# Reduced Order Models using Graph Theoretic Approaches for Physical Systems

## Applications of non-local calculus on finite weighted graphs

Matthew Duschenes, Krishna Garikipati

November 10, 2021

Computational Physics Group, Applied Physics - University of Michigan

# Outline

1. Introduction
2. Reduced Order Modelling
3. Graph Theoretic Approaches
4. Results

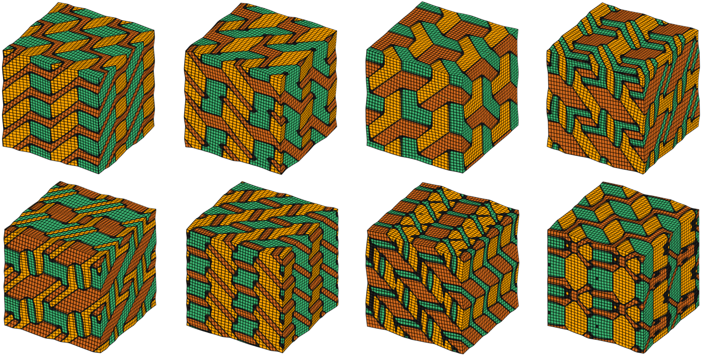


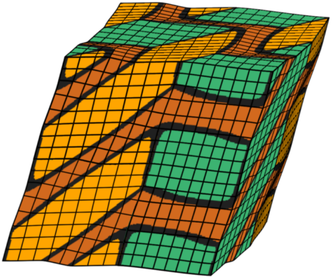
**Figure 1:** Example phase-field microstructures (Banerjee et al., *Comput. Methods* **351** (2019)).

# Introduction

# Mechano-Chemical Processes

- Multi-crystalline solids, with composition $c$ and strain $\mathbf{E}$ dependent phase transitions

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



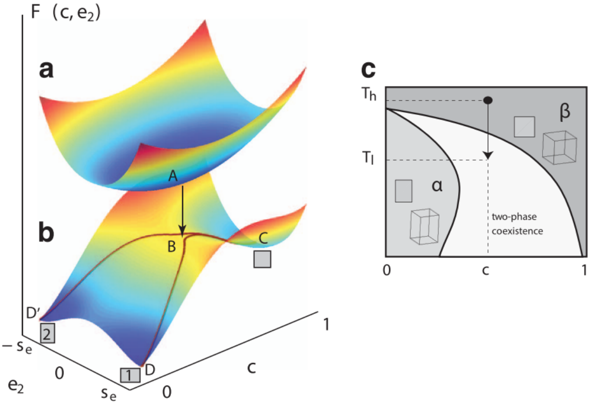



**Figure 2:** Free energy density landscape over $c - e_2$ fields (Rudraraju et al., *npj Comput. Mater.* **2** (2017)).

# Microstructure Evolution in 2 Dimensions

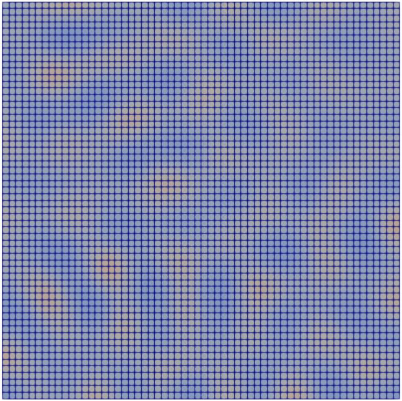


**Figure 3:** Composition $c$ phase field evolution.

# Reduced Order Modelling

# Quantities of Interest

Spatially dependent $f(x) \rightarrow$ Volume averaged $F$

- Chemical quantities:

$$\{c(x),\ \mu(x)\}\ \rightarrow\ \{\varphi_\alpha,\ l_\alpha,\ N_\alpha\}_{\alpha=\{\square,\square+,\square-,\dots\}}$$

- Mechanical quantities:

$$\{\mathbf{F}(x), \mathbf{E}(x),\ \mathbf{P}(x), \dots\} \rightarrow \{\bar{\mathbf{F}}, \bar{\mathbf{E}},\ \bar{\mathbf{P}}, \dots\}$$

- Free Energy quantities:

$$\{\psi(x),\ \psi_{\text{mech}}(x),\ \psi_{\text{chem}}(x), \dots\}\ \rightarrow\ \{\Psi,\ \Psi_{\text{mech}},\ \Psi_{\text{chem}}, \dots\}$$

