Reduced Order Models using Graph Theoretic Approaches for Physical Systems

Introduction to Graph Theory and its Applications in Continuum Physics

Matthew Duschenes

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Computational Physics Group, Applied Physics - University of Michigan

Outline

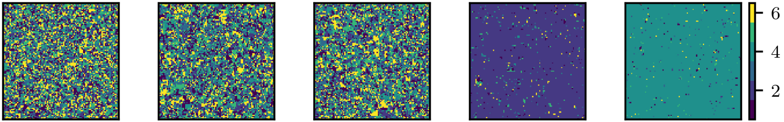


Figure 1: Monte Carlo simulation of quenched $q = 6$ state Pott's model.

Introduction

Continuum Physics

- Systems in continuum physics framework, with solids and fluids represented by quantities $f(x,t)$ over continuous material volumes

$$x \in \Omega_t,\ t \in [0,T].$$

- Time evolution of reference body:

$$\varphi_t : \Omega_0 \to \Omega_t,$$

$$X \to x = \varphi_t(X) \equiv X + u(X,t),$$

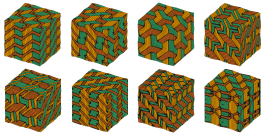


Figure 2: Example microstructures (Banerjee et al., Comput. Methods **351** (2019).).

Mechano-Chemical Processes

- Multi-crystalline solids, with composition c and strain E dependent phase transitions
- Symmetries of system used to construct relevant order parameters

$$\eta = \{c, e_2 = \frac{1}{\sqrt{2}}(E_\perp - E_\parallel)\},$$

for binary solid, and lattice in $d = 2$ dimensions

- Landau free energy approach:

$$\psi = \psi_{\mathrm{hom}} + \psi_{\mathrm{grad}}$$

- Resulting equilibrium states of solids develop distinct phase field patterns, called microstructures

Mechano-Chemical Spinodal Decomposition

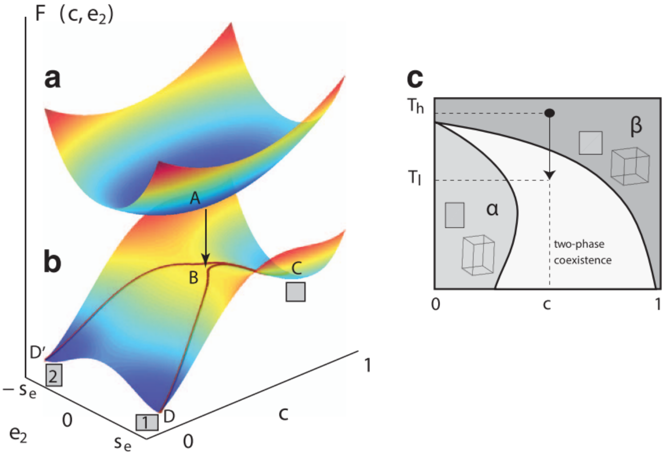
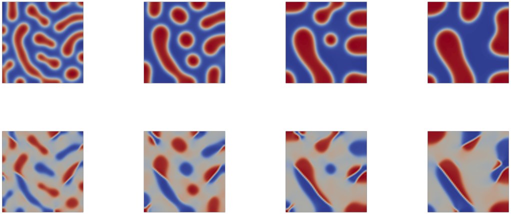


Figure 3: Free energy density landscape over $c - e_2$ fields [1].

Microstructures in $d = 2$



(a) $100\mu s$ **(b)** $200\mu s$ **(c)** $500\mu s$ **(d)** $750\mu s$

Figure 4: Microstructure Phase Field Evolution,
Top row: c, Bottom row: e_2.

Quantities of Interest

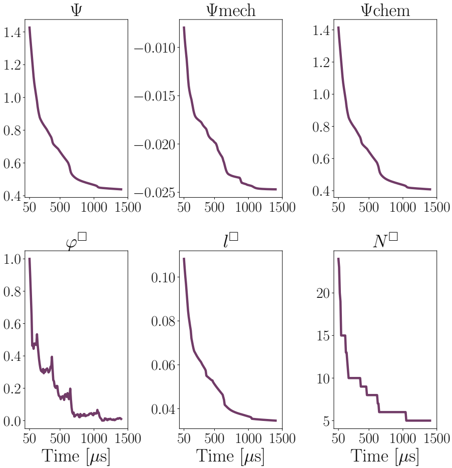


Figure 5: Quantities of interest over phase field evolution.

