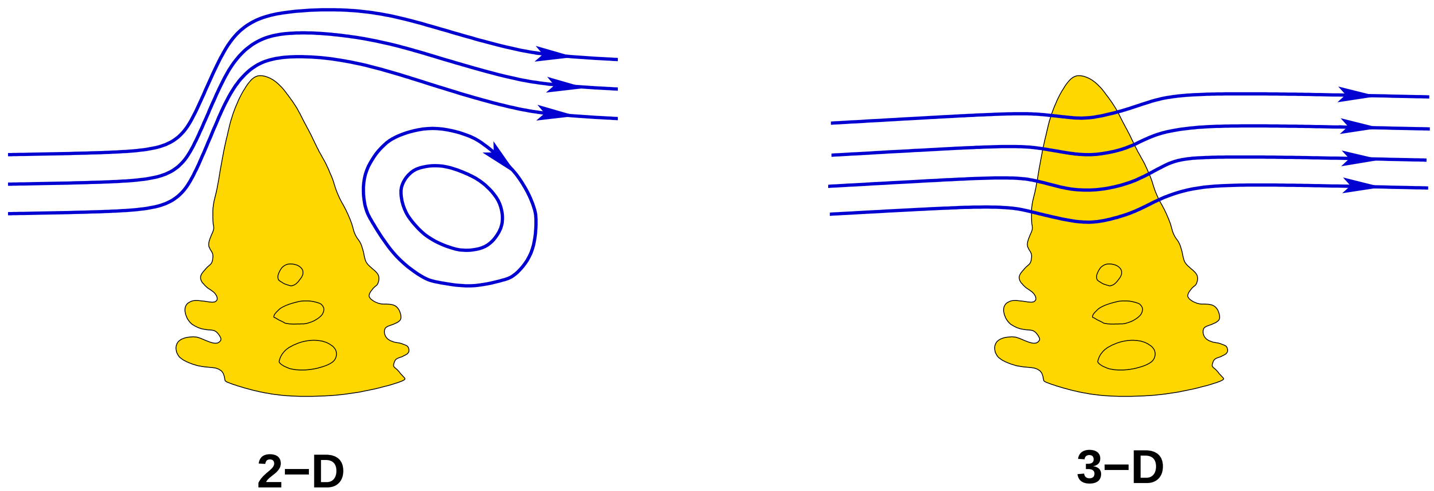
Another approach to the length scale problem

- Combine FDM and random walkers (Plapp and Karma, PRL, 2000):
  - § Solve using combined FDM/Random walker method
  - § Inner fine FDM mesh includes dendrite
  - § Outer diffusion field solved using random walkers
  - § Match solutions at boundary





