MGI and Applied Mathematics

Robert V. Kohn
Courant Institute, NYU

MGI Workshop, Jan 2016

Overview

Mandate: Discuss the interface between applied mathematics and materials science.

Goal: Communicate, through examples,

- some recent tools and algorithms you may be able to use;
- some communities you may be interested in challenging;
- some recent successes in the spirit of MGI.

A key point: for greatest impact, mathematics and computing should participate early – helping to identify the questions (not just the answers).

Outline

(1) Designing materials or structures

- finding better shape-memory materials
- 3D printable structures with specified elastic response

(2) Motion of interfaces or defects

- annealing of polycrystals, or coarsening of foams
- the phase-field-crystal approach to motion of defects

(3) Extraction of data from simulations or images

- image processing of (approximately) crystalline structures

(4) Linking length scales

- dislocation densities and plasticity

(5) Linking time scales

- finding barriers, pathways, and transition rates

NOTE: algorithms and theory are distributed throughout. In many cases both play key roles.

(1) Designing materials or structures

- finding better shape-memory materials
- 3D printable structures with specified elastic response

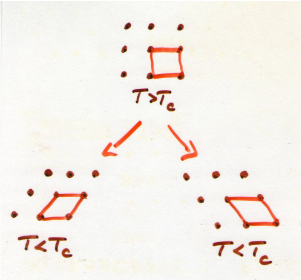
Finding better shape-memory materials

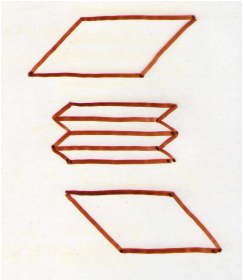
Shape-memory materials get their special properties from a martensitic phase transformation.

- If room-temperature structure is the low-symmetry phase, material sustains large deformation at low stress but recovers reference shape upon heating. This shape-memory effect is useful for actuation and energy conversion.
- If room-temperature structure is the high-symmetry phase, material sustains large deformation at low stress but recovers reference shape upon unloading. This pseudo-elastic behavior is used eg in cardiac stents and dental wire.

Mechanism: Large deformation is achieved (at low stress) by changing the arrangement of the phases.

2D schematic



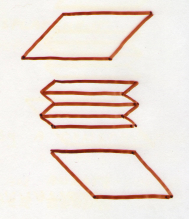


Better shape-memory materials, cont'd

Problem: Most shape-memory materials have considerable hysteresis, and fatigue under cyclic loading.

Idea: Fatigue is from plastic deformation, present since stress-free phase mixtures are very special (hard to nucleate, and to change).

In 2D schematic, transf strain B maps a square to a parallelogram, i.e. $B = \begin{pmatrix} 1 & \pm a \\ 0 & 1 \end{pmatrix}$. Stress-free mixture requires layering (twinning) with well-chosen normal.



Progress: For special (non-generic) choices of the transformation strain B there are many additional stress-free microstructures. Such materials have less hysteresis and less fatigue.

Examples found by varying composition in known shape-memory alloys. Particular success in $Zn_{45}Au_{30}Cu_{25}$.