Quantities of Interest

- Chemical quantities:

$$\{c(x),\ c\}$$

- Mechanical quantities:

$$\{e_2(x),\ E,\ P\}$$

- Free Energy quantities:

$$\{\Psi_{\text{tot}},\ \Psi_{\text{chem}},\ \Psi_{\text{mech}},\ \Psi_{\text{couple}}\}$$

- Phase Mixture quantities:

$$\{\varphi^{\alpha},\ l^{\alpha},\ N^{\alpha}\}_{\alpha=\{\square,\,\sqsubset\!\sqsupset,\ldots\}}$$

Conventional Computational Methods

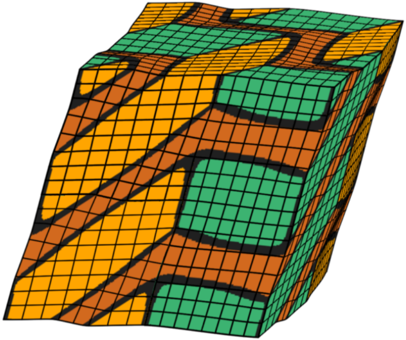


Figure 5: Example strain state microstructure with colours representing local cubic or tetragonal lattice structures (Banerjee et al., Comput. Methods **351** (2019).).

Computational Methods

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  - Deep Neural Network
  - Convolution Neural Network
  - Knowledge Based Neural Network
- Statistical Inference (Walle and Asta, Model. Simul. Mater. **10** (2002).)
  - Monte Carlo
  - Bayesian Approaches
  - Regression Analysis

Graph Theoretic Approaches

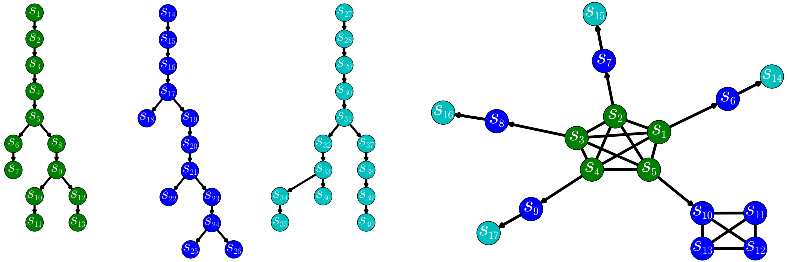
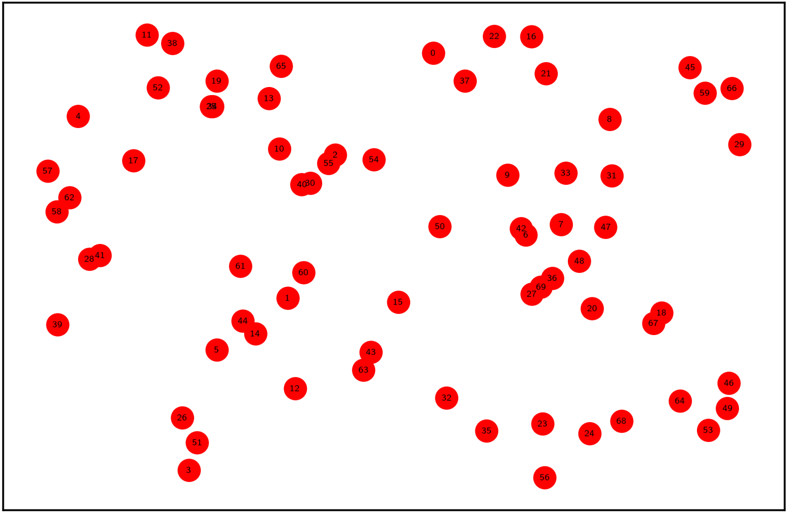
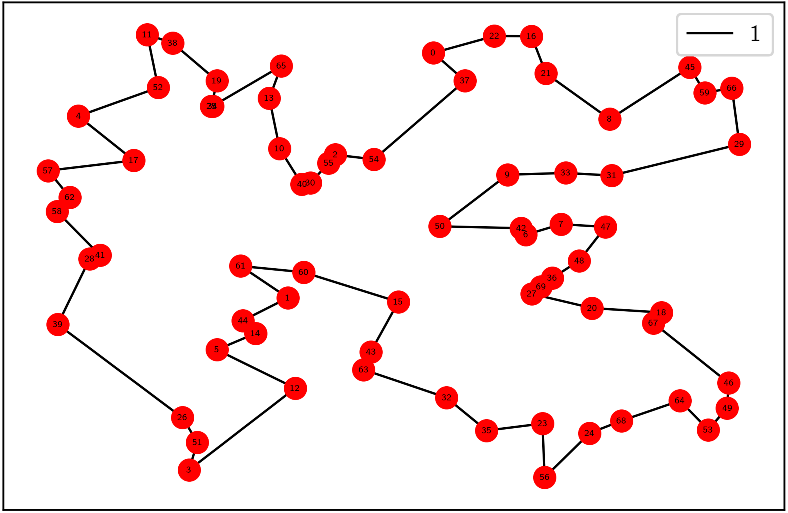