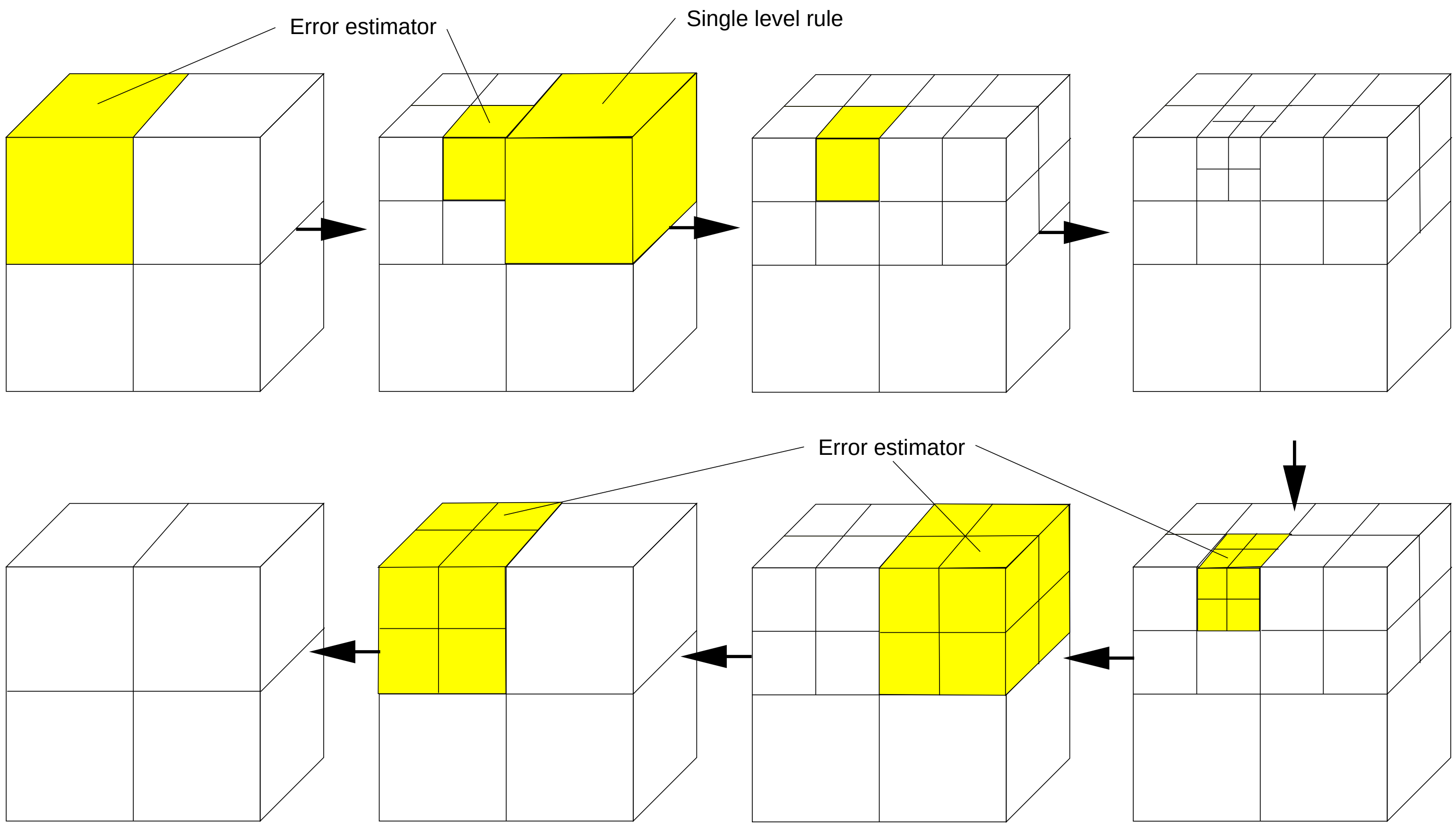
3D dendritic growth with fluid flow



- 3D nature is essential (Dantzig and Chao, IUTAM, 1986)
  - § 2D transport: Fluid must flow up and over the tip
  - § 3D transport: Vertical and horizontal flow around the tip
- Formulation (Beckermann, Diepers, Steinbach, Karma and Tong, JCP, 1999)
  - § Volume averaged form
  - § Special source to get correct drag force

Adaptive grid procedure in 3D

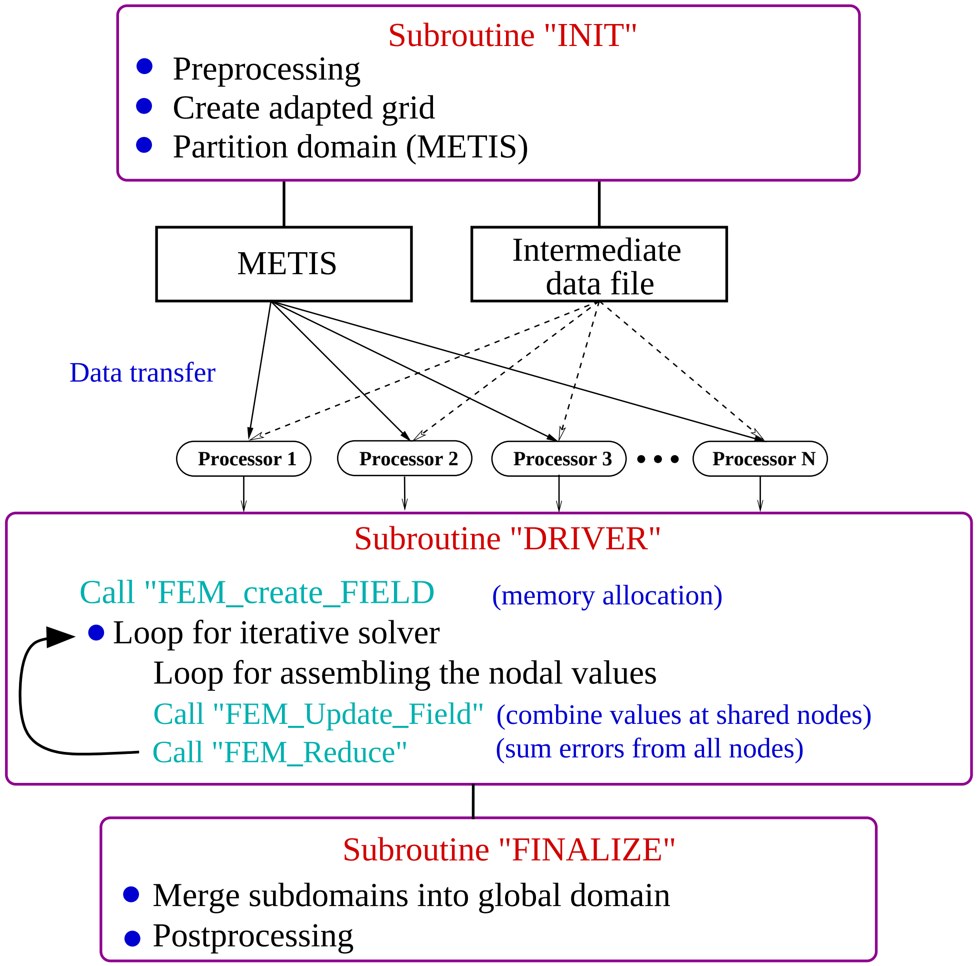
- Octree data structure
- Disconnected nodes handled by constraints