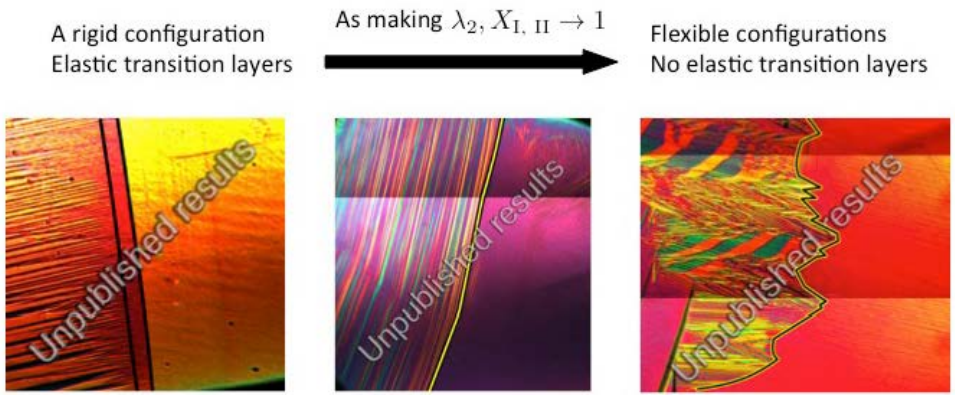
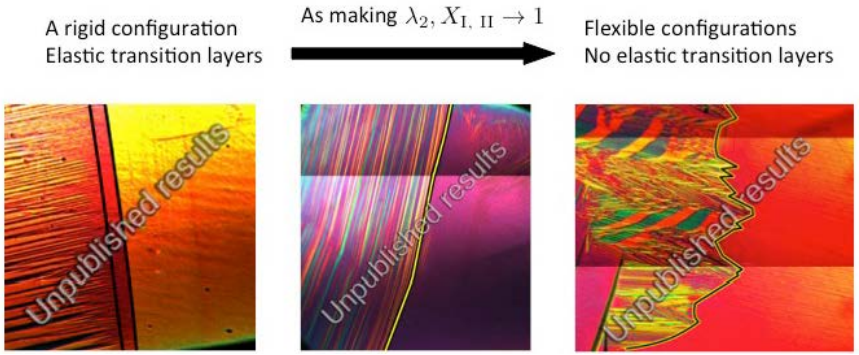


Image from Xian Chen's site http://www.tc.umn.edu/∼chen1561/research.html

Better shape-memory materials, cont'd



Some MGI-related thoughts:

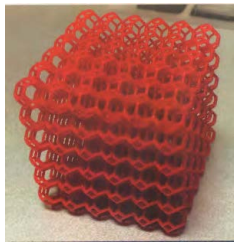
- Examples were found experimentally, because present theory doesn't predict lattice parameters as a function of composition.
- Desirable effects at special, non-generic lattice parameters are hard to find by interpolating between (more generic) examples.
- Success came from understanding the role of microstructure.

Some references:

- X. Chen, V. Srivastava, V. Dabade, and R.D. James, J Mech Phys Solids 61:12 (2013) 2566-2587
- Y. Song, X. Chen, V. Dabade, T.W. Shield, and R.D. James, Nature 502 (2013) 85-88.

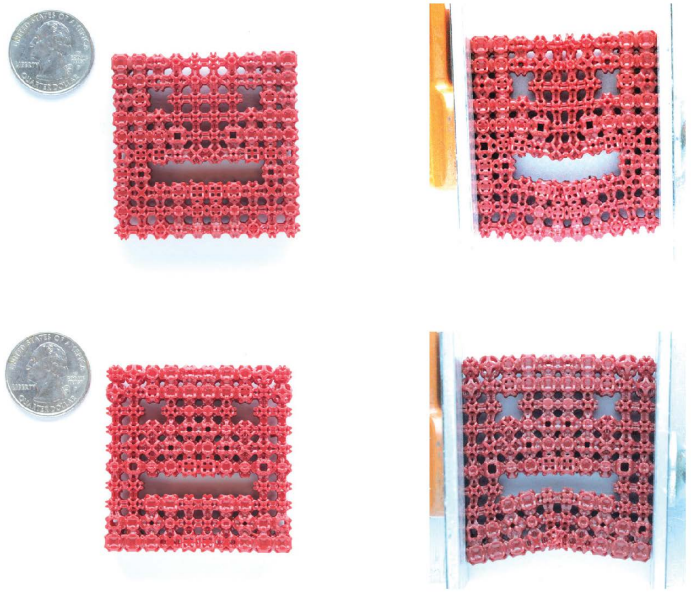
3D printable structures with specified elastic response

3D printing (stereolithography) permits the manufacture of lightweight porous structures. Structure is built up one layer at a time.



Cost of manufacture is independent of complexity, but there are some restrictions: the printer has limited resolution, and each layer must be supported by the one below it.