Figure 6: Example directed and undirected graphs, with varying levels of connectivity.

Graph Theory Applications



Graph Theory Applications



Graph Theory Formalism

Let a graph

$$G = G(V, E; \chi, \theta),$$

be comprised of a set of elements, or vertices

$$i \in V,$$

with relationships between elements described by a set of edges between vertex pairs

$$e = (i, j) \in E,$$

and tuples of quantities associated with each vertex

$$\chi = \{\chi_i^\mu\},$$

and edge

$$\theta = \{\theta_{ij}^\nu\}.$$

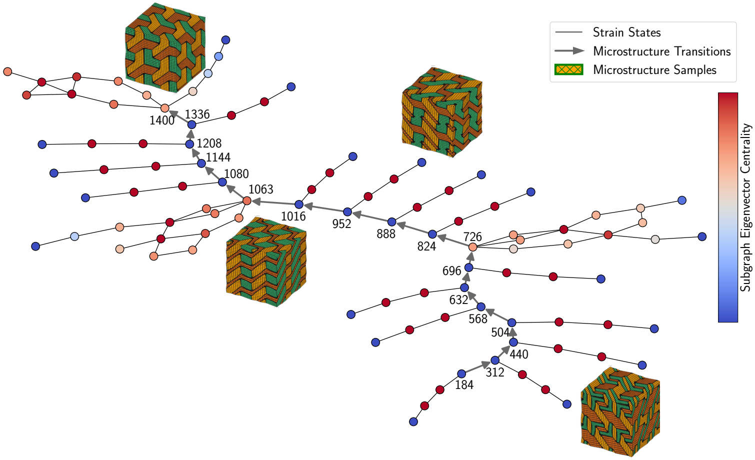


Figure 7: Visualization of microstructure evolution using graph theoretic approach and centrality measures.

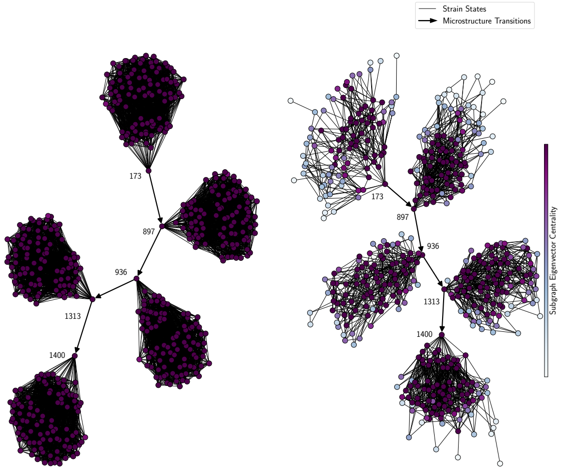


Figure 8: Visualization of microstructure evolution using graph theoretic approach and centrality measures.