Parallel implementation of 3D code

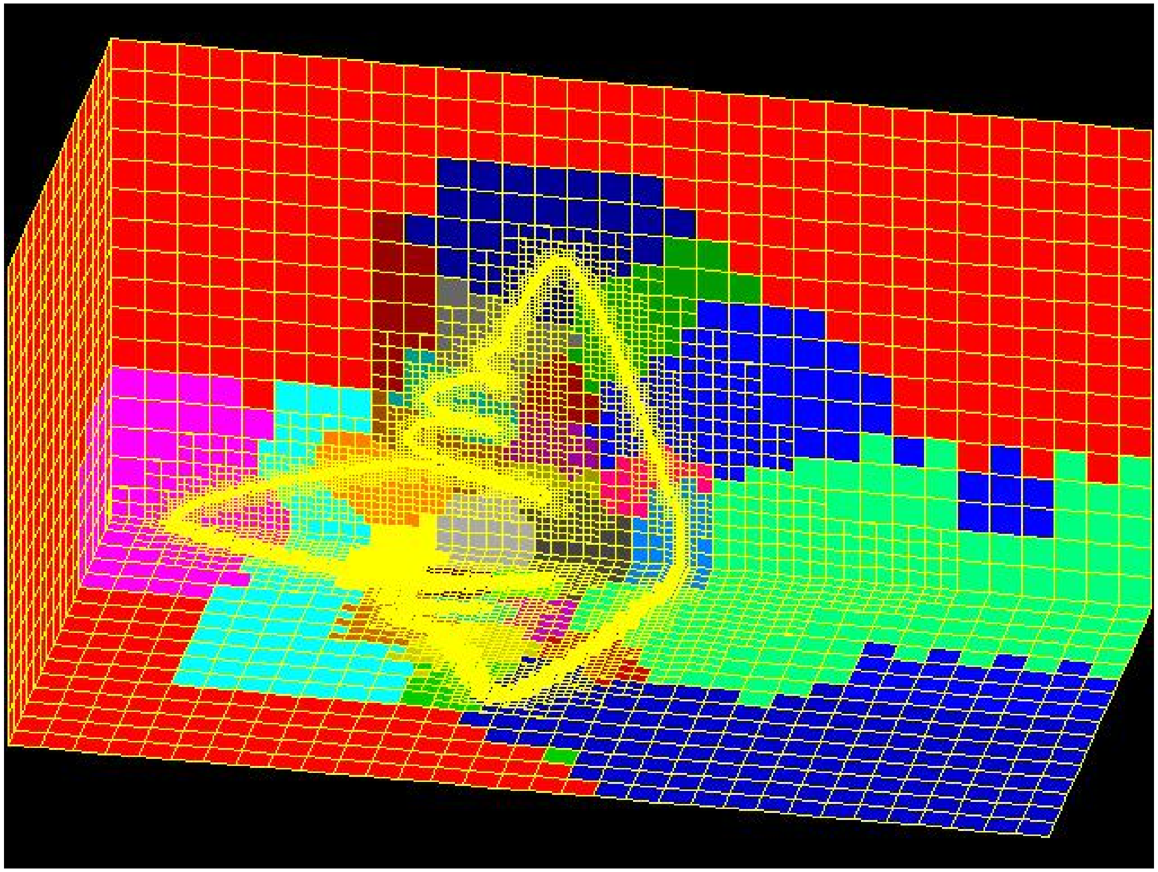
- Need large speedup factors ($\mathcal{O}(100)$)
- Domain decomposition not obvious
- Strategy
  - Distributed memory
  - CHARM++
- Code details
  - Explicit time stepping for phase-field, implicit for others
  - Flow computed using semi-implicit approximate projection method
  - Element-by-element conjugate gradient solver