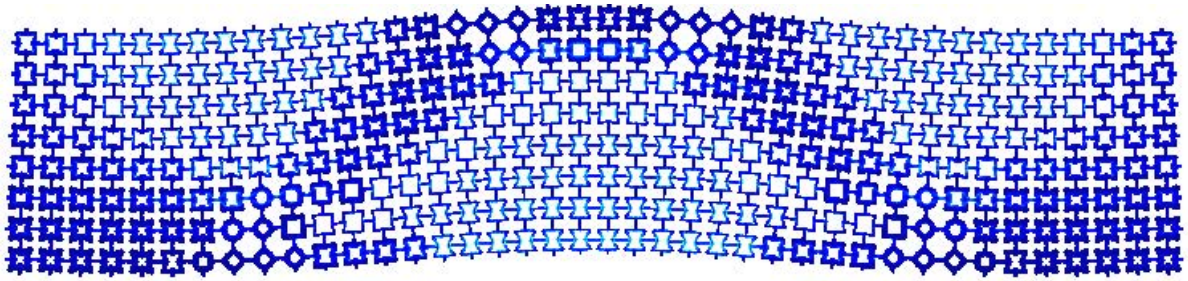
A design problem: Make a lightweight, printable structure with specified response to a given load.



3D printable structures, cont'd

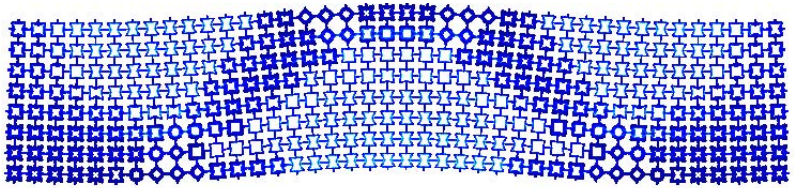
STEP 1 Find a continuously-varying Hooke's law $C_{ijkl}(x)$, defined on the given shape, whose elastic response has the desired character.

STEP 2 Realize $C(x)$ by a locally periodic composite whose cell structure varies with x.



A key detail: choose topology of period cell and keep it fixed, so neighboring cells connect properly despite their varying structure.

3D printable structures, cont'd



Some MGI-related thoughts:

- This is my own MGI project (with D. Zorin, J. Ricci, and Y. Zhang). Goal is to combine techniques that were previously separate: topology optimization and 3D printing.
- The subject is just getting started. Long-term goals include: controlling how microstructure meets curved boundaries; varying pore size; avoiding large stresses and/or brittle fracture; real applications such as bone scaffolds.

Reference:

- J Panetta, Q Zhou, L Malomo, N Pietroni, P Cignoni, D Zorin, ACM Transactions on Graphics 34:4, paper 135, 2015

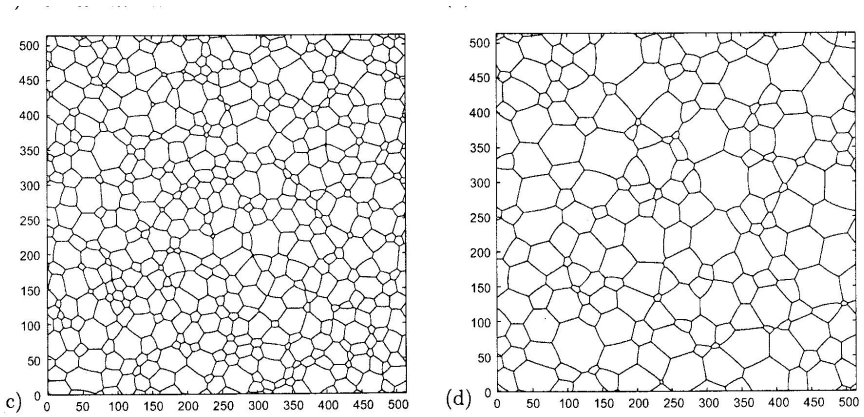
(2) Motion of interfaces or defects

- annealing of polycrystals, or coarsening of foams
- the phase-field-crystal approach to motion of defects

Annealing of polycrystals, or coarsening of foams

Moving interfaces are crucial to many materials science problems.

Changes of topology make such problems difficult to simulate. Even theoretical questions – such as whether the evolution is uniquely determined (indep of numerical solution scheme) is often unclear.

