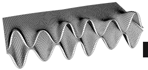
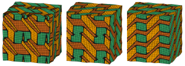
# Reduced Order Models Using a Non-Local Calculus on Finite Weighted Graphs





**Matthew Duschenes, Siddhartha Srivastava & Krishna Garikipati**

Applied Physics, Mechanical Engineering, and
Michigan Institute for Computational Discovery & Engineering
University of Michigan, Ann Arbor

July 26, 2021

arXiv:2105.01740



**USNCCM #309 Data-Driven Science**

# Outline

1. Systems of Interest

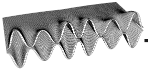
2. Graph Theoretic Approaches

3. Applications

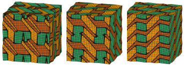
1. Systems of Interest

2. Graph Theoretic Approaches

3. Applications



# Diffusion Processes



Consider a local diffusion process for a scalar field $\phi(x,t)$, driven by gradient-flow:

$$\frac{\partial \phi}{\partial t} = - M_\phi \frac{\delta \psi}{\delta \phi} \tag{1}$$

which can be described by a free energy density

$$\psi = f(\phi) + \lambda |\nabla \phi|^2 \tag{2}$$

where the Landau $f$ is algebraic in $\phi$, and the total free energies are

$$\Psi = \int_\Omega d\Omega \ \psi \ , \quad F = \int_\Omega d\Omega \ f \ , \quad G = \int_\Omega d\Omega \ |\nabla \phi|^2 \ , \quad F' = \int_\Omega d\Omega \ f' \ . \tag{3}$$

# Reduced Order Modelling

Can we use global observables, such as the field's moments:

$$\varphi_k = \frac{1}{\Omega}\int_\Omega d\Omega \quad \underbrace{I(\phi)}_{\text{indicator function}} \quad \phi^k \tag{4}$$

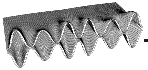
or its derivatives

$$\varphi_{\nabla^k} = \frac{1}{\Omega}\int_\Omega d\Omega \; I(\phi)\; \nabla^k \phi \; , \qquad \varphi_{\nabla_k} = \frac{1}{\Omega}\int_\Omega d\Omega \; I(\phi)\; |\nabla\phi|^k \tag{5}$$

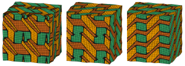
or functional derivatives (and how may we precisely define these?)

$$\frac{\delta\Psi}{\delta\varphi_k}, \; \frac{\delta\Psi}{\delta\varphi_{\nabla^k}}, \; \frac{\delta\Psi}{\delta\varphi_{\nabla_k}} \quad \ldots \tag{6}$$

to develop a reduced order model?



# Models of Interest



We aim to find a model for a global gradient-flow (Banerjee *et al.*, *Comp. Meth. App. Mech. Eng.*, **351**, (2019)):

$$\frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi}\left(\varphi_k, \varphi_{\nabla^k}, \varphi_{\nabla_k}, \frac{\delta \Psi}{\delta \varphi_k}, \cdots\right) \tag{7}$$

and a free energy functional representation

$$\Psi = \Psi\left(\varphi_k, \varphi_{\nabla^k}, \varphi_{\nabla_k}, \frac{\delta \Psi}{\delta \varphi_k}, \cdots\right). \tag{8}$$

**Taken's Theorem**: (Stark, *J. Nonlinear Sci.*, **351**, (1999))
For $\phi(x,t) \in \mathscr{M} \subset \mathbb{R}^d$, a mapping $P \ : \ \phi(x,(k+1)\tau) = P_\tau(\phi(x,k\tau))$, and an observable, $\varphi[\phi] \in \mathbb{R}$, $\exists$ an embedding

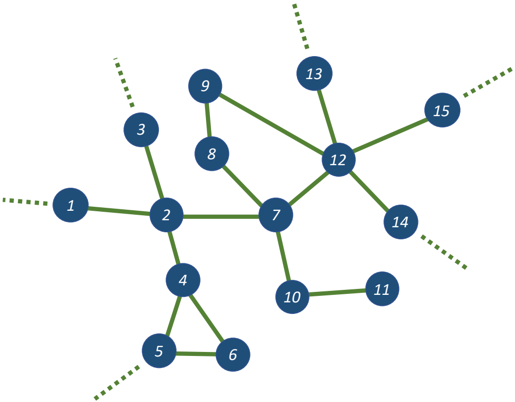
$$\mathscr{T} : \mathscr{M} \to \mathbb{R}^n, \quad \mathscr{T}[\phi(x,t)] = \{\varphi^{(1)}, \phi^{(2)}, \dots, \varphi^{(n)}\} \tag{9}$$

for $(P, \varphi)$ *dense* and *open* in $D^r \times C^r(\mathscr{M}, \mathbb{R})$ for $n \geq 2d+1$ observations.