Framework for parallelization by CHARM++



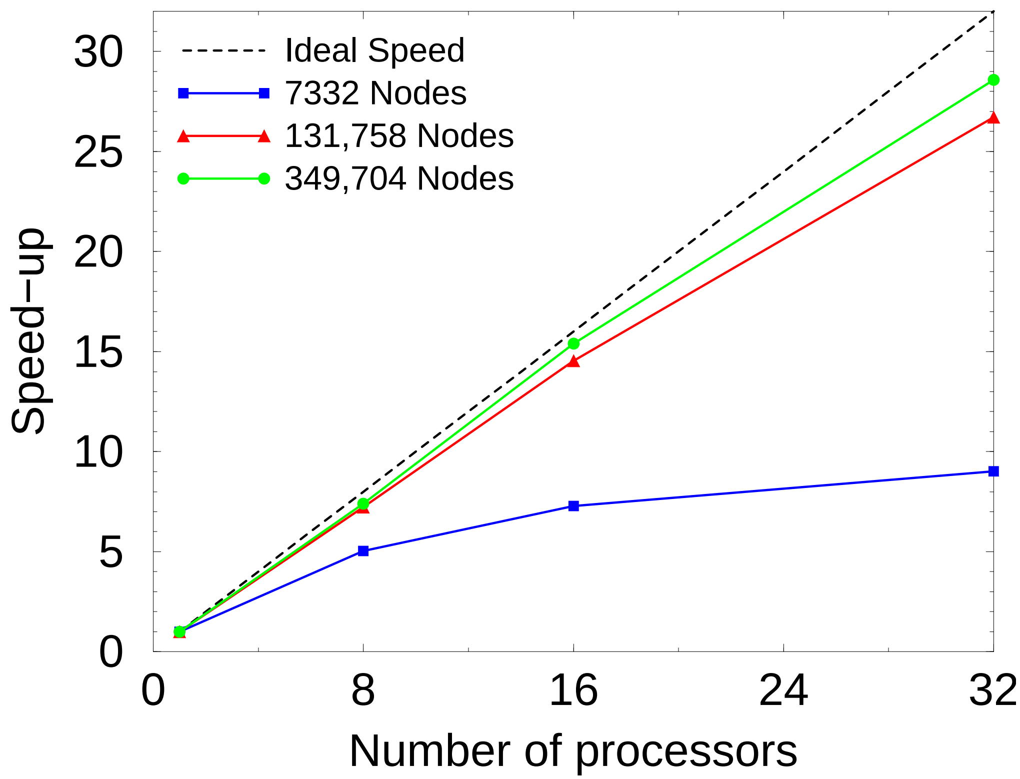
Domain decomposition

- Processor assignment for 32 processors (METIS)



Parallel performance of code

- Perform 20-100 time steps on a single mesh
- Speed-up approaches ideal as mesh size increases