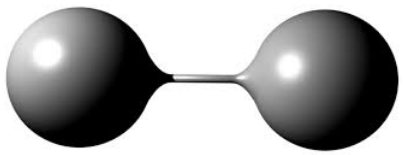


Annealing of a polycrystal is a good example. Geometric model (Mullins): same crystalline material in each grain, with different orientations. Interfaces have surface energy (depending on orientation of neighboring grains, and that of interface). Surface evolution is "steepest descent for surface energy" (in same sense that linear heat eqn $u_t = \Delta u$ is steepest descent for $\int |\nabla u|^2 \, dx$).

Annealing of polycrystals, cont'd

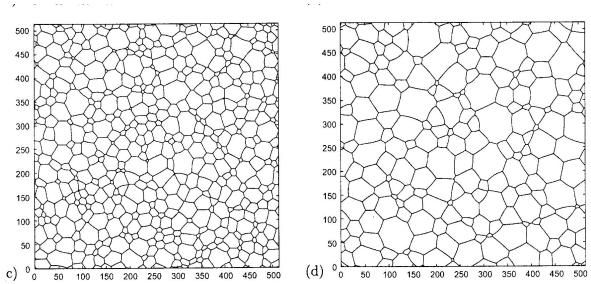
Methods for solving two-phase problems have seen much progress in past 30 years:

- numerics via level-set methods, diffuse-interface approximations, and thresholding-type algorithms;
- theory via viscosity solutions.



Multiphase problems are harder. Older tools include:

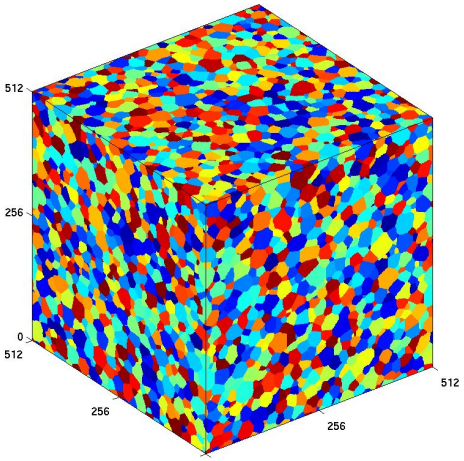
- front-tracking (difficult even in 2D);
- n-state Potts models (noisy; limited control of anisotropy);
- diffuse interface models with vector-valued order parameter (stiff; limited control of anisotropy).

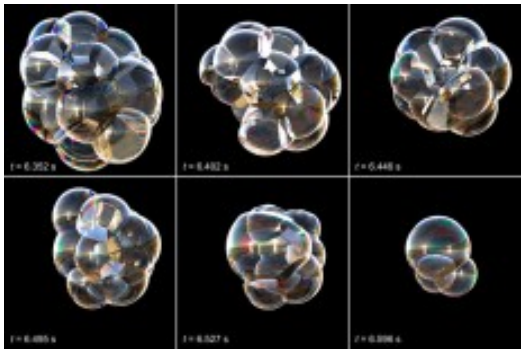


Annealing of polycrystals, cont'd

Newer tools include:

- front tracking in 3D (Lazar, Mason, MacPherson & Srolovitz), based on classification of local changes of topology;
- thresholding-type methods with controlled anisotropy (Esedoglu, Elsey & Smereka; Esedoglu & Otto);
- the Voronoi-implicit interface method (Sethian & Saye, applied also to foams and other multiphysics systems).





images: M Elsey, S Esedoglu & P Smereka (left); Sethian & Saye (right)

Annealing of polycrystals, cont'd

Some MGI-related thoughts:

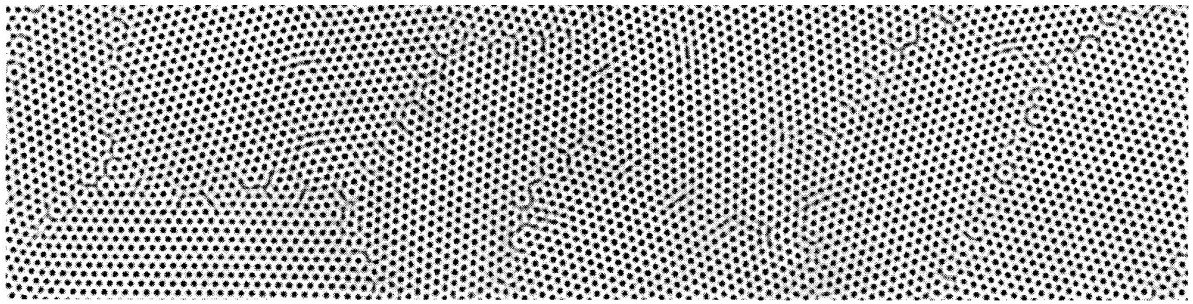
- In almost every area of materials science we need bigger, better, and more accurate simulations. Advances in hardware will help, but improved algorithms are also crucial.
- Algorithmic challenges are best addressed through well-chosen examples. This audience has many such examples.
- MGI emphasizes interaction of theory, simulation, and experiment. Development of improved algorithms can be an enabling technology.

References:

- E Lazar, J Mason, R MacPherson, D Srolovitz, Acta Mater 59 (2011) 6837-6847
- M Elsey, S Esedoglu, P Smereka, Acta Mater 61 (2013) 2033-2043
- S Esedoglu, F Otto, Comm Pure Appl Math 68 (2015) 808-864
- R Saye, J Sethian, Science 340:6133 (2013) 720-724

The phase-field-crystal approach to motion of defects

For polycrystals, the geometric model omits a lot of physics. Grains can rotate. Interfaces have structure (arrays of dislocations). For very small grains, continuum approxn may not be adequate.



Phase field crystal method offers an alternative. Introduced in 2002, it uses Cahn-Hilliard-type dynamics, for a functional that prefers periodic structures but tolerates defects. Simplest case:

$$E = \int \tfrac{1}{2}(\Delta u + u)^2 - \tfrac{\delta}{2}u^2 + \tfrac{1}{4}u^4; \qquad u_t = \Delta \tfrac{\delta E}{\delta u} = \Delta((\Delta + 1)^2 u - \delta u + u^3)$$

- Captures atomic-scale effects, including grain rotation and the anisotropy of surface energy
- Little is known about relationship to the more classical geometric model.

The phase-field-crystal approach, cont'd

Some remarks:

- Annealing of polycrystals is just one application. Phase field crystal method has many uses, both static (eg grain boundary structure) and dynamic (eg motion of dislocations and defects).
- MD with a pair potential has similar atomic resolution. But PFC simulations have no noise.
- The pictures are great, but is the evolution physically correct?

Selected references:

- K Elder, M Grant, Phys Rev E 70 (2004) 051605 (the method)
- P Voorhees and K-A Wu, Acta Mater 60 (2012) 407-419 (grain rotation)
- M Elsey, B Wirth, ESAIM: MMAN 47 (2013) 1413-1432 (a numerical scheme with no timestep restriction)

(3) Extraction of data from simulations or images

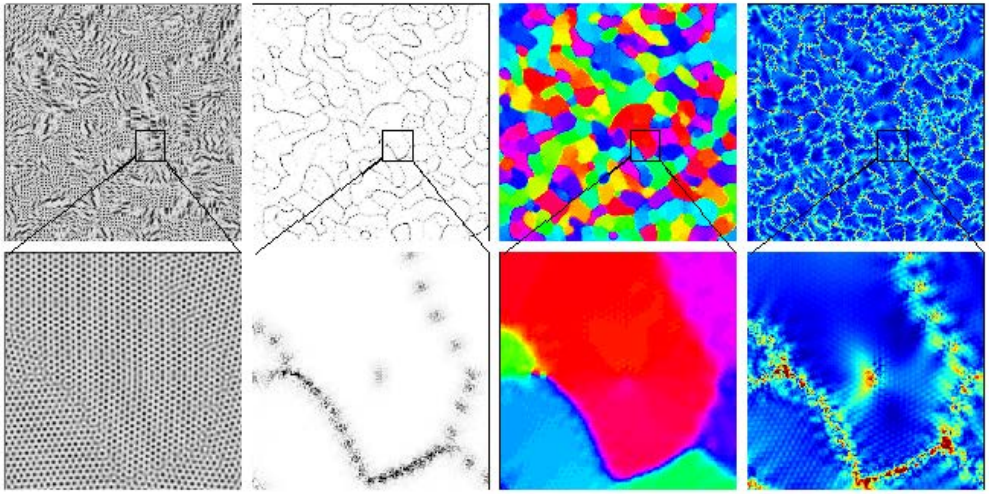
- image processing of (approximately) crystalline structures

