The Gibbs Open Source Thermodynamics Project and Integrated Computational Materials Engineering (ICME)

Reactive Metals Workshop

February 19, 2009

Adam C. Powell, IV

Opennovation

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Overview

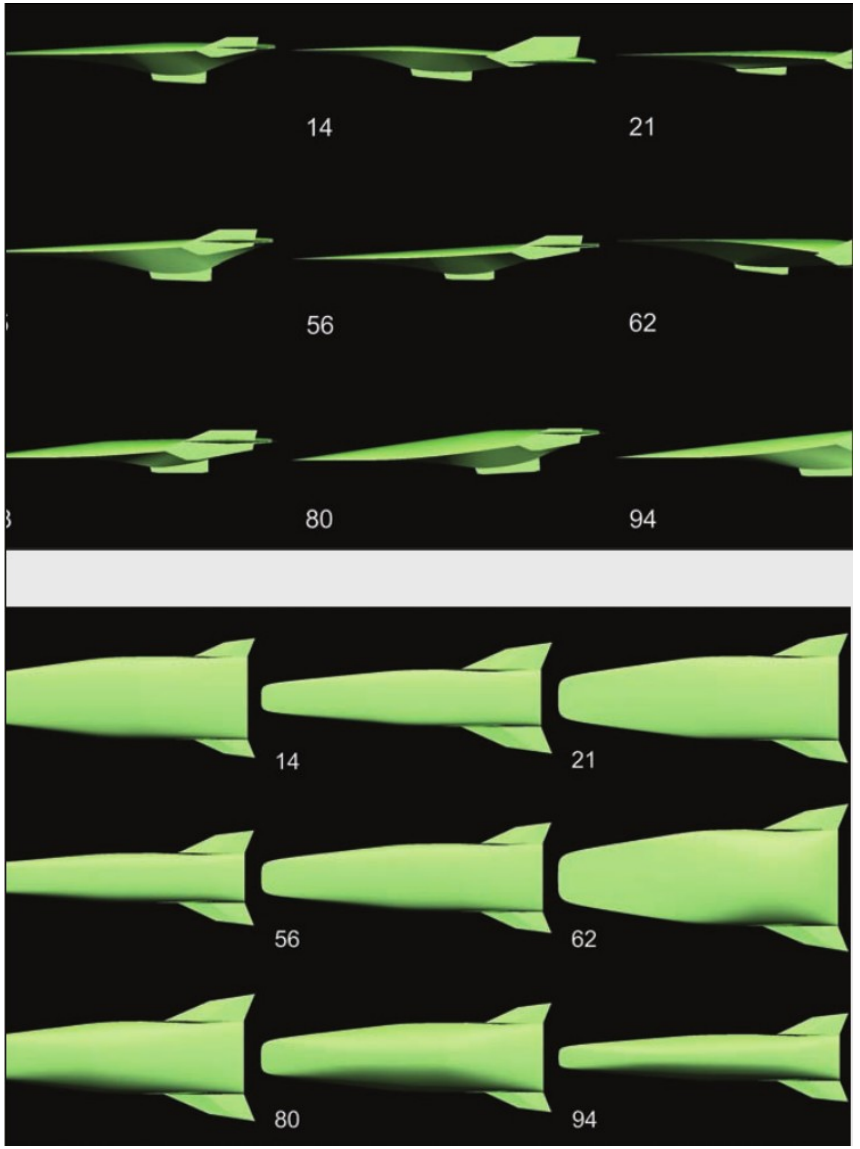
- ICME brief intro
- Thermodynamics: Gibbs Project
- Other tools:
  - Phase field: RheoPlast
  - Statistical mechanics: ATAT
  - Ab initio: abinit
- Summary

Motivations for ICME

- Product design cycle: 2-4 years
- Materials design cycle: 10-20 years!
- Application-specific materials development is impossible, hence materials *selection*
- New materials models and model integration accelerate development
- Broaden design space with application-specific materials

Geometry

- Geometric flexibility allows shape optimization for a given part's needs
- ICME: do the same for materials design



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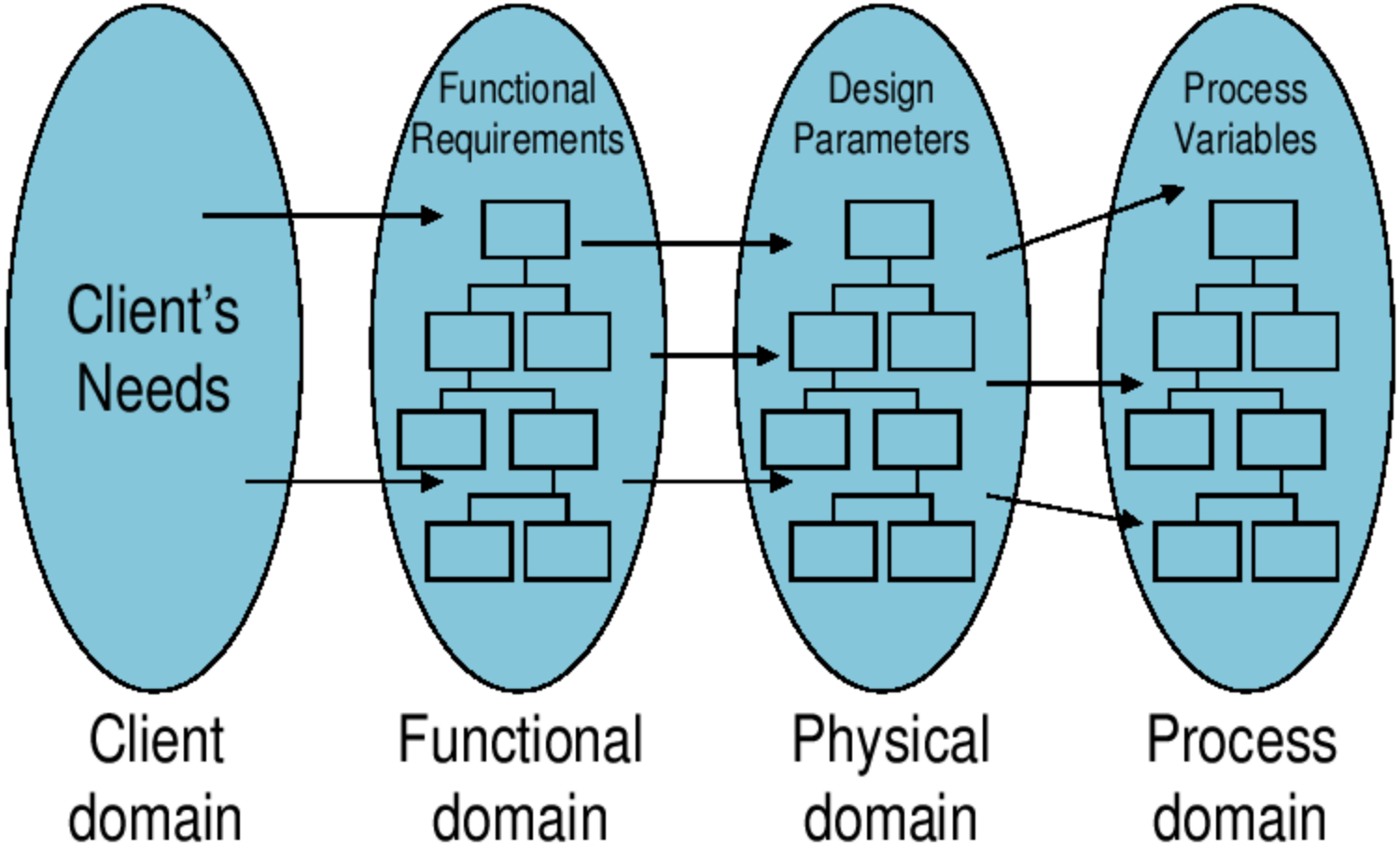
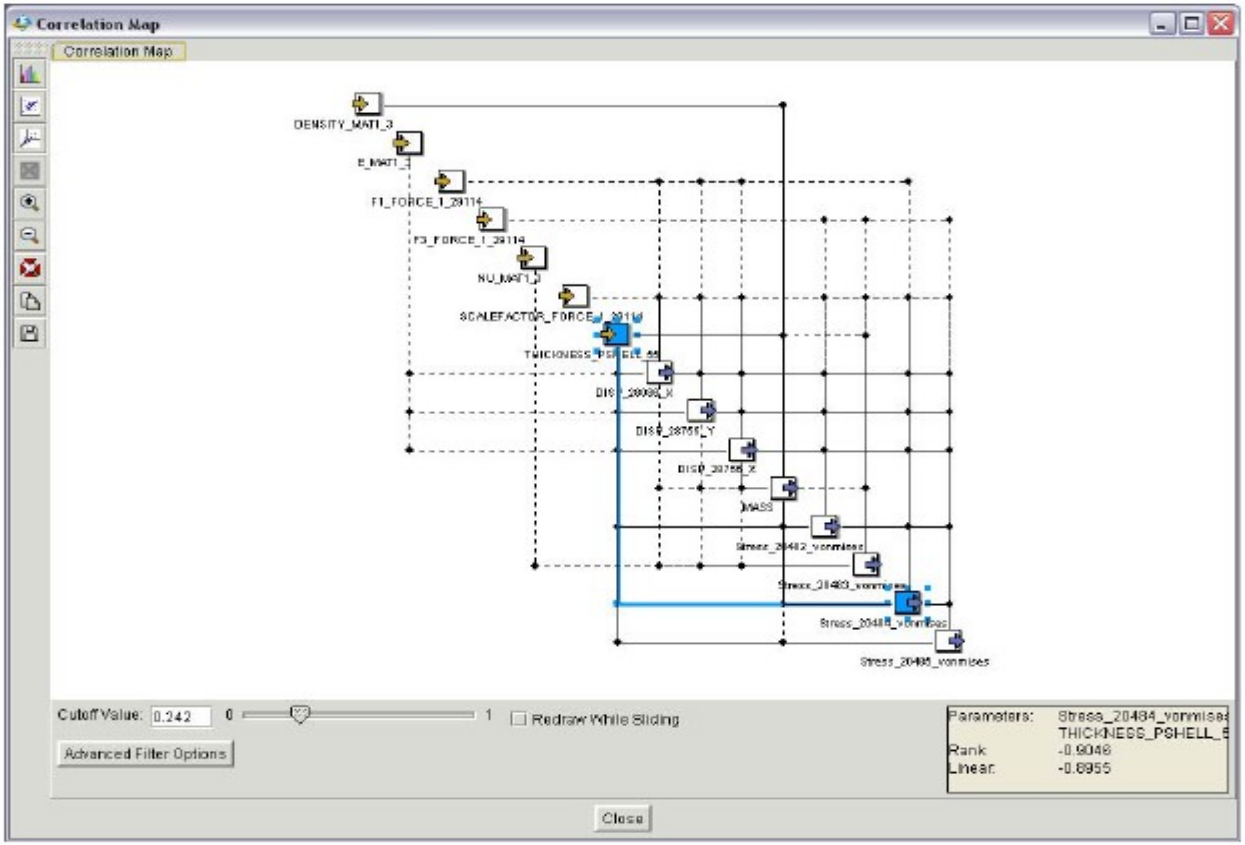
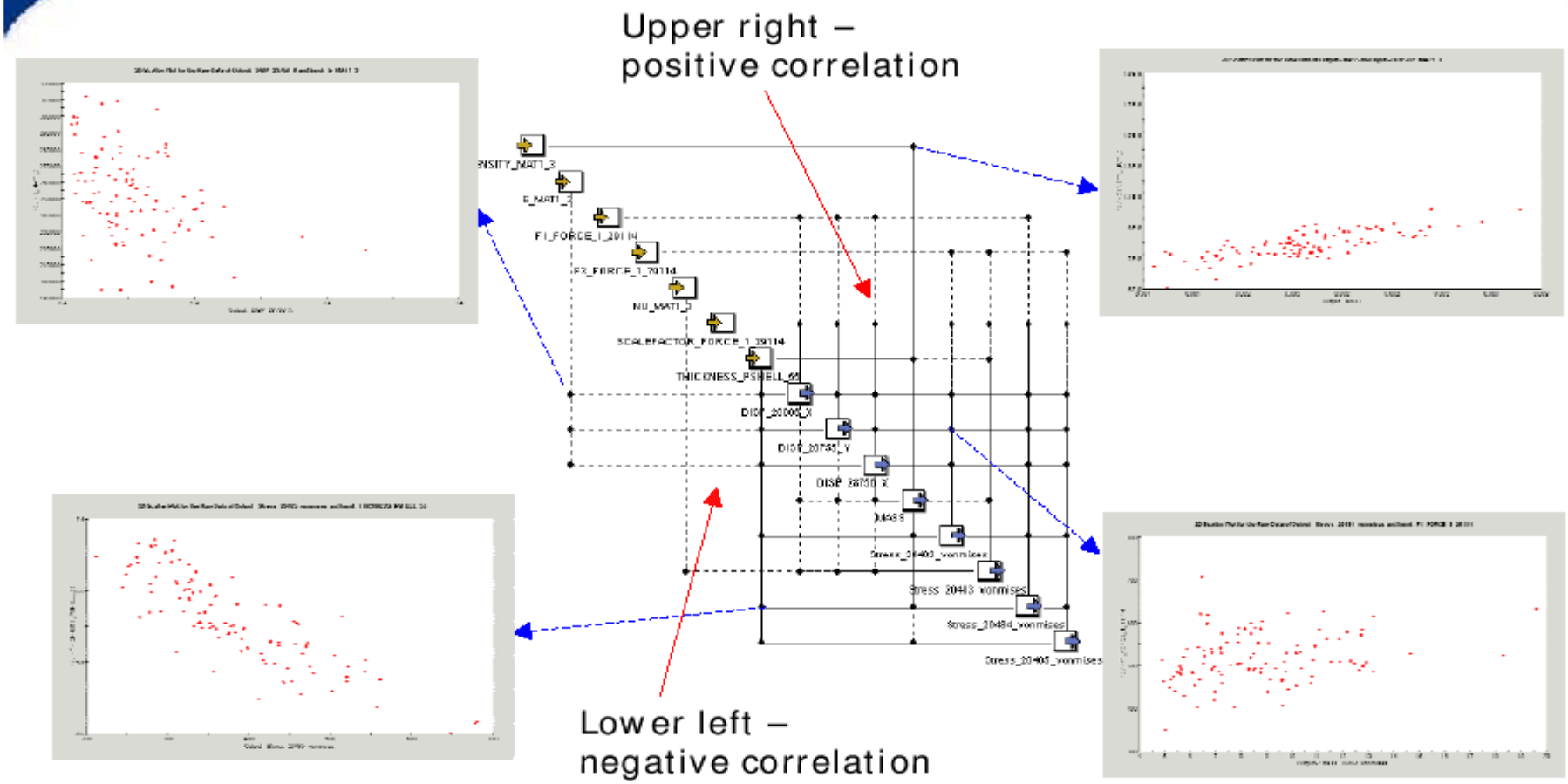
Engineering Systems Approach (N. Suh)