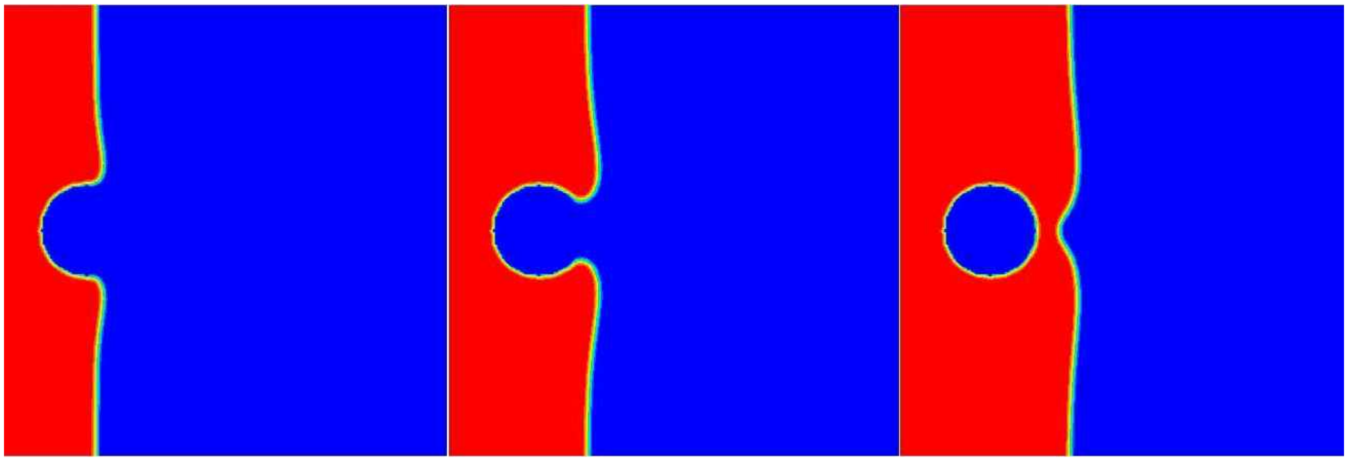


Biological application

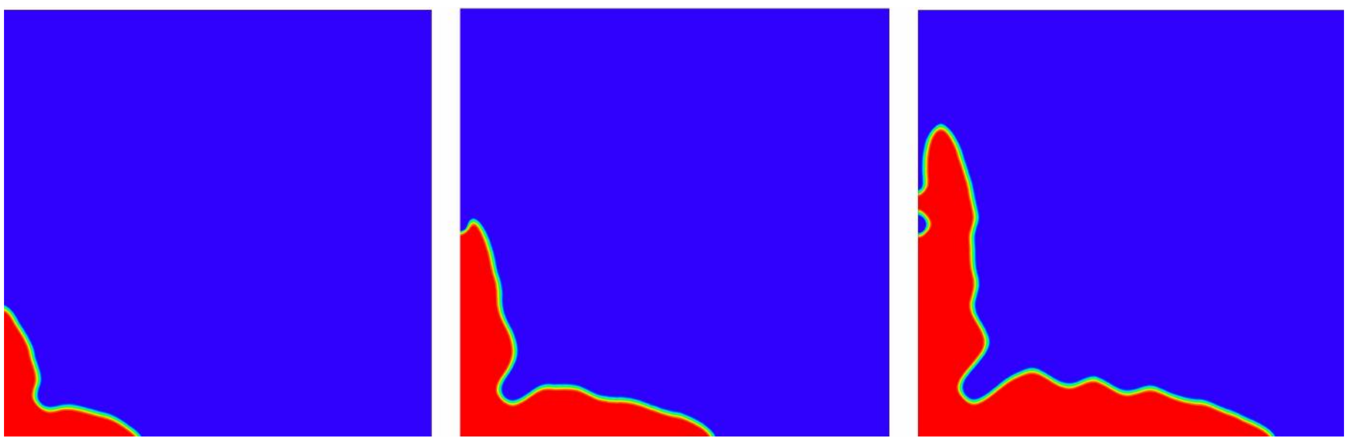
- Cryobiology: freezing cells for preservation
- Cells segregate from freezing ice
  - Local concentration important
  - Minimize mechanical damage
- Frog blood (Rapatz, Menz and Luyet, Cryobiology, 1966)

Modeling particle interaction

- Fixed particles, engulfed by interface



- Changes in dendritic growth patterns



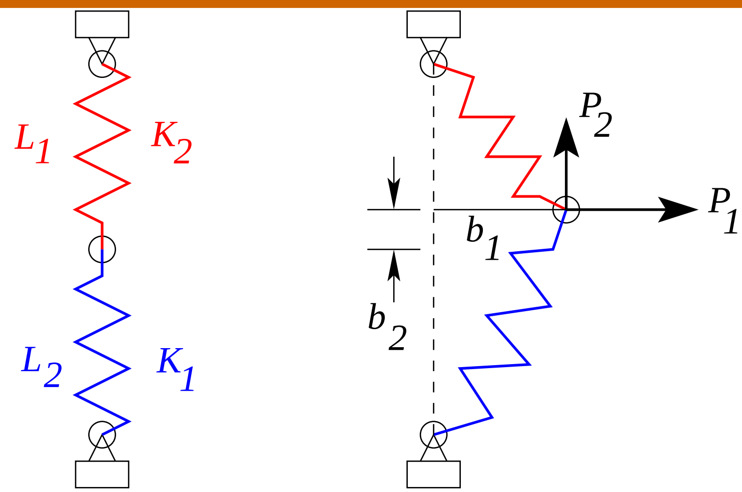
Summary: dendritic growth

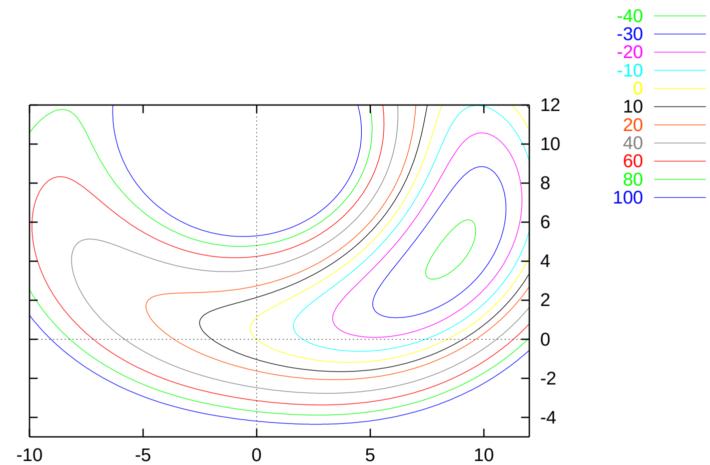
- Dendritic growth is complex pattern selection problem
- Multiple length scales can be resolved using adaptive grids
- Fluid flow has a profound effect on structure evolution
- 2D is different from 3D
- High Δ is different from low Δ
- Adaptive, 3-D Navier-Stokes, phase field code enables comparison to experimental observations
- More than one way to solve this problem!