1. Systems of Interest

2. Graph Theoretic Approaches

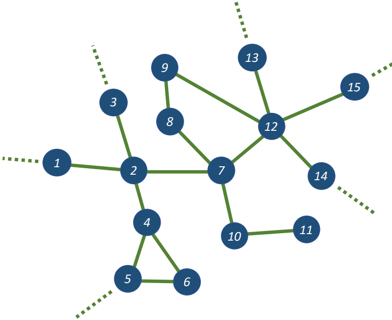
3. Applications



1
2
3
4
5
6
7
8
9
10
11
12
13
14
15

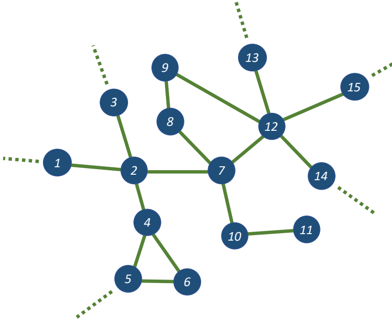
# Graph Theory Formalism

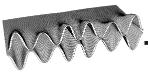
- State Vertices and State Dimensions: $V = \{1, 2, \ldots, n\}, \quad \chi = \{1, 2, \ldots, p\}$
- State Vector: $X = \{x = \{x^\mu\}_{\mu \in \chi} \;:\; x \in V\}$
  $i.e)\; X = \{x = \{\, \varphi_k,\, \varphi_{\nabla^k},\, \varphi_{\nabla_k}, \Psi, \ldots\} \;:\; x \in V\}$
- State Transition Edges: $E = \{(x, y) \;:\; x, y \in V\}$
- Edge Weights: $w = \{w(x, y) \;:\; (x, y) \in E\}$
- Neighborhoods of Adjacent Vertices:
  $\delta = \{\delta(x) = \{y \in V \;:\; (x, y) \in E\} \;:\; x \in V\}$
- Derived Quantities (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008)):
  $i.e)\; D = \{\{\varphi(x),\, \frac{\delta \Psi}{\delta \varphi_k}(x),\, \frac{\delta \Psi}{\delta \varphi_{\nabla^k}}(x),\, \frac{\delta \Psi}{\delta \varphi_{\nabla_k}}(x), \ldots\} \;:\; x \in V\}$



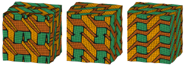
# Graph Theory Formalism

- State Vertices and State Dimensions: $V = \{1, 2, \ldots, n\}, \quad \chi = \{1, 2, \ldots, p\}$
- State Vector: $X = \{x = \{x^\mu\}_{\mu \in \chi} \ : \ x \in V\}$
  $i.e)\ X = \{x = \{\ \varphi_k,\ \varphi_{\nabla^k},\ \varphi_{\nabla_k}, \Psi, \ldots\}\ :\ x \in V\}$
- State Transition Edges: $E = \{(x, y)\ :\ x, y \in V\}$
- Edge Weights: $w = \{w(x, y)\ :\ (x, y) \in E\}$
- Neighborhoods of Adjacent Vertices:
  $\delta = \{\delta(x) = \{y \in V\ :\ (x, y) \in E\}\ :\ x \in V\}$
- Derived Quantities (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008)):
  $i.e)\ D = \{\{\varphi(x),\ \frac{\delta \Psi}{\delta \varphi_k}(x),\ \frac{\delta \Psi}{\delta \varphi_{\nabla^k}}(x),\ \frac{\delta \Psi}{\delta \varphi_{\nabla_k}}(x), \ldots\}\ :\ x \in V\}$

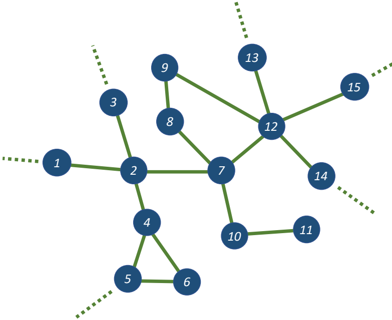


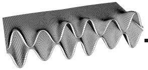


# Graph Theory Formalism

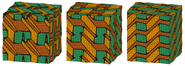


- State Vertices and State Dimensions: $V = \{1, 2, \ldots, n\}, \quad \chi = \{1, 2, \ldots, p\}$
- State Vector: $X = \{x = \{x^\mu\}_{\mu\in\chi} \ : \ x \in V\}$
  *i.e)* $X = \{x = \{\ \varphi_k,\ \varphi_{\nabla^k},\ \varphi_{\nabla_k}, \Psi, \ldots\} \ : \ x \in V\}$
- State Transition Edges: $E = \{(x, y) \ : \ x, y \in V\}$
- Edge Weights: $w = \{w(x, y) \ : \ (x, y) \in E\}$
- Neighborhoods of Adjacent Vertices:
  $\delta = \{\delta(x) = \{y \in V \ : \ (x, y) \in E\} \ : \ x \in V\}$
- Derived Quantities (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008)):
  *i.e)* $D = \{\{\varphi(x),\ \frac{\delta\Psi}{\delta\varphi_k}(x),\ \frac{\delta\Psi}{\delta\varphi_{\nabla^k}}(x),\ \frac{\delta\Psi}{\delta\varphi_{\nabla_k}}(x), \ldots\} \ : \ x \in V\}$