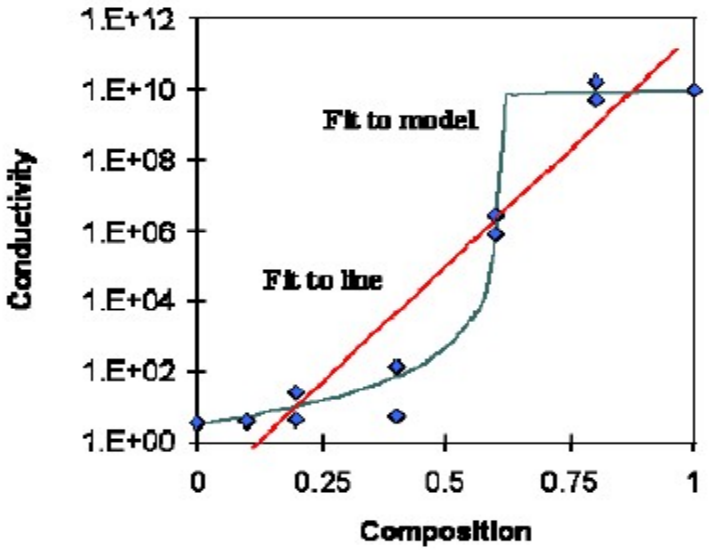
Results: System Level Cause & Effect



Results – Correlation Map



Electronic Materials Data Matching: Conductivity of a Composite

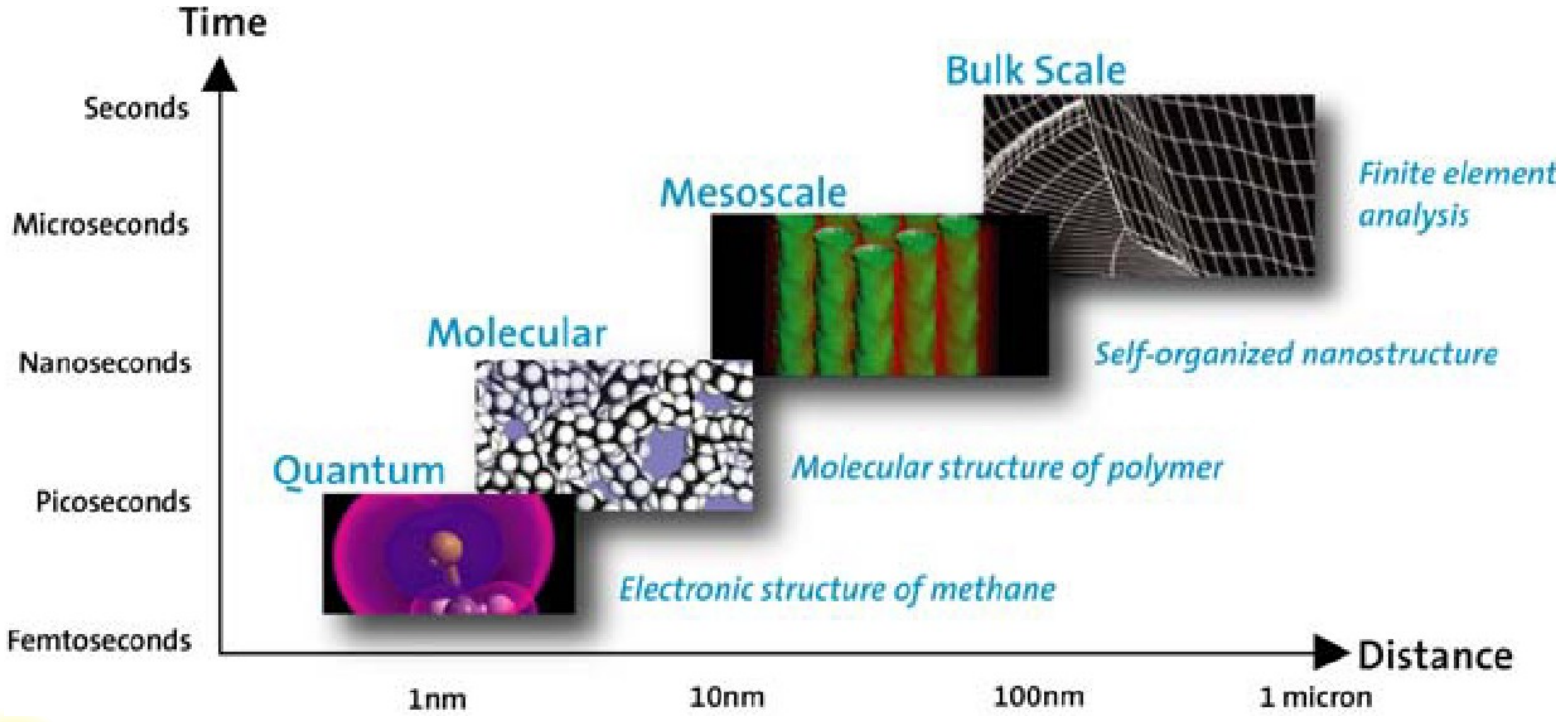


$$(v_i)\frac{\sigma_i^{1/s}-\sigma_m^{1/s}}{\sigma_i^{1/s}+\left(\frac{1}{\phi_c}-1\right)\sigma_m^{1/s}}+(v_c)\frac{\sigma_c^{1/s}-\sigma_m^{1/s}}{\sigma_c^{1/s}+\left(\frac{1}{\phi_c}-1\right)\sigma_m^{1/s}}=0$$