Optimal design

- Have become adept at complex modeling
- Make transition from *analysis* to *design*
- Use simulations to improve design, or identify parameters
- Pose as an optimization problem:
  - § Identify *design variables* $\boldsymbol{b}$
  - § Solve problem for a given design $\boldsymbol{u}(\boldsymbol{b})$
  - § Minimize (or maximize) and objective function $G(\boldsymbol{u}, \boldsymbol{b})$
  - § Possible constraints $F(\boldsymbol{u}, \boldsymbol{b})$
- Design space is "orthogonal" to analysis space

Example: Equilbrium of two springs





- Equilibrium position is minimum potential energy P

$$
\begin{aligned}
P \;=\; & \frac{1}{2}K_1\left(\sqrt{b_1^2+(L_1-b_2)^2}-L_1\right)^2 + \\
& \frac{1}{2}K_2\left(\sqrt{b_1^2+(L_2+b_2)^2}-L_2\right)^2 - P_1 b_1 - P_2 b_2
\end{aligned}
$$

- How do you find minimum?
  - § Generate contours (response surface) and select
  - § Pick starting point and search discrete points

Solution strategies

- Each design implies a full simulation for $\boldsymbol{u}(\boldsymbol{b})$
- Simulations are costly $\Rightarrow$ limited number of designs
- Efficient search strategies require *sensitivities*, $dG/d\boldsymbol{b}$
- "Forward problem:" $\boldsymbol{R}(\boldsymbol{u}, \boldsymbol{b}) = 0$
  - § Solve by Newton-Raphson iteration

$$\boldsymbol{R}(\boldsymbol{u}^{i+1}, \boldsymbol{b}) = 0 = \boldsymbol{R}(\boldsymbol{u}^{i}, \boldsymbol{b}) + \left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}}\right|_i \boldsymbol{\Delta u} + \cdots$$

  - § Truncate and rearrange

$$\left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}}\right|_i \boldsymbol{\Delta u} = -\boldsymbol{R}(\boldsymbol{u}^{i}, \boldsymbol{b})$$

  - § Update $\boldsymbol{u}^{i+1} = \boldsymbol{u}^{i} + \boldsymbol{\Delta u}$
  - § Iterate to convergence

Sensitivity evaluation

- Finite difference evaluation of sensitivity very costly
- $dG/d\boldsymbol{b}$ involves "response sensitivity" $\partial\boldsymbol{u}/\partial\boldsymbol{b}$

$$\frac{dG}{d\boldsymbol{b}} = \frac{\partial G}{\partial \boldsymbol{b}} + \frac{\partial G}{\partial \boldsymbol{u}} \cdot \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{b}}$$

- Direct differentiation of forward problem wrt $\boldsymbol{b}$

$$\frac{d\boldsymbol{R}}{d\boldsymbol{b}} = 0 = \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{b}} + \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}} \cdot \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{b}}$$

- Rearrange to evaluate response sensitivity:

$$-\left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}}\right)^{-1} \cdot \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{b}} = \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{b}}$$

- Efficient implementation
  - Uses *same* tangent matrix as the forward problem
  - $\partial\boldsymbol{R}/\partial\boldsymbol{b}$ reforms force vector

Example: Nonlinear FEM heat conduction

- Interpolation using shape functions

$$T = \boldsymbol{N}\boldsymbol{T}; \quad \nabla T = \begin{bmatrix} \boldsymbol{N}_x \\ \boldsymbol{N}_y \\ \boldsymbol{N}_z \end{bmatrix} \boldsymbol{T} = \boldsymbol{B}\boldsymbol{T}$$

- Analysis, after assembly

$$\boldsymbol{R} = 0 = \boldsymbol{K}\boldsymbol{T} - \boldsymbol{F}$$

  - § Isoparametric form

$$\boldsymbol{K} = \int_V \boldsymbol{B}^T k(T) \boldsymbol{B} dV = \int_{V_r} \boldsymbol{J}^{-T} \boldsymbol{B}_r^T k(T) \boldsymbol{J}^{-1} \boldsymbol{B}_r |\boldsymbol{J}| dV_r$$

- Tangent matrix $\partial \boldsymbol{R}/\partial \boldsymbol{T} = \boldsymbol{K} + (\partial \boldsymbol{K}/\partial \boldsymbol{T})\boldsymbol{T} + \partial \boldsymbol{F}/\partial \boldsymbol{T}$

$$\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{T}} = \int_V \boldsymbol{B}^T \frac{dk}{dT} \boldsymbol{N} \boldsymbol{B} dV$$