# Quantities of Interest

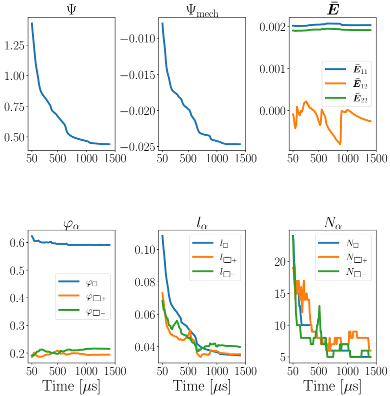



**Figure 4:** Quantities of interest over phase field evolution.

# Models of Interest

- Free Energy Functional Representation:

$$\psi = \psi_{\text{hom}}(c, \mathbf{E}) + \psi_{\text{grad}}(\nabla c, \nabla \mathbf{E}) \rightarrow \Psi = \Psi(\varphi_\alpha, \bar{\mathbf{E}})$$

- Phase Volume Fraction Dynamics:

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J} = 0 \rightarrow \frac{\partial \varphi_\alpha}{\partial t} = f(\varphi_\beta, \bar{\mathbf{E}}, \frac{\partial^n \Psi}{\partial \varphi_\gamma \cdots \partial \bar{\mathbf{E}}})$$

# Graph Theoretic Approaches

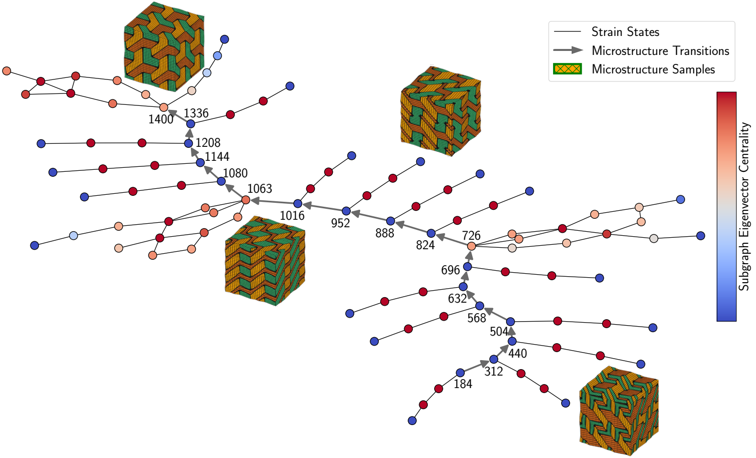
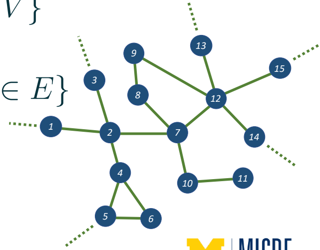



**Figure 5:** Visualization of microstructure evolution using graph theoretic approach and centrality measures.

# Graph Theory Formalism

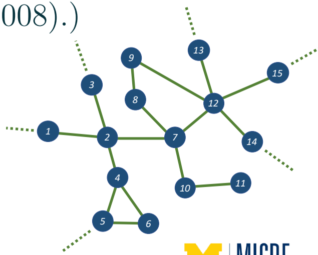
A graph $G = G(V, E; x, w)$ contains:

- State Vertices: $V = \{1, 2, \ldots, n\}$
- State Transition Edges: $E = \{e = (i, j) : i, j \in V\}$
- State Vector: $x = \{\{x_i^\mu\}_{\mu=\{1\ldots p\}} : i \in V\}$
  *i.e)* $x = \{\{\Psi_i, \bar{\mathbf{E}}_i, \varphi_{\alpha_i},\ l_{\beta_i},\ N_{\gamma_i}\} : i \in V\}$
- Edge Weights: $w = \{w(x_i, x_j) : (i, j) \in E\}$



# Non-Local Calculus

- Functional representations and differential equations require a basis of operators
- States of a system may be unstructured, not lending themselves to typical finite difference approaches
- Discrete $p$-dimensional manifold of graph allows for a rigorous non-local calculus to be defined (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008).)



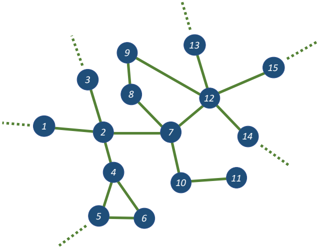
# Derivative Definitions

- Partial derivatives:

$$\frac{\partial u(x_i)}{\partial x^\mu} \approx \frac{\delta u(x_i)}{\delta x^\mu} \equiv \frac{1}{n}\sum_{j\in V}(u(x_j)-u(x_i))(x_j^\mu - x_i^\mu)w(x_i,x_j)$$

- Taylor series:

$$\begin{aligned} u(x_i) \approx u(x_1) &+ \sum_{\mu=\{1\ldots p\}} \gamma^\mu \frac{\delta u(x_1)}{\delta x^\mu}\Delta x_{1i}^\mu \\ &+ \frac{1}{2}\sum_{\mu,\nu=\{1\ldots p\}} \gamma^{\mu\nu}\frac{\delta^2 u(x_1)}{\delta x^\mu \delta x^\nu}\Delta x_{1i}^\mu \Delta x_{1i}^\nu \\ &+ \cdots \end{aligned}$$