Image processing of (approx) crystalline structures

Matt Elsey and Benedikt Wirth had a new scheme for PFC dynamics. To show its power, they did large-scale polycrystal simulations.

Problem: How to extract meaningful data from the result?

Their approach: seek a matrix-valued function $F(x)$ (mapping reference lattice to deformed lattice) that (i) is faithful to image, (ii) has small $\int |\mathrm{curl}(F)|\, dx$.



FAR LEFT PFC simulation (2048×2048)
CENTER LEFT Dislocations (curl of F)
CENTER RIGHT Lattice orientation (grains)
FAR RIGHT Elastic strain ($|(F^T F)^{1/2} - I|$)

Image processing, cont'd

Some related work:

- Segmentation into grains without identifying dislocations (Elsey, Wirth)
- A Fourier-type method for finding the local $F(x)$ (Lu, Yang, Wirth)
- Application to art history – canvas weave analysis (Lu, Yang, Brown, Daubechies, Ying)

Some MGI-related thoughts:

- Getting information from large-scale simulations is a cross-cutting pbm
- This work used methods from image processing and signal processing
- In other settings, methods from machine learning may be useful

Some references:

- M Elsey & B Wirth, Multiscale Modeling & Simulation 12 (2014) 1-24
- M Elsey & B Wirth, J Sci Comp 63 (2014) 279-306
- H Yang, J Lu, W Brown, I Daubechies, L Ying, IEEE Signal Processing Mag 32 (2015) 55-63
- J Lu, B Wirth, H Yang, arXiv:1501.06254

(4) Linking length scales

- dislocation densities and plasticity

Dislocation densities and plasticity

Dislocation motion is the atomic-scale mechanism of plastic deformation.

Simulation of interacting dislocations is difficult. Useful for benchmarking macroscopic models, but not feasible for macroscopic problems.

Continuum plasticity models are useful but phenomenological. The relationship to to dislocation dynamics is unclear. Limited ability to capture size effects.

Dislocation density models have been explored. But link to 3D macroscopic behavior is problematic.

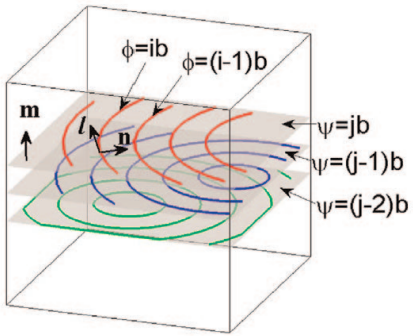
Recent progress: a new approach to dislocation densities, focusing on the density of dislocations in each slip plane.

Dislocation densities, cont'd

Key idea (Yang Xiang et al): focus on dislocations with a given Burgers vector b. Introduce two potential functions, ϕ and ψ:

surfaces $\psi = \text{const}$ are slip planes;

$\phi =$ amt of plastic slip across plane (reflecting dislocation density).



In practice there are several slip systems. Use several pairs $\{(\phi_j, \psi_j)\}$, one for each slip system.

In fcc metals, dislocations move mainly in their slip planes by glide. In this case there's an evolution law for ϕ_j:

$$\partial_t \phi_j + v_j |\nabla \phi \times n_j| = s_j$$

where $n_j = \nabla\psi_j / \nabla\psi_j$ is the slip plane normal, v_j is the dislocation glide velocity, and s_j is a source term (reflecting presence of Frank-Read sources). Velocity v_j depends on the Peach-Koehler force, which is a nonlocal functional of the dislocation densities.