Composite conductivity should behave according to the McLachlan Equation. Fitting the parameters of this equation with gives a completely curve fit than an linear approximation. iSIGHT datamatching component enables this application. **Dr. Julie Runyan, Dr. Rosario Gerhardt GT**

Computational Materials

- Tools: DFT, MD, MC, crystal plasticity, OOF, thermo, phase field, FEM

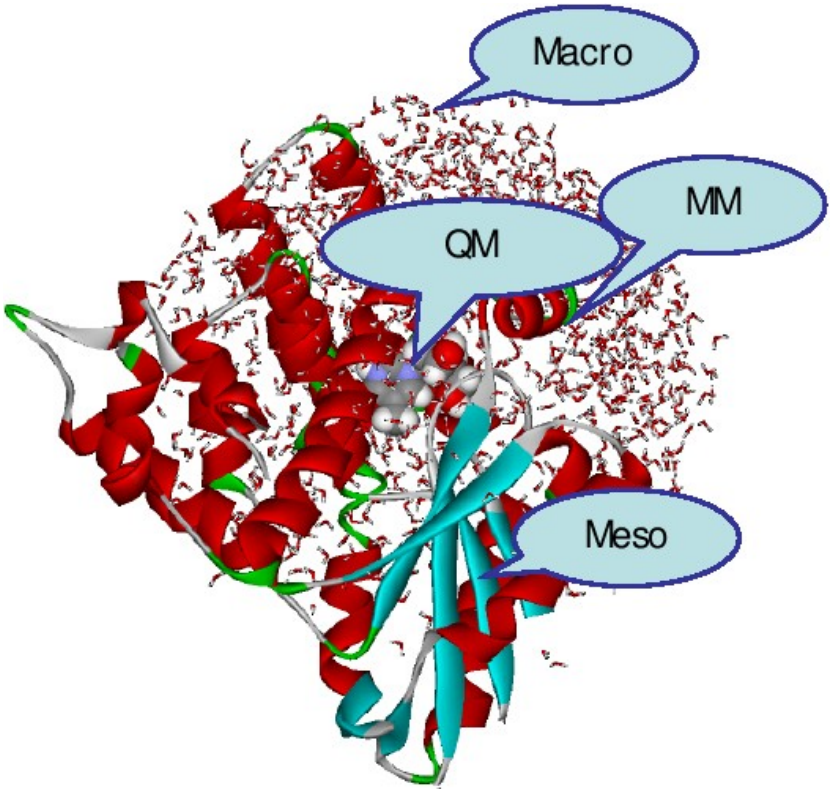


Linking Strategies

- Direct full coupling: very difficult, narrow utility
- Weak coupling: large-scale models call smaller-scale ones as needed
- Databases: store results of small-scale models for later retrieval
- Use models to “fill in the gaps” *e.g.* Ceder alloy intermetallic prediction

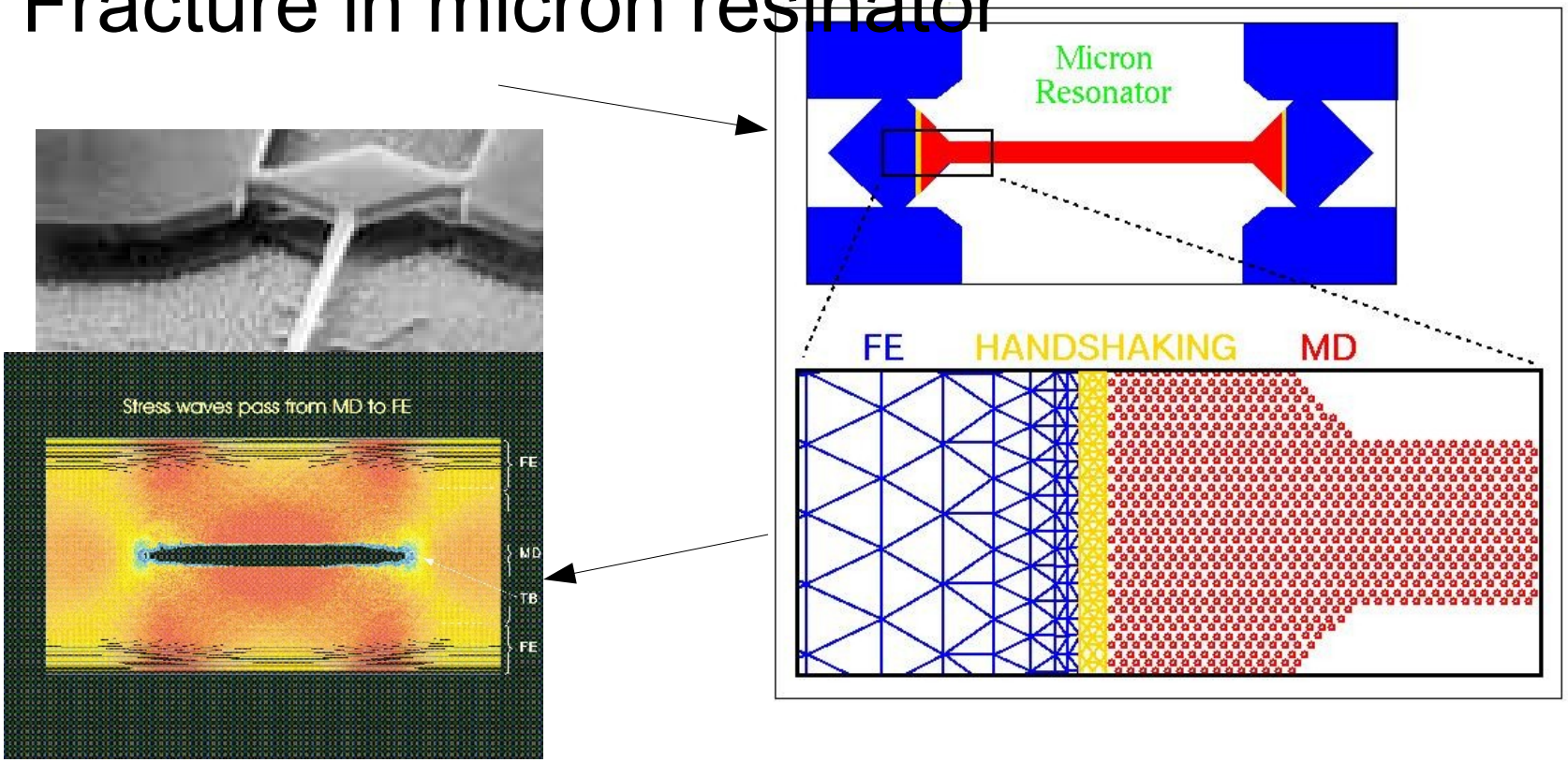
Linking Strategies

- Direct full coupling: very difficult, narrow utility



Brittle Fracture Simulation

Fracture in micron resinator



http://physci.llnl.gov/divisions/hdivision/EOS_MaterialsTheory/ourStaff/Rudd/GrandChallenge/grandChall.html

ICME Databases

- Store small-scale simulation results for large-scale model use
- Large-scale models "pull" data as necessary by interpolation or modeling