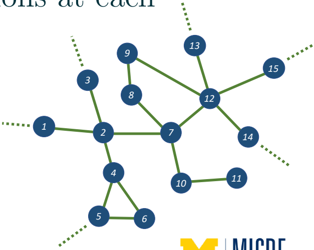


# Edge Weight Constraints

In order to ensure consistency with differential calculus

$$\frac{\delta u(x_i)}{\delta x^\mu} = \frac{\partial u(x_i)}{\partial x^\mu} + O\left(\sum_{j\in V}(x_j^\nu - x_i^\nu)(x_j^\theta - x_i^\theta)(x_j^\mu - x_i^\mu)w(x_i, x_j)\right),$$

the weights are constrained to obey equations at each vertex $i$.



# Edge Weight Constraints

Possible forms of radially symmetric weights:

- Gaussian:

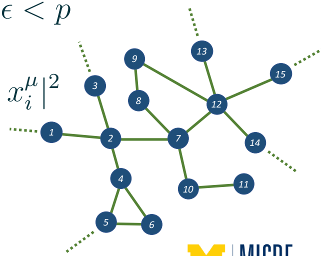
$$w(r) = Ce^{-\frac{1}{2}\frac{r^2}{\sigma^2}}$$

- Polynomial:

$$w(r) = C\left(\frac{\sigma}{r}\right)^{2+\epsilon}\ ,\ 0 < \epsilon < p$$

where

$$r^2 = r(x_i, x_j)^2 = \sum_{\mu=\{1\ldots p\}} |x_j^\mu - x_i^\mu|^2$$



# Results

# Stepwise Regression

- Operators rejected based on statistical tests (F-test) for how likely it is for the operator to be irrelevant

# Stepwise Regression

- Operators rejected based on statistical tests (F-test) for how likely it is for the operator to be irrelevant
- Statistical tests relate fitting loss, and model complexity

# Stepwise Regression

- Operators rejected based on statistical tests (F-test) for how likely it is for the operator to be irrelevant
- Statistical tests relate fitting loss, and model complexity
- Model becomes increasingly parsimonious

# Stepwise Regression

- Operators rejected based on statistical tests (F-test) for how likely it is for the operator to be irrelevant
- Statistical tests relate fitting loss, and model complexity
- Model becomes increasingly parsimonious
- Linear regression used, but other, i.e) Bayesian approaches are possible

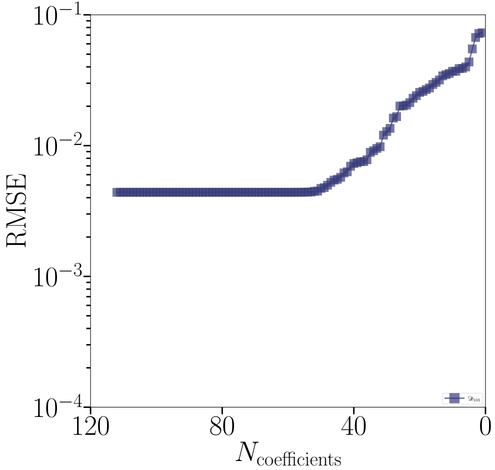



**Figure 6:** Stepwise regression loss curve as model becomes more parsimonious

# Phase Volume Fraction Dynamics

Cahn-Hilliard Equation:

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

Model:

$$\frac{\partial \varphi_\alpha}{\partial t} = f(\varphi_\beta, l_\gamma, N_\delta, \bar{E}_{ij}, \frac{\partial^q \Psi}{\partial \varphi_\beta \cdots \partial \bar{E}_{ij}})$$

# Phase Volume Fraction Dynamics

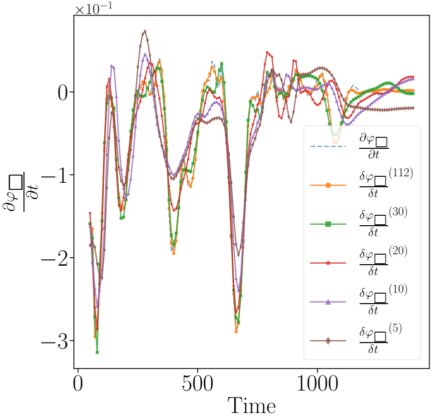



**Figure 7:** Fitted curves for decreasing number of operators for the square phase volume fraction dynamics as a function of polynomials of operators present in the Cahn-Hilliard equation.