Dislocation densities, cont'd

Reference: Y Zhu, Y Xiang, J Mech Phys Solids 84, 2015, 240-253 (includes application to dependence of yield stress on size in micropillars)

Some MGI-related thoughts:

- Linking models on different length scales is a grand-challenge, cross-cutting problem.
- Plasticity is just one of many examples. Others in this talk: links between microstructure and macroscopic behavior in shape-memory materials, and in 3D-printed composites.

(5) Linking time scales

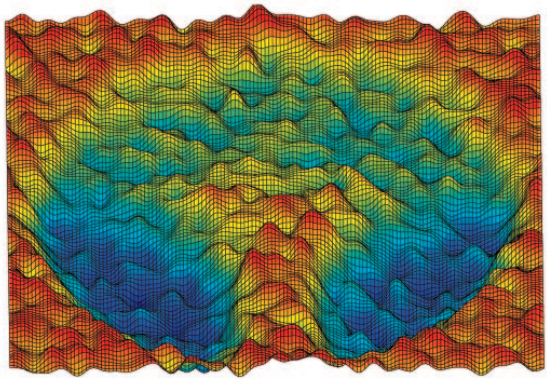
- methods for finding barriers, pathways, and transition rates

Finding barriers, pathways, and transition rates

Thermal fluctuations play a crucial role in structural transitions. Examples include

- the evolution of a crystal surface, as atoms move from site to site (KMC models need transition rates)
- the nucleation of a new phase (critical nucleus is a saddle point in the energy landscape)

Usually the energy landscape is high-dimensional, and only accessible numerically.



- Mapping of energy landscape is infeasible, due to high dimension.
- Direct stochastic simulation of transitions is infeasible, since they take too long.

Finding barriers, pathways, & transition rates, cont'd

Many algorithms have emerged from physics & chemistry communities, including:

- the nudged elastic band method (for finding saddle btwn two minima);
- the dimer method (for finding saddle points)
- hyperdynamics (a principled scheme for accelerating rare events)
- transition path sampling (a Monte-Carlo-like scheme in path space)

An applied math community has emerged around the analysis, improvement, and application of such algorithms. Still young, but many outcomes including some new methods:

- the minimal action method (for transition paths in non-gradient systems)
- the finite-temperature string method (for complex energy landscapes)
- the climbing string method (for finding saddle points)

An analogy: 50 years ago the finite element method was widely used by engineers. Sometimes it worked, sometimes it didn't. Numerical analysis provided much clarification. Math can help here too.

Finding barriers, pathways, & transition rates, cont'd

Some MGI-related thoughts, as noted earlier:

- Advances in computer hardware will help, but improved algorithms will be crucial.
- MGI emphasizes interaction of theory, simulation, and experiment. Algorithmic improvement can be an enabling technology.

Selected references by mathematicians:

- W E, W Ren, E Vanden-Eijnden, J Phys Chem B 109 (2005) 6688 (string method)
- W Ren, E Vanden-Eijnden, J Chem Phys 138 (2013) 134105 (climbing string method)
- J Zhang, Q Du, SIAM J Numer Anal 50 (2012) 1899-1921 (dimer method)
- N Guttenberg, A Dinner, J Weare, J Chem Physics 136 (2012) 234103 (transition path sampling)
- D Aristoff, T Lelievre, G Simpson, AMRX 2014(2), 2014, 332-352 (parallel replica method)

Stepping back

Mathematics can help. Today's examples captured a few of the many ways, involving

- designing materials or structures
- algorithms and models for evolving interfaces and moving defects
- extraction of data from simulations or images
- linking length scales
- linking time scales

This audience faces many such challenges. For greatest impact, mathematics and computing should participate early – helping to identify the questions (not just the answers).

Where to find this type of mathematician? Some upcoming events:

- SIAM Conference on Mathematical Aspects of Materials Science, May 8-12, 2016.
- IPAM has a program on Understanding Many-Particle Systems with Machine Learning, Sept - Dec 2016. (IPAM = Institute for Pure and Applied Mathematics, an NSF-funded institute at UCLA.)