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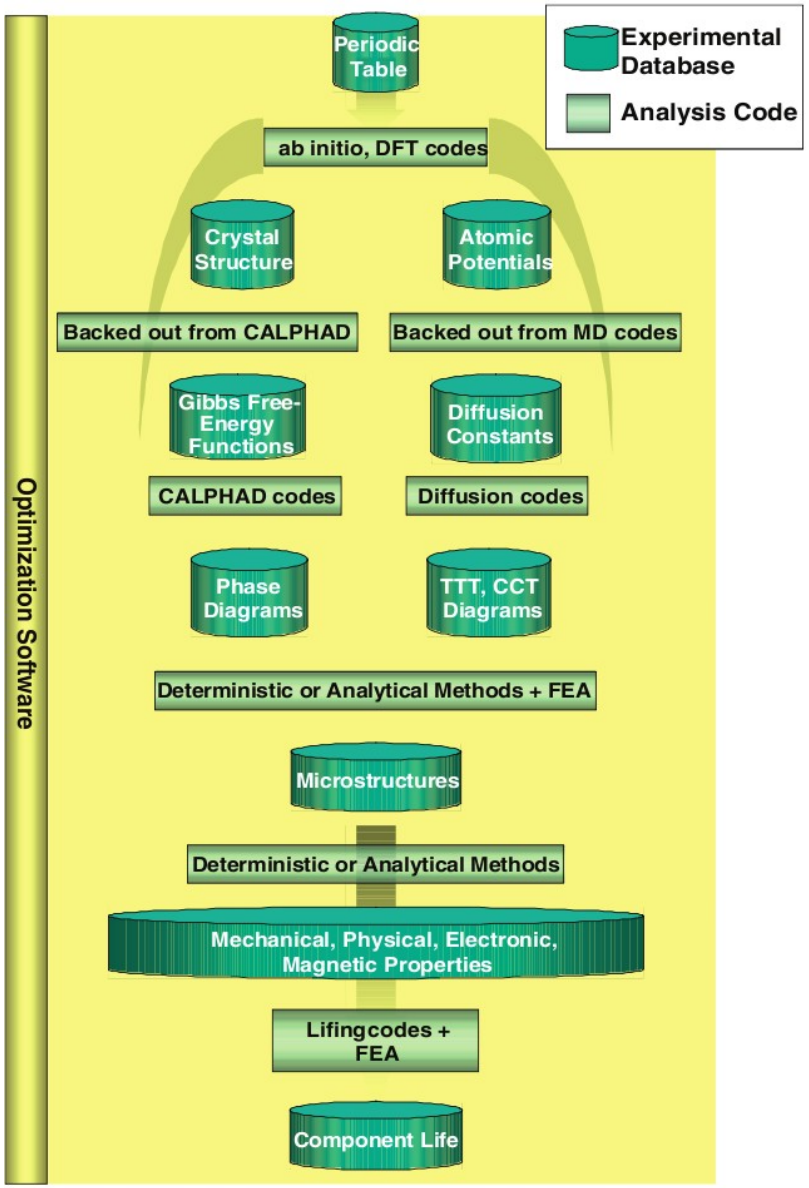
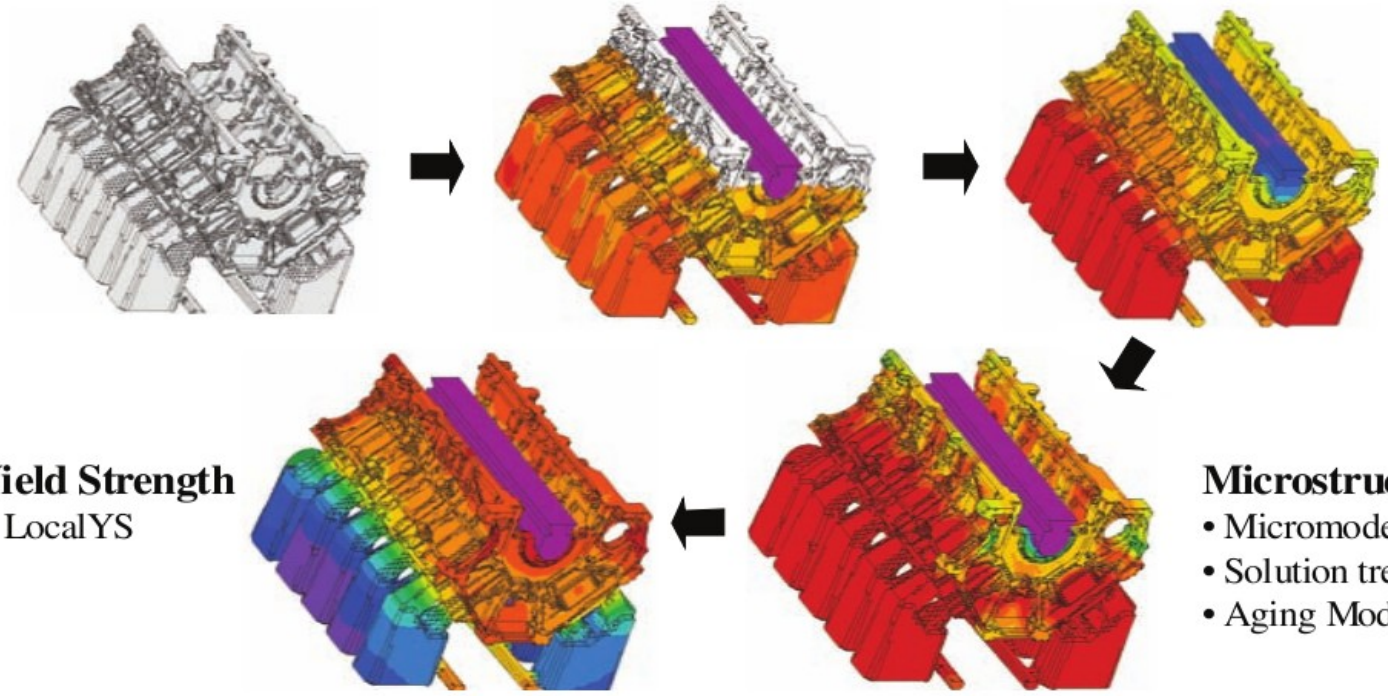


Ford Virtual Aluminum Casting

Initial Geometry
•CAD Geometry and Mesh

Filling
•Accurate filling Profile (ProCast, OPTCAST)

Thermal Analysis
•Boundary Conditions (OPTCAST)
•Fraction solid Curves (ThermoCALC)



Yield Strength
• LocalYS

Microstructure (Al_2Cu)
• Micromodel (MicroMod, PanDat)
• Solution treatment (Dictra)
• Aging Model (NanoPPT, PanDat)

Simulate changes with new alloys—and processes!

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Open Source ICME Tools

- Current capabilities:
  - *Ab initio* DFT quantum mechanics: **abinit**
  - Statistical mechanics: **ATAT**
  - CALPHAD Thermodynamics: **Gibbs***
  - Molecular dynamics: **LAMMPS**
  - Phase field structure formation: **RheoPlast**
  - Macroscopic mechanics: OOF, several others
- Needed:
  - Property prediction *e.g.* crystal plasticity

CALPHAD Thermodynamics

- CALculate PHAse Diagrams
- Estimate energy parameters by theory and experiments
- Single component to binary, ternary, etc. interaction coefficients
- Share free energy functions with phase field models

Gibbs Project

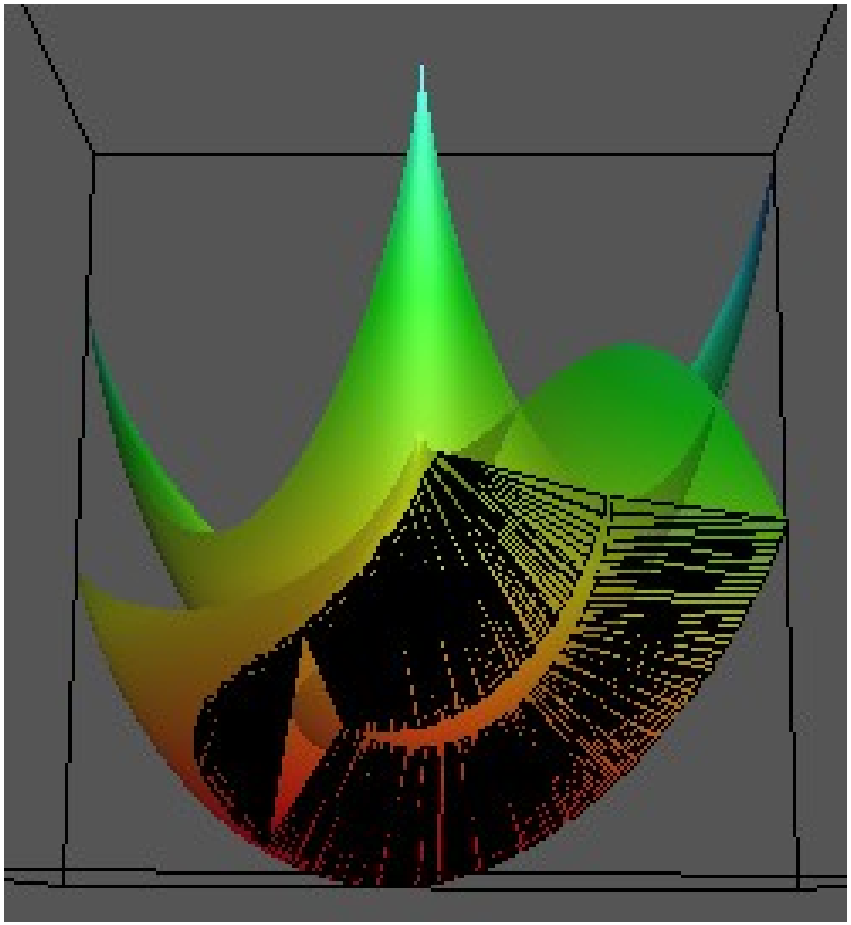
- Why no open source thermodynamics?
- What would we do with open source thermodynamics?
  - Informatics, automated DFT, vector/tensor
- Adam Powell, Edwin Garcia, Raymundo Arroyave
- Calculate phase diagrams from free energy functions
- Proof-of-concept ternary calculator

Gibbs Algorithm

- Start with a grid of points
- Calculate free energy and derivatives at each point
  - Repeat for each phase
- Calculate the convex hull of all points
- Identify multi-phase facets, refine them
- Send data to visualization
- Very fast!

Gibbs Output

- “Solid” with miscibility gap and “liquid”
- Eutectic sliver and three-phase region

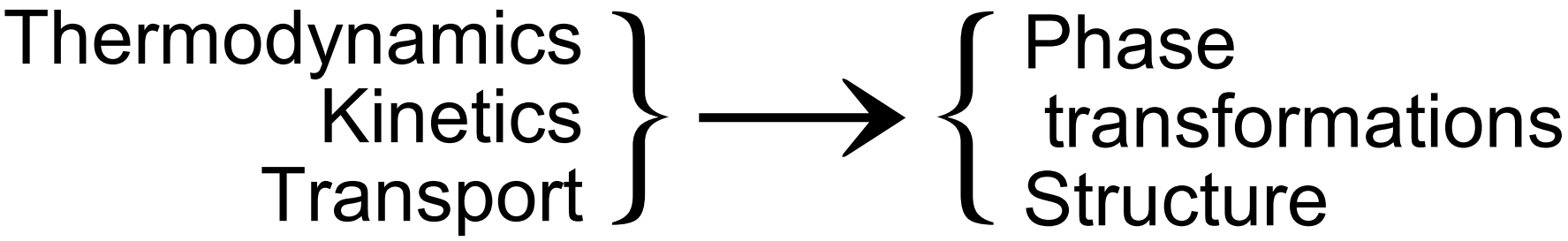


Next Steps

- Full temperature-composition phase diagrams
- Optimal fit to experimental data
- Python front-end
- Informatics: thermo & diffusion data format
  - Illinois Institute of Technology IMI proposal
- ATAT integration
- Anisotropic thermodynamics...
- http://teaching.matdl.org/teachingarchives/wiki/Ternary