# Free Energy Functional Representation

Free Energy Density:

$$\psi = \psi_{\text{hom}}(c, \mathbf{e}) + \frac{1}{2}\kappa|\nabla c|^2 + \frac{1}{2}\gamma|\nabla \mathbf{e}|^2$$

Taylor Series:

$$\begin{aligned}
\Psi(\varphi_{\alpha_k}, \bar{\mathbf{E}}_k) = {} & \gamma^0 \Psi(\varphi_{\beta_0}, \bar{E}_{ij_0}) \\
& + \ \gamma^{\varphi_\beta} \frac{\partial \Psi(\varphi_{\beta_0}, \bar{E}_{ij_0})}{\partial \varphi_\beta} \Delta \varphi_{\beta_{0k}} \\
& + \ \gamma^{\bar{E}_{ij}} \frac{\partial \Psi(\varphi_{\beta_0}, \bar{E}_{ij_0})}{\partial \bar{E}_{ij}} \Delta \bar{E}_{ij_{0k}} \\
& + \ \cdots
\end{aligned} \tag{1}$$

# Free Energy Functional Representation

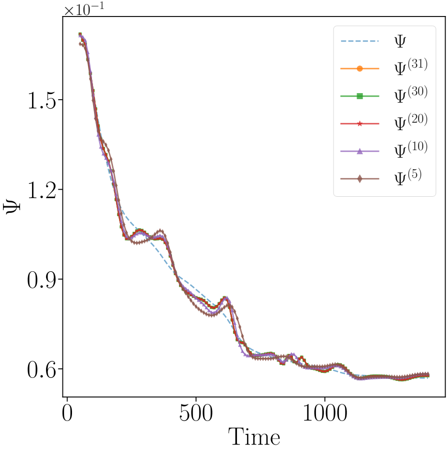



**Figure 8:** Fitted 2$^{\text{nd}}$ order Taylor series representation of the total free energy, for a decreasing number of operators.

# Summary

- *Low dimensional representation* of high dimensional systems
- *Non-local* discrete calculus is rigorous and analogous to differential calculus operators
- Constraints on edge weights ensure *consistency*, however pose numerical issues
- Reduced order models can be computed using *basis* of graph operators
- Very *general* framework for many system scales and types of physics

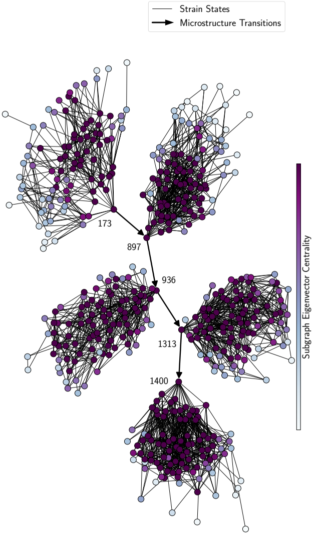
# Thank you!

<u>Computational Physics Group</u>:

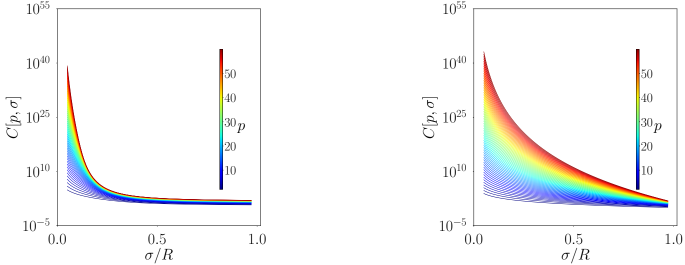
- Dr. Krishna Garikipati
- Dr. Xiaoxuan Zhang
- Dr. Zhenlin Wang
- Dr. Gregory Teichert
- Elizabeth Livingston

<u>Collaborators</u>:

- Dr. Brendan Kochunas
- Dean Price
- Thomas Folk



# Weight Scalings

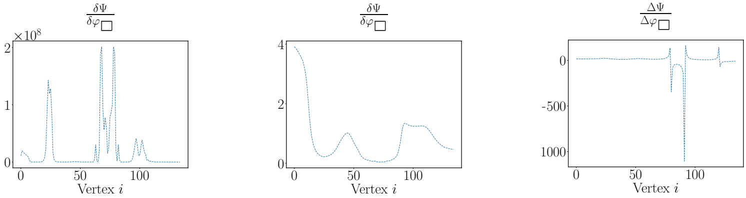



**(a)** Gaussian

**(b)** Polynomial

**Figure 9:** Weight constraint scales for various $p$ values, as a function of weight extent $\sigma$. $\epsilon = \frac{p}{2}$ for the polynomial weights.

# Derivatives




**(a)** Gaussian **(b)** Polynomial **(c)** Finite Difference

**Figure 10:** Comparison of derivatives at each vertex index for Gaussian, Polynomial, and Finite Difference weights.