Non-Local Calculus

- Non-local operators over n-dimensional space of discrete states (Gilboa and Osher, Multiscale Model. Simul., **7** (2008).)
- Each state i has an associated tuple of quantities $\{x_i^\mu\}$, as well as *scalars* $u(x_i)$, and *vectors* $v(x_i, x_j)$
- Distance metric d_{ij} chosen to define edge *weights* w_{ij}
- Unlike for Finite Difference approaches, differences between *all* states are accounted for
- Rigorous definitions lead to self-adjointness and divergence-like theorems, and therefore conventional calculus operators are well defined

Derivative Definitions

- Partial derivatives:

$$\frac{\delta u(x_i)}{\delta x_i^\mu} \approx \frac{\partial u(x_i)}{\partial x_i^\mu} \equiv \sum_j (u(x_j) - u(x_i))(x_j^\mu - x_i^\mu) w_{ij},$$

- Taylor series:

$$u(x_i) \approx u(x_0) + \sum_{\{\mu\}} \gamma^{\{\mu\}} \frac{\delta u}{\delta x^\mu}_i \bigg|_{x_0} \Delta x_i^\mu + \frac{1}{2} \sum_{\{\mu,\theta\}} \gamma^{\{\mu,\theta\}} \frac{\delta^2 u}{\delta x^\mu \delta x^\theta} \bigg|_{x_0} \Delta x_i^\mu \Delta x_i^\theta + \ldots \text{(h.o.t)}.$$

Reduced Order Modelling

- Initial assumptions on general form of model or PDE for dynamics based on lower dimensional representation

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- Model fitting using regression, Bayesian approaches, machine learning ...
- Cross validation and model predictions (Wang et al., Comput. Methods Appl., **356** (2019).)

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- Model becomes increasingly parsimonious
- Linear regression used, but other, i.e) Bayesian approaches are possible

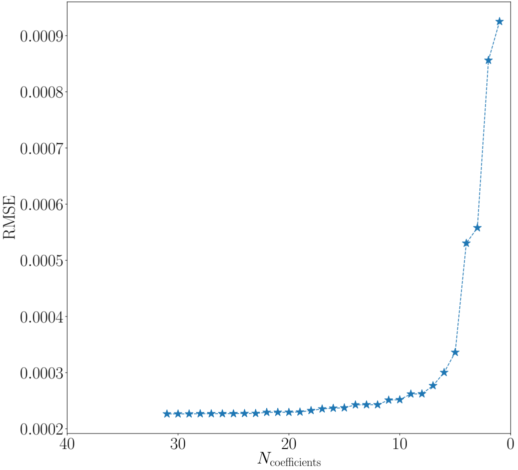

Figure 9: Stepwise regression loss curve as model becomes more parsimonious

Results

Results - Phase Volume Fractions

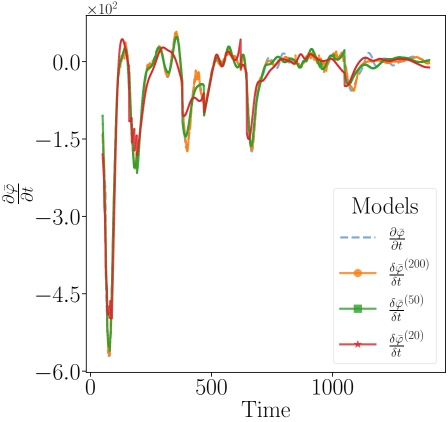

Figure 10: Fitted curves for decreasing number of operators for phase volume fraction first order dynamics, using a monomial basis.

Results - Neutron Cross Sections

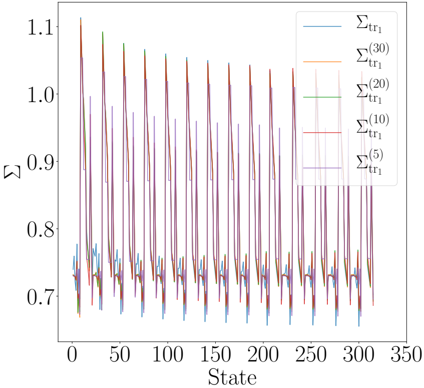

Figure 11: Fitted curves for decreasing number of operators for transport cross section, using a Taylor series basis (Kochunas et al., Unpublished (2020).).

Summary

- Graph theoretic approaches offer a low dimensional representation of high dimensional systems
- Non-local discrete calculus allows rigorous and analogous calculus operators to be computed
- Reduced order models can be computed and fit for predictions using data from conventional methods
- Very general framework for many system scales and types of physics
  - Condensed matter systems
  - Neutron transport equations
  - Biological systems such as pattern formation

Thank you!

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