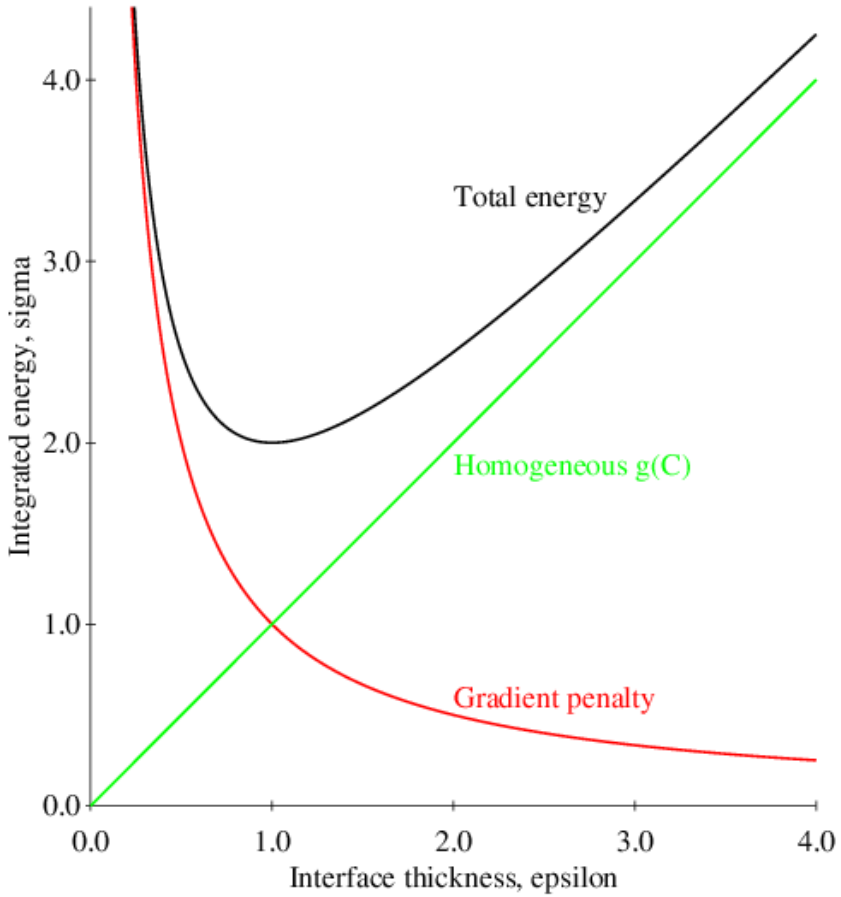
Phase Field Modeling

- Useful for modeling multi-phase systems with interfaces undergoing topology change
  - Solve one equation everywhere
  - No need to create or move an interface
  - “Diffuse interface” arises from equations
  - Maximize entropy or minimize free energy



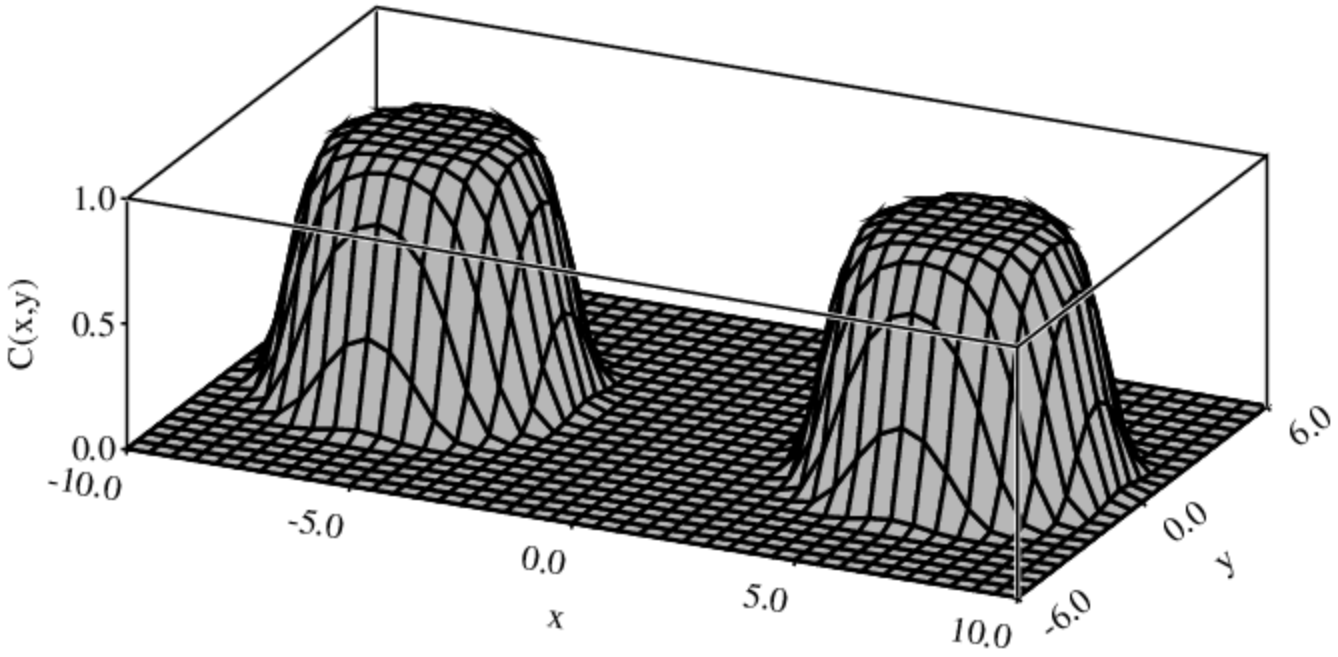
Diffuse Interface

- Free energy:
  $F = \int [\beta\, g(C) + \tfrac{1}{2}\, \alpha\, |\nabla C|^2]\, dV$
- Homogeneous ~ thickness
- Grad penalty ~ 1/thickness
- Result:
  $\sigma \sim (\alpha\beta)^{1/2}$
  $\varepsilon \sim (\alpha/\beta)^{1/2}$

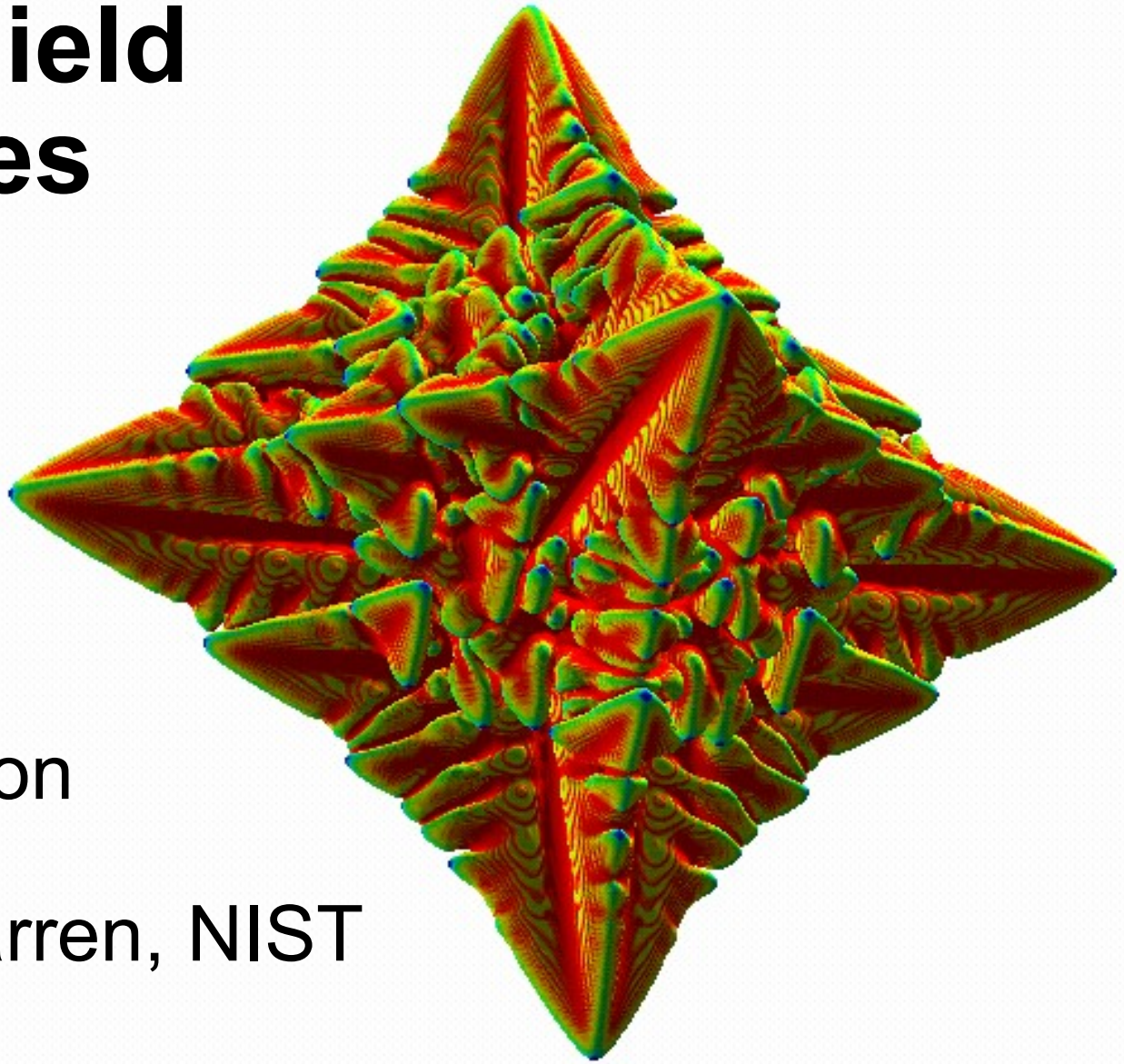


Why Diffuse Interface?

