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Multiscale Modeling Methods for Materials Science

Machine-Learning via Genetic Programming for Multiscale Modeling

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Multiscaling via Symbolic Regression

Overview

Multiscale simulations by coupling traditional methods have proven inadequate because of the range of scales, detailed information needed from finer scales, and the prohibitively large numbers of variables then required. Thus, for multiscale simulations (spatial and temporal) we must provide data from finer (atomic) scales that is reliable, avoids the need for determining "hidden variables" at various scales, and is computational inexpensive.

Abstract

We employ Symbolic-Regression via *Genetic-Programming* – a *Genetic Algorithm* that evolves computer programs – to represent the atomic-scale details needed to simulate processes at time and lengths pertinent to experiment, or even to reveal pertinent correlations that determine the relevant physics or chemistry at differing scales.

We provide three recent examples involving regression of:
i) constitutive behavior for an aluminum alloy,
ii) diffusion barriers for multiscale kinetics on alloy surfaces,
iii) semi-empirical quantum-chemistry potentials that avoid potentially irrelevant transition states but get excited-state reaction pathways.

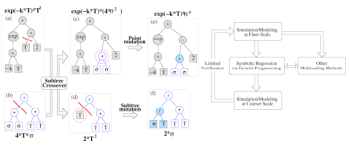
***Genetic Programming* is a genetic algorithm that *evolves* computer programs, requiring:**

Representation: programs represented by trees
- Internal nodes contain functions
  - e.g., {+, -, *, /, ^, log, exp, sin, AND, if-then-else, for}
- Leaf nodes contain terminals
  - e.g., Problem variables, constants, Random numbers

Fitness function: Quality measure of the program

Population: Candidate programs (individuals)

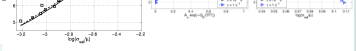
Genetic operators:
- **Selection:** "Survival of the fittest".
- **Recombination:** Combine parents to create offspring.
- **Mutation:** Small random modification of offspring.



1. Evolving Constitutive Relations

Goal: Evolve constitutive "law" between macroscopic variables from stress-strain data with multiple strain-rates for use in continuum finite-element modeling.

Flow stress vs. temperature-compensated strain rate for AA7055 [Padilla, et al. (2004)].
- GP fits both low- and high-strain-rate data well.



- Automatic identification of transition point via a complex relation, *g*, which models a step function.

$$y = 10^{\left[1 - \frac{3\sigma}{\mu}\sqrt{6 + \sqrt{\left|A_1 c^{-\frac{3\sigma}{\mu}} - \frac{2\sigma}{\mu}\right|}\left\{1 - \frac{3\sigma}{\mu}A_1 c^{-\frac{3\sigma}{\mu}}\left(1 - A_1^2 c^{-\frac{6\sigma}{\mu}} + \frac{2\sigma}{\mu}\right)\right\}}\right]}$$

- GP identifies "law" with two competing mechanisms

$$\dot{\varepsilon} = \frac{c_\alpha}{g\left\{\epsilon, \exp\left(\frac{1}{RT}\right)\right\}} \exp\left(\frac{1}{RT}\right)\left(\frac{\sigma}{\mu}\right)^d \left[1 - \frac{\sigma}{\mu_s}\right]$$

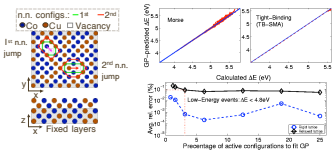
  – 5-power law modeling creep mechanism
  – 4-power law modeling as-yet-unknown mechanism.

2. Multi-Timescale Kinetics Modeling

Goal: To advance dynamics simulation to experimentally relevant time scales.

- Molecular Dynamic (MD) or Kinetic Monte Carlo (KMC) based methods fall short 3–9 orders in real time.
  – Unless ALL the *diffusion barriers* are known in Table.
  – Table KMC has 10^9 increase in "simulated time" over MD at 300K.
- Symbolically-Regressed KMC (sr-KMC)
  – Use MD to get *some* barriers.
  – *Machine learn* via GP *all* barriers as a regressed *in-line function call*, i.e. "table-look-up" KMC is replaced by function.