Sensitivity evaluation

- Parameter identification: $k = k(\boldsymbol{b})$

$$\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{b}} = \frac{\partial \boldsymbol{K}}{\partial \boldsymbol{b}} \boldsymbol{T} = \int\limits_V \boldsymbol{B}^T \frac{\partial k}{\partial \boldsymbol{b}} \boldsymbol{B} dV$$

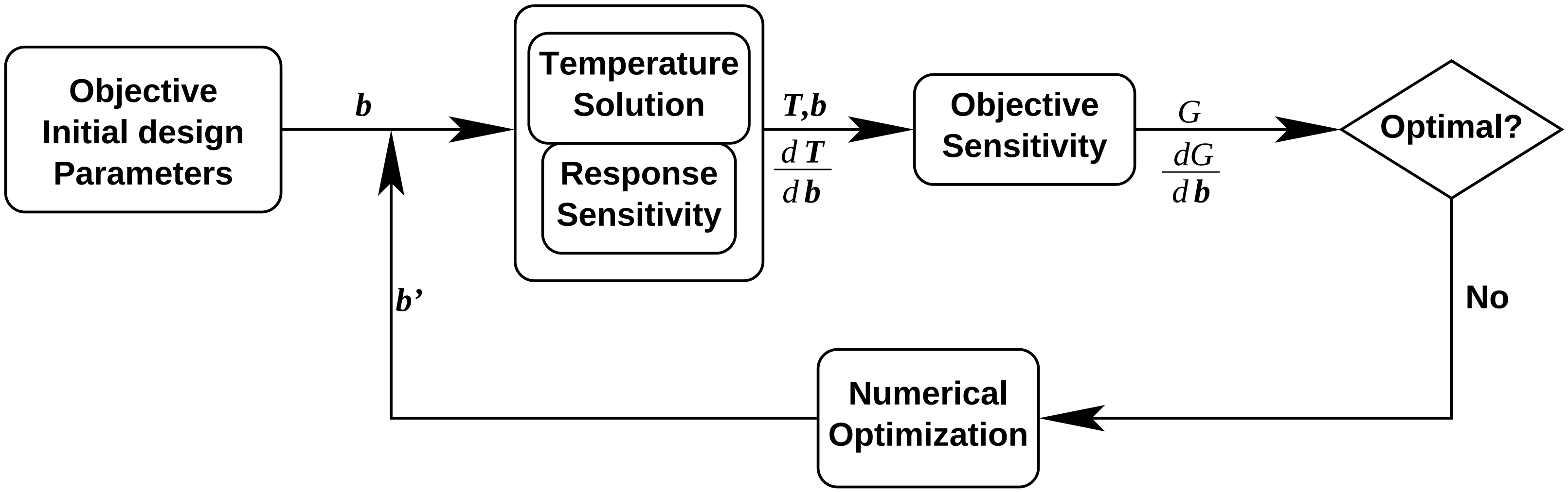
- Shape optimization: $\boldsymbol{J} = \boldsymbol{J}(\boldsymbol{b})$

$$\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{b}} = \int\limits_{V_r} \left(\frac{\partial \boldsymbol{J}^{-T}}{\partial \boldsymbol{b}} \boldsymbol{B}_r^T k(T) \boldsymbol{J}^{-1} \boldsymbol{B}_r + \boldsymbol{J}^{-T} \boldsymbol{B}_r^T k(T) \frac{\partial \boldsymbol{J}^{-1}}{\partial \boldsymbol{b}} \boldsymbol{B}_r + \right.$$
$$\left. \boldsymbol{J}^{-T} \boldsymbol{B}_r^T k(T) \boldsymbol{J}^{-1} \boldsymbol{B}_r \mathrm{tr} \left(\boldsymbol{J}^{-1} \frac{\partial \boldsymbol{J}}{\partial \boldsymbol{b}} \right) \right) |\boldsymbol{J}| dV_r$$

- Form multiple right hand sides and back-substitute

$$-\left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{T}} \right)^{-1} \cdot \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{b}} = \frac{\partial \boldsymbol{T}}{\partial \boldsymbol{b}}; \qquad \frac{dG}{d\boldsymbol{b}} = \frac{\partial G}{\partial \boldsymbol{b}} + \frac{\partial G}{\partial \boldsymbol{T}} \cdot \frac{\partial \boldsymbol{T}}{\partial \boldsymbol{b}}$$