- Physical interpretation: rough interface, solute trapping, spinodal decomposition
- Facilitates topology changes



Phase Field Examples

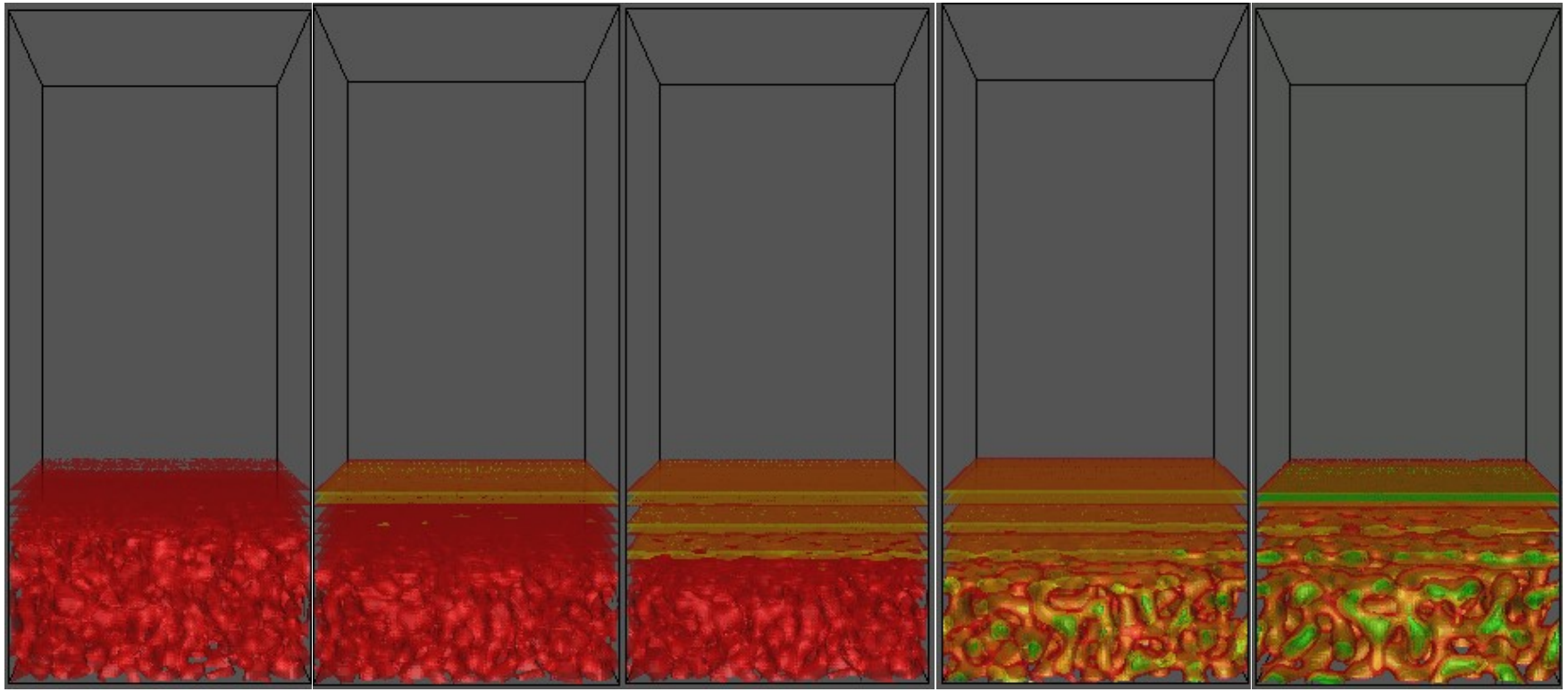


Solidification
Dendrite
James Warren, NIST

RheoPlast Phase Field Code

- Parallel FD infrastructure based on PETSc
- Modules:
  - Binary/ternary Cahn-Hilliard
  - Vector-valued Allen-Cahn
  - Navier-Stokes: *V-P*, *V-ω*
  - Electrical potential
  - Shear strain
- Full coupling between modules permits numerous simulation possibilities

Polymer Membrane Casting



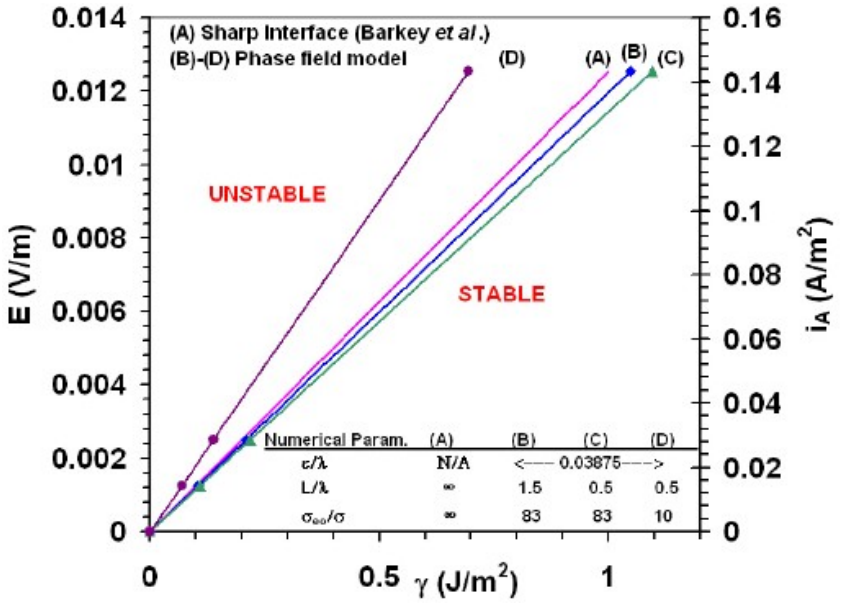
Five snapshots in an immersion precipitation simulation

3-D Electromigration

- Anode instability decay
- Cathode instability growth
- Short circuit
- Connection breaks
- Interface breakdown
- Broken oxide

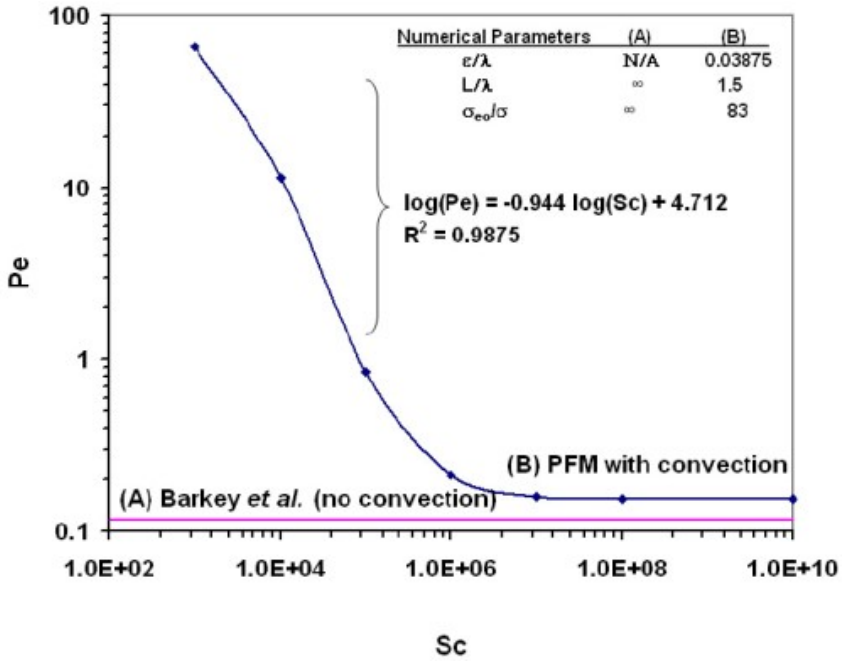
Benchmark: Stability Analysis

- Barkey et al. 1989: growth of a sinusoidal cathode perturbation
- Simulation: fix wavelength, test critical voltage and surface tension



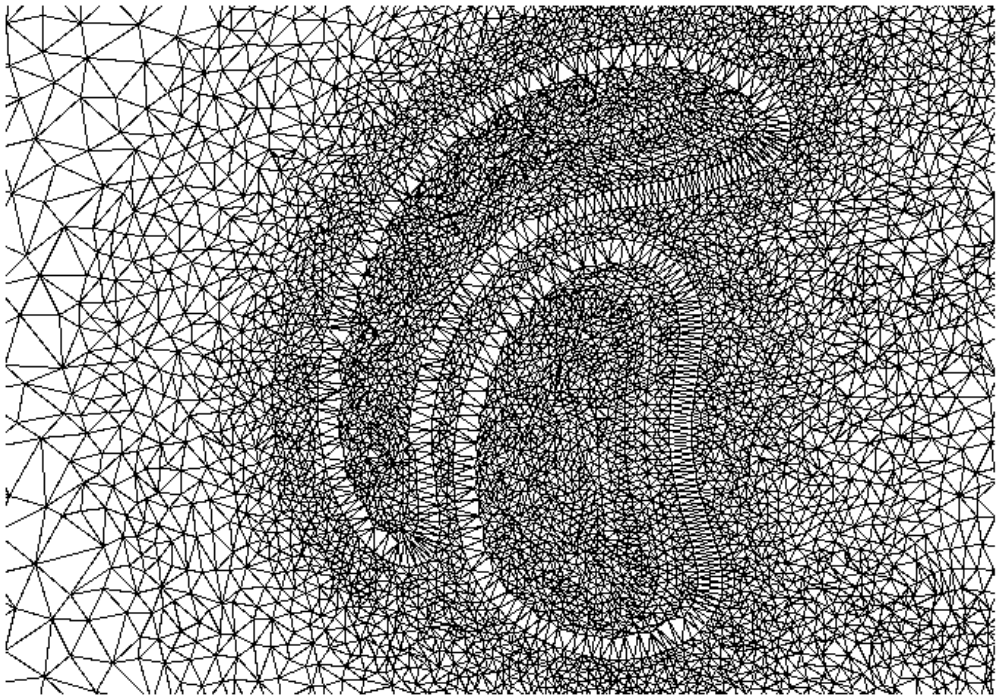
Stability Analysis: Viscosity

- Dimensionless viscosity: Schmidt number $\mu/\rho D$
- High viscosity behaves like a solid
- Low viscosity: new stability criterion



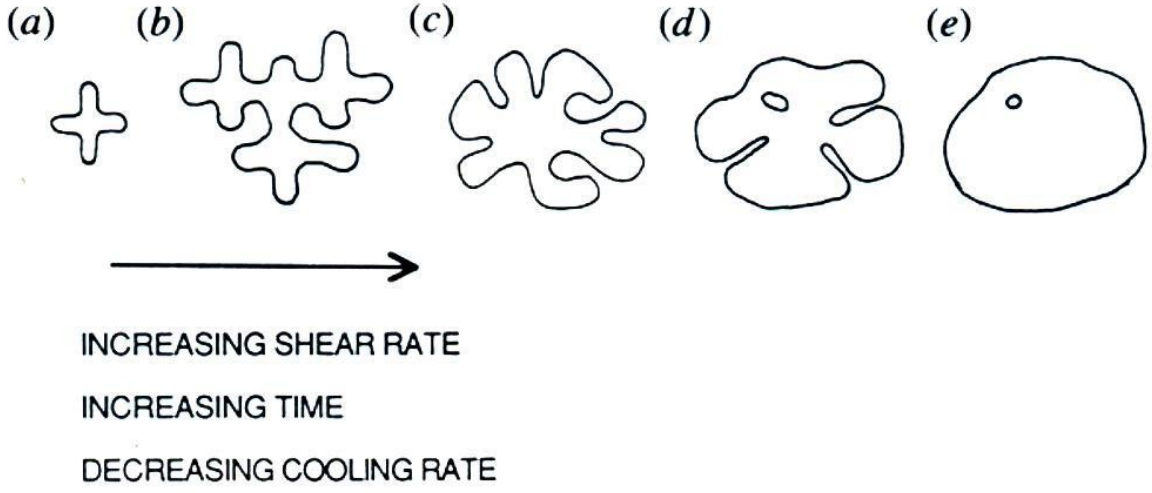
Fluid-Structure Interactions

- Navier-Stokes equations in fluid, elastic mechanics in solid
- Match traction, displacement at interfaces
- Example: blood flow, membrane as elastic solid