# Graph Theory Formalism



- State Vertices and State Dimensions: $V = \{1, 2, \ldots, n\}, \quad \chi = \{1, 2, \ldots, p\}$

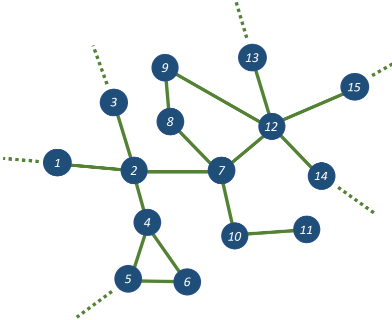
- State Vector: $X = \{x = \{x^{\mu}\}_{\mu \in \chi} \ : \ x \in V\}$
  *i.e)* $X = \{x = \{\ \varphi_k,\ \varphi_{\nabla^k},\ \varphi_{\nabla_k}, \Psi, \ldots\}\ :\ x \in V\}$

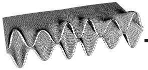
- State Transition Edges: $E = \{(x, y)\ :\ x, y \in V\}$

- Edge Weights: $w = \{w(x, y)\ :\ (x, y) \in E\}$

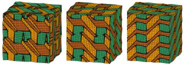
- Neighborhoods of Adjacent Vertices:
  $\delta = \{\delta(x) = \{y \in V\ :\ (x, y) \in E\}\ :\ x \in V\}$

- Derived Quantities (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008)):
  *i.e)* $D = \{\{\varphi(x), \frac{\delta\Psi}{\delta\varphi_k}(x), \frac{\delta\Psi}{\delta\varphi_{\nabla^k}}(x), \frac{\delta\Psi}{\delta\varphi_{\nabla_k}}(x), \ldots\}\ :\ x \in V\}$

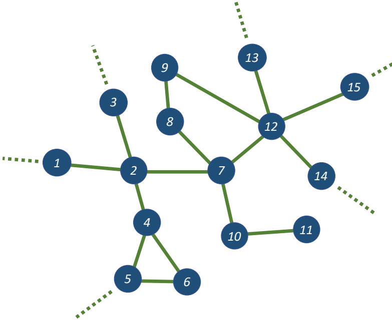




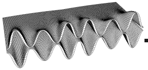
# Graph Theory Formalism



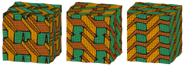
- State Vertices and State Dimensions: $V = \{1, 2, \ldots, n\}, \quad \chi = \{1, 2, \ldots, p\}$
- State Vector: $X = \{x = \{x^\mu\}_{\mu \in \chi} \ : \ x \in V\}$
  *i.e)* $X = \{x = \{\ \varphi_k,\ \varphi_{\nabla^k},\ \varphi_{\nabla_k}, \Psi, \ldots\}\ :\ x \in V\}$
- State Transition Edges: $E = \{(x, y)\ :\ x, y \in V\}$
- Edge Weights: $w = \{w(x, y)\ :\ (x, y) \in E\}$
- Neighborhoods of Adjacent Vertices:
  $\delta = \{\delta(x) = \{y \in V\ :\ (x, y) \in E\}\ :\ x \in V\}$



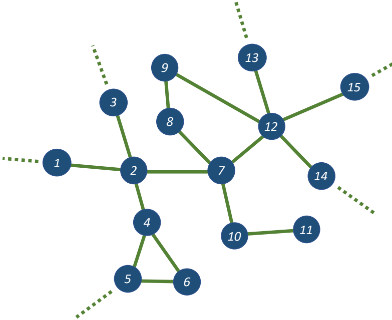

- Derived Quantities (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008)):
  *i.e)* $D = \{\{\varphi(x),\ \frac{\delta\Psi}{\delta\varphi_k}(x),\ \frac{\delta\Psi}{\delta\varphi_{\nabla^k}}(x),\ \frac{\delta\Psi}{\delta\varphi_{\nabla_k}}(x), \ldots\}\ :\ x \in V\}$



# Graph Theory Formalism



- State Vertices and State Dimensions: $V = \{1, 2, \ldots, n\}, \quad \chi = \{1, 2, \ldots, p\}$
- State Vector: $X = \{x = \{x^\mu\}_{\mu\in\chi} \ : \ x \in V\}$
  *i.e)* $X = \{x = \{\ \varphi_k,\ \varphi_{\nabla^k},\ \varphi_{\nabla_k}, \Psi, \