Application: Surface-vacancy-assisted migration in phase-segregating Cu_xCo_{1-x}

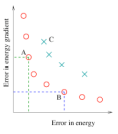


- GP predicts all barriers with 0.1–1% error using explicit calculations for 3% of the barriers (0.3% with cluster expansion).
  – Standard basis-set regression *fails*.
  – sr-KMC approach provided, for this problem:
    – 10^2 decrease in CPU time for barrier calculations.
    – 10^3–10^6 less CPU time per time-step vs. on-the-fly methods.
- Could combine with pattern-recognition methods, or temperature-accelerated MD, to model more complex cooperative dynamics.

3. On-Going: Multiscale Modeling in Excited-State Reaction Chemistry

Goal: Functional augmentation & rapid multi-objective re-parameterization of semiempirical methods to obtain reliable pathways for excited-state reaction chemistry.

- *Ab Initio* methods: accurate, highly expensive
- Semiempirical (SE) methods: approximate, inexpensive
  – Reparameterization based on few *ab initio* data
  – Involves optimization of multiple objectives, such as fitting simultaneously limited *ab initio* energy and energy-gradients of various chemical excited-states or conformations.
  – Augmentation of functions may be needed
- Propose: Multi-objective GAs for reparameterization
  – Obtain set of non-dominated solutions in parallel.
  – *Avoid* potentially irrelevant pathways, arising from SE-forms.
  – GP for functional augmentation, e.g., symbolic regression of core-core repulsions.



Semi-empirical potential parameterizations lead to differing solutions, or competing solutions. Using GA/GP we can find optimal potentials and avoid pathways from dominating but irrelevant solutions.

- solution C is dominate over A.
- solutions A and B are non-dominate.

Summary

Symbolic regression via genetic programming (GP) is a robust method for bridging methods across multiple scales. Unlike traditional regression methods, symbolic regression via GP adaptively evolves both the functional relation and regression constants for transferring key information from finer to coarser scales, and is inherently parallel.

The present results indicate that GP-based symbolic regression is an effective and promising tool for multiscaling. We believe that GP-based symbolic regression holds promise in other multiscaling areas, such as finding chemical reaction pathways mentioned above. Moreover, the flexibility of GP makes it readily amenable to hybridization with other multiscaling methods leading to enhanced scalability and applicability to more complex problems.

Acknowledgement

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New Concepts and Methods for Modeling Complex Dynamical Systems

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Complex Dynamical Systems

Dynamical systems and their manifestations are ubiquitous in everyday life, from earthquakes to weather changes, and in modern society, from magnetic devices to nuclear reactors. These systems are intrinsically complex because of the presence of **long-range interactions** and **non-linear dynamics**, and often because of the presence of nonequilibrium **external forcing**, e.g., by applying electrostatic field, magnetic field, or by irradiation with energetic projectiles.

Our recent results focus on the connection between external noise (1), and internal noise (3), on critical behavior and self-organization. We have also devised a new experimental set-up for the study of fractals dynamics (2). We have used computer simulations to elucidate the structure of triblock copolymer gels (4).

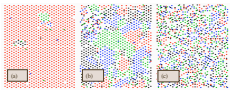
1. Self-Organization of Chemical Order in Alloys Driven by Irradiation

Materials under irradiation are dissipative systems, and as such, they are susceptible to self-organize (SO). Twofold interest:
- Fundamental: excellent test bed of the theory driven systems since microscopic mechanisms are well identified and can be varied in a controlled manner experimentally.
- Practical: self-organization can be used to synthesize functional nanocomposites with tunable scales

Irradiation with energetic ions creates displacement cascades, resulting in disordered zones in chemically ordered alloys. At finite temperatures, this disorder competes with thermally activated reordering.

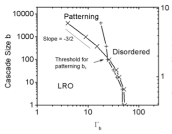
We used kinetic Monte Carlo simulations and analytic modeling to identify that self-organization of the chemical order field can take place when the cascade size exceeds a threshold value.