Phase Field+FSI Applications

- Semi-solid metals
- Electrodeposition with cross-flow
- Polymer membrane structure with moving solids



FSI with Phase Field

- Lagrangian and ALE methods:
  - Nodes move with fluid or solid
  - Nodes with boundary comprise interface
  - Different equations in different phases
- Phase field:
  - No sharp boundary between fluid and solid
  - Same equation everywhere
- Combination: Mixed Stress method

$$\rho \frac{D\vec{v}}{Dt} = \nabla \cdot [p(C)\sigma_e + (1 - p(C))\sigma_f] + \vec{F}$$

FSI/Phase Field First Cut

- Assume incompressible fluid and solid
- Pressure enforces incompressibility

$$\sigma = -PI - p(C)\tau_e - (1 - p(C))\tau_f, P = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

- Newtonian fluid, solid with pure shear

$$\tau_f = -\eta(\nabla\vec{v} + \nabla\vec{v}^T) \qquad \tau_e = -G\gamma_e$$

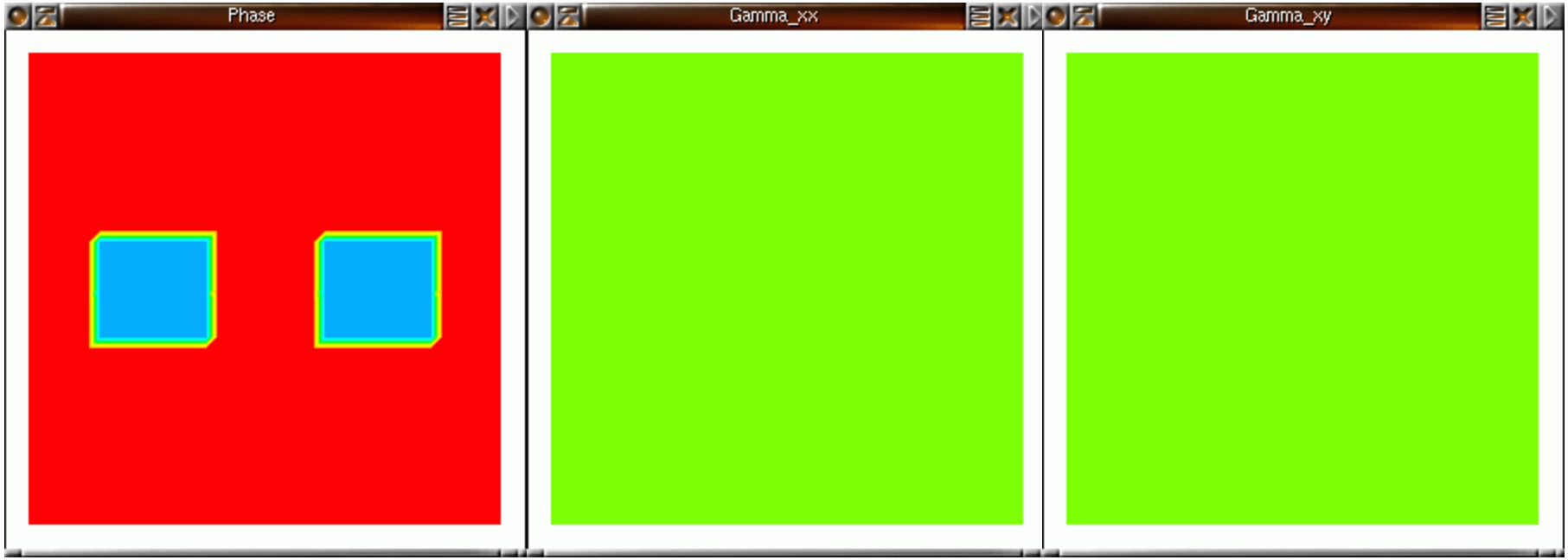
- Coupling between velocity, vorticity, strain

$$\frac{D}{Dt}\begin{pmatrix} \gamma_{xx} \\ \gamma_{xy} \end{pmatrix} = \begin{pmatrix} 2\partial v_x/\partial x \\ \partial v_x/\partial y + \partial v_y/\partial x \end{pmatrix} + \begin{pmatrix} -2\omega\gamma_{xy} \\ 2\omega\gamma_{xx} \end{pmatrix}$$

- Fields: velocity, pressure, shear strain

Impinging Particles

Composition: XX Strain: XY Strain:

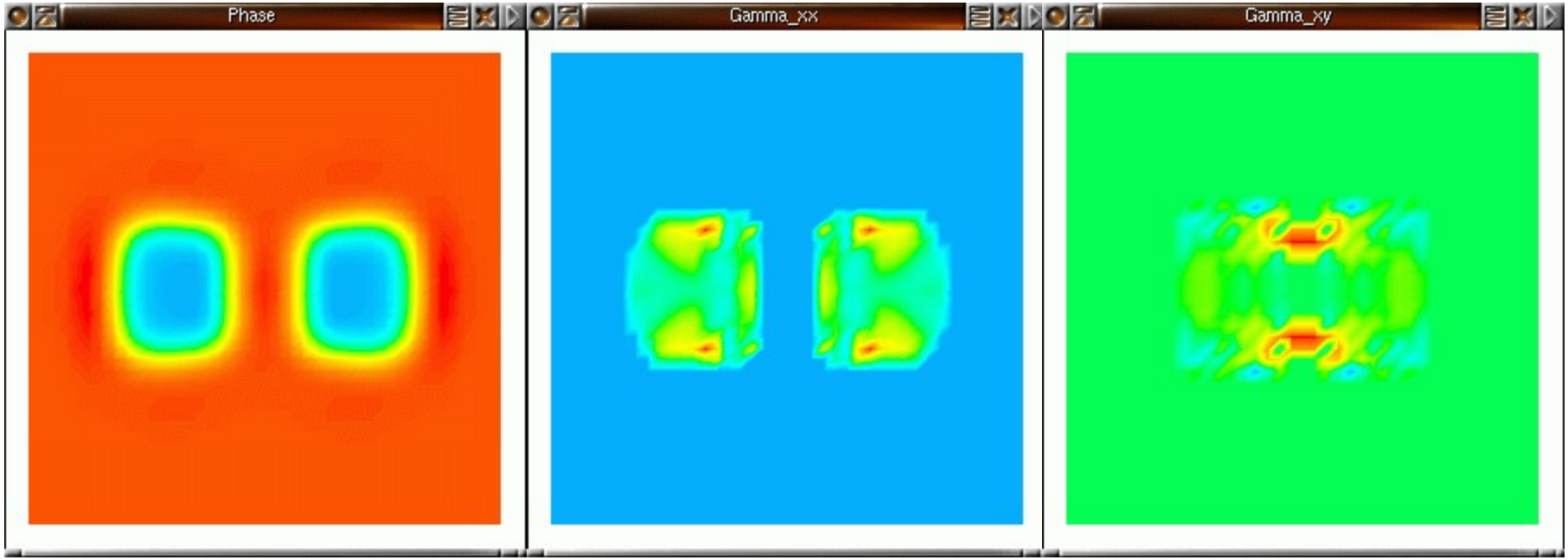


Impinging Particles

Composition:

XX Strain:

XY Strain:



Impinging Particles

Composition:

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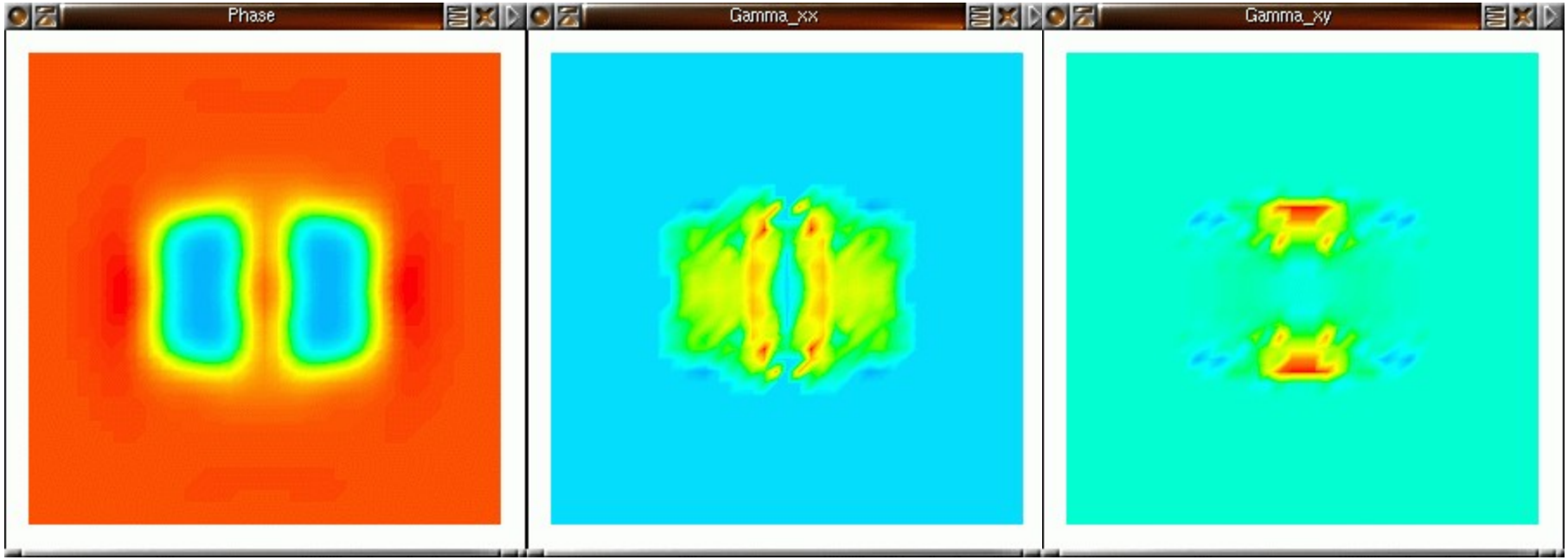