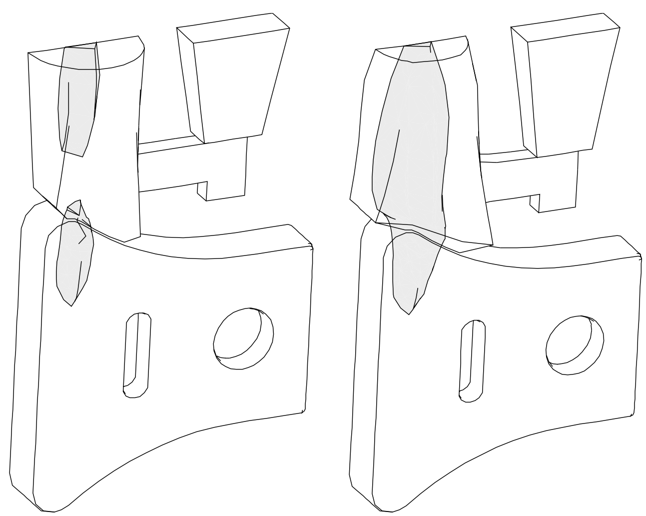
Optimization strategy



- Link to standard analysis codes
- Requires access to code for efficient sensitivity evaluation

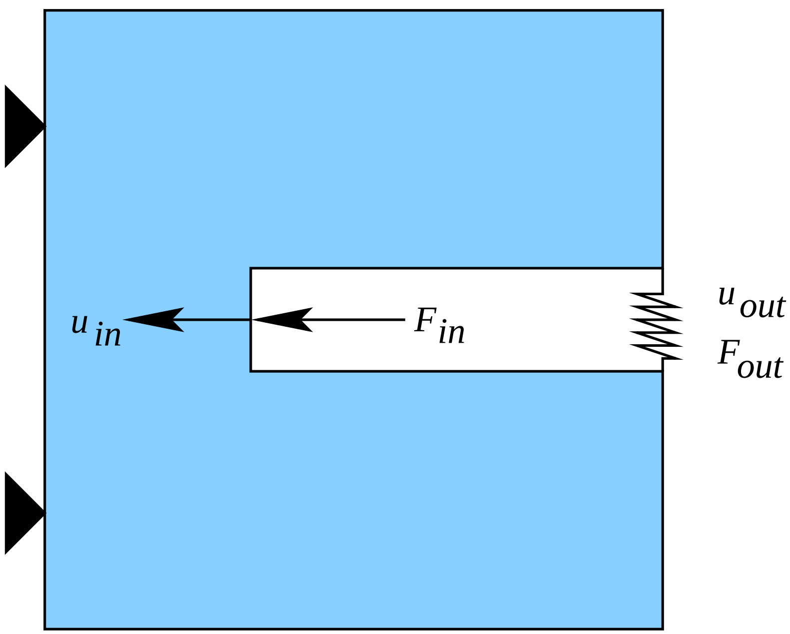
Example: Hammer casting simulation

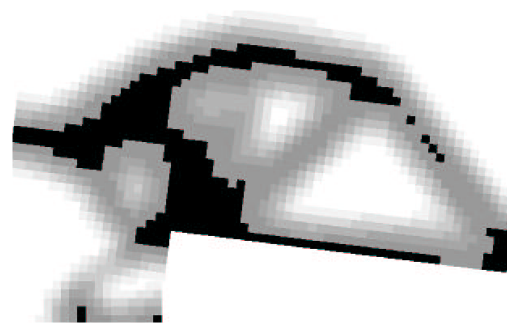
- Original design produced porosity
- Optimization problem
  - § Design variables parameterize riser dimensions
  - § Objective: Minimize riser volume
  - § Constraint: Connected freezing path from part to riser
  - § Solution: 24 designs evaluated, 5 line searches (total $\mathcal{O}$(week)



Topology optimization

- Work of Bruns and Tortorelli
- Material density ρ_e in each element becomes a design variable
- Compliant mechanism
  - Maximize F_{out}/F_{in}
  - Discrete values through penalization of values $0 < \rho_e < 1$
  - Nonlinear (geometric) elastic analysis





Features of inverse problems

- Powerful method for improving product design, identifying parameters
- Must be able to quantify objectives
- Problems are ill-posed
- Solutions are not unique
  - § Regularization can be used, e.g.,

$$G = G_0 + \sum_{i=1}^{N} a_i b_i^2$$

- Some strategies can trap local minima
- Multiple analyses need to be run
- Multiple objectives can be complicated to include

Conclusion

- Multiscale phenomena exist across a range of disciplines
- Mathematics can be similar
  - Disparate array of length scales
  - Moving interfaces driven by long range fields
- Numerous approaches to modeling
- Optimization methods extend analysis capability
  - Fashion design from analysis tools
  - Parameter identification
- Questions?