Three possible steady states for the order field in a A_3B alloy that displays $L1_2$ ordering



Maps of B atoms at steady state under irradiation with increasing disordering rate:
(a) $\Gamma_a = 1\ s^{-1}$;
(b) $\Gamma_a = 10\ s^{-1}$;
(c) $\Gamma_a = 100\ s^{-1}$.
Each one of the 4 ordering variants is displayed with one color

KMC Dynamical phase diagram

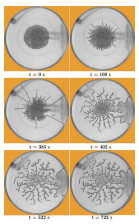


Impacts and perspectives
- Demonstrate the key role played by extrinsic length scales in dynamical self-organization
- Potential application for Fe-Pt exchange spring-magnets, which require $A1\text{-}L1_0$ or $L1_2\text{-}L1_0$ nanocomposites
- Alloy-specific simulations by Genetic-Programming KMC

2. Fractals in Electrochemical Systems

Two major difficulties in experimental studies of dynamics of fractals are:
1) time scales are either too fast (as in dielectric breakdown) or too slow (as in river formation)
2) control of experimental parameters are out of the researchers' hands.

We design a new model system by placing conductive particles in a viscous dielectric medium, to which an electrical field is applied. The mechanical relaxation time scales become much slower than the electrical relaxation time scales. This experimental set-up resolves the two major issues involved in studying dynamic fractal formation.



Relaxation sequence starting from a compact initial condition:

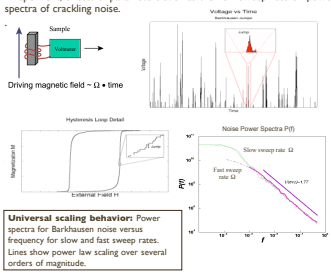
Before time τ =400s, the unconnected particles form chains that compete to reach the grounded electrode.

After τ = 400s, one of the chains meets ground and all other chains quit reaching. The network proceeds to form from the single connected chain.

Networks formed are nearly space-filling, with mass dimensions between 1.74 and 1.9.

3. Hysteresis, Noise, and Domain Wall Dynamics in Magnets

We investigate *Crackling Noise* – a jerky response to slowly varying force – such as Barkhausen noise, superconducting vortex Avalanches, earthquakes, and shape memory alloys. Such materials all respond to an external driving force or field with crackling noise. We study *universal*, *i.e.* detail independent, effects of parameters such as the field sweep rate on power spectra of crackling noise.



Universal scaling behavior: Power spectra for Barkhausen noise versus frequency for slow and fast sweep rates. Lines show power law scaling over several orders of magnitude.

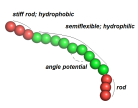
Effect of long-range (LR) demagnetizing field studied by zero temperature random field Ising model. Two generic behaviors identified for magnetization subloops:
- with LR field, response similar to self-organized critical systems
- without LR field, avalanche size distribution displays history-induced critical scaling

Very good agreement with experiments on CoPt and CoPt/CrB thin films.

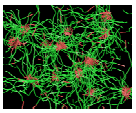
4. Gelation in Triblock Copolymer Solutions

Petka *et al.* [Science **281**, 389 (1998)] demonstrated that triblock copolymers with a water-soluble domain flanked by two rod-like hydrophobic end blocks are capable of undergoing reversible gelation in response to changes in pH or temperature.

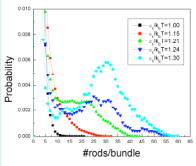
However, the microscopic structure and the dynamics of this system during the gelation process as well as their interconnection are difficult to clarify using experimental methods. We have used molecular dynamics simulations to investigate a coarse-grained model of this system and to address the above-mentioned questions.



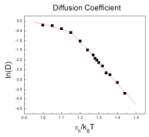
Model triblock copolymer

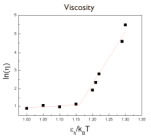


Snapshot of resulting structure



Probability distribution function of #rods/bundle peaks suggests formation of interconnected bundles that make up the gel structure. Percolation threshold corresponds to ε_b/k_BT=1.15





Key Findings
- Onset of percolation coincides with bundle formation and leads to slow-down of dynamics, but occurs much earlier than actual gelation
- Both short-range and long-range order are being established upon decrease of temperature