Impinging Particles

Composition:

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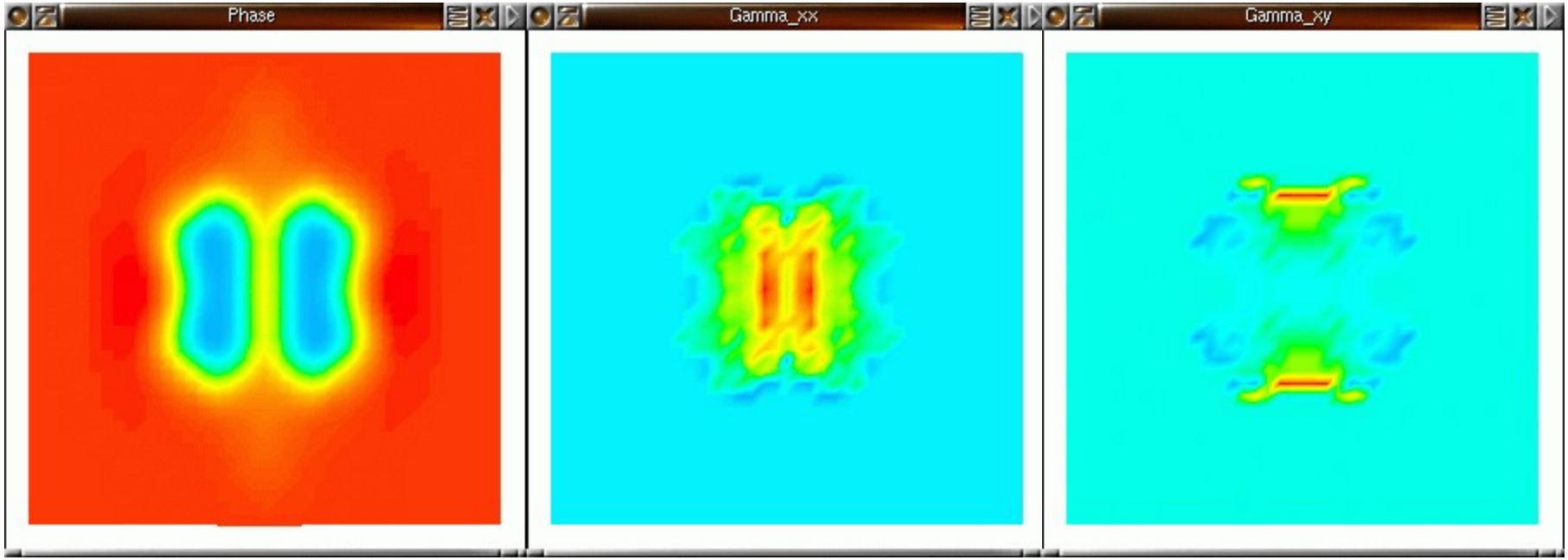
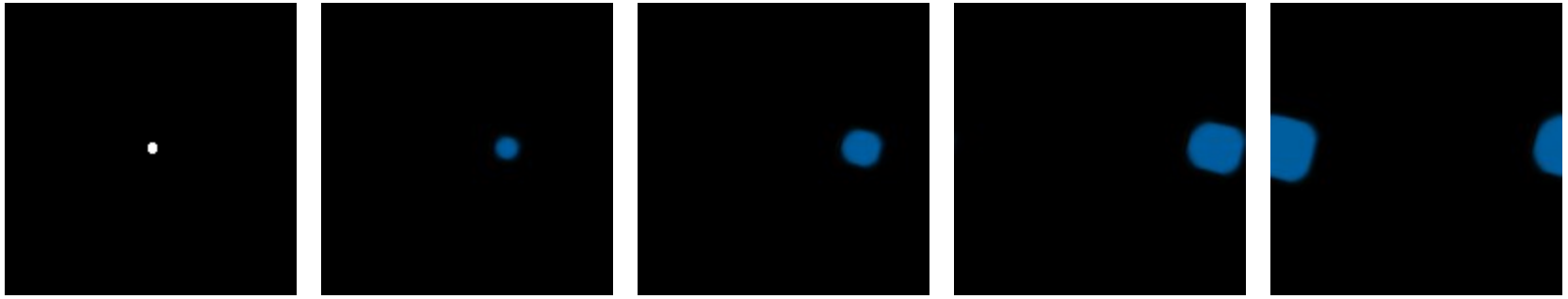
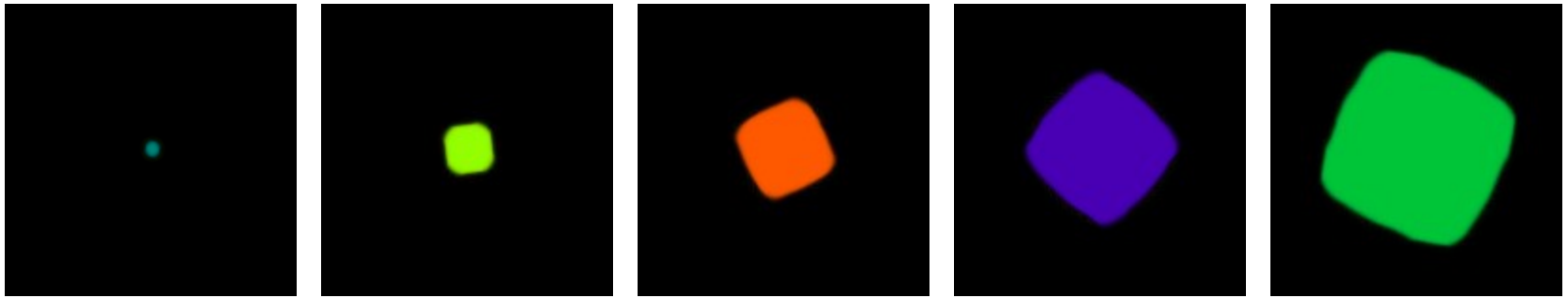


Anisotropic Growth+Motion



With rotation:

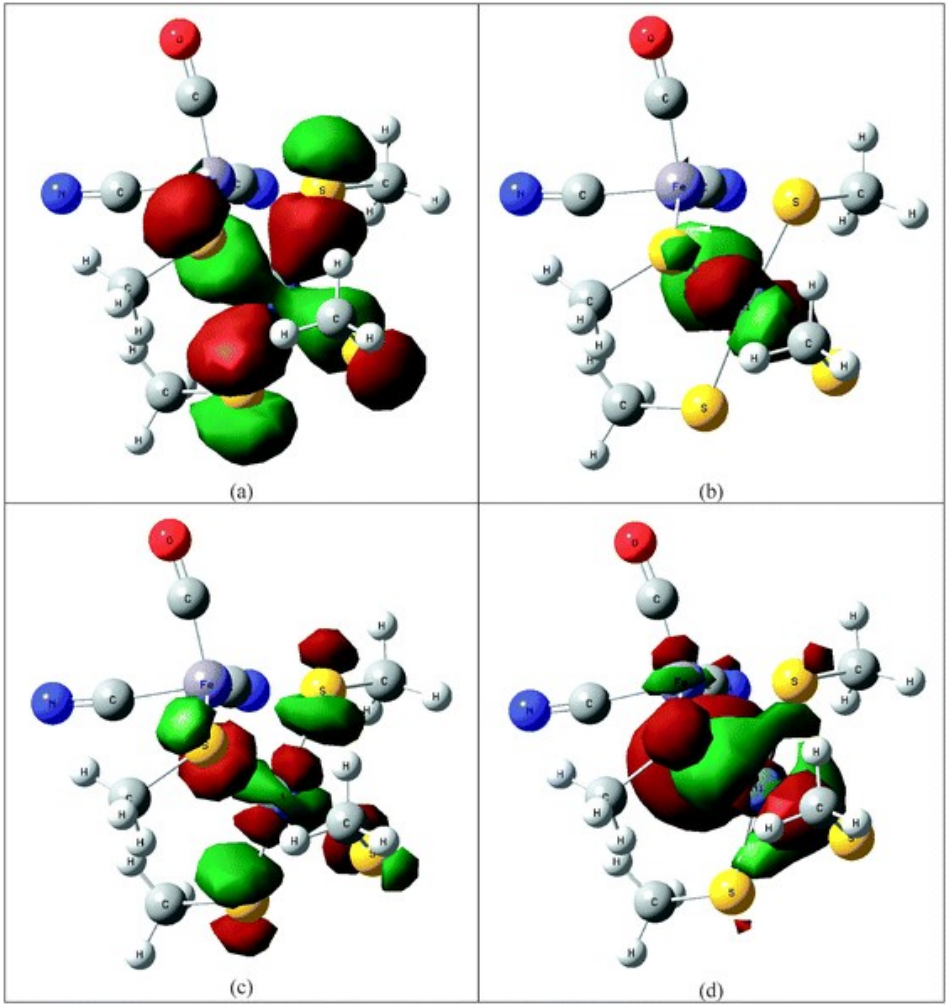


ATAT

- Calculate ground states by *ab initio*/DFT
- Entropy calculations:
  - Cluster expansion to estimate configurational
  - Phonon band structure for vibrational
  - Electron band structure for electronic
- Feed free energy to CALPHAD and Phase Field codes
- Problem: difficult to run!

Ab Initio/DFT

- Multiple atom → multiple electron → single electron
- Calculate energy, entropy, electron & phonon band structure
- Weaknesses: slow; oxides and liquids not accurate



Summary

- Integrated Computational Materials Engineering promise to reduce materials cycle time, deliver part-specific materials design
- Expanded design space could result in significant performance improvement
- Open Source tools here now and under development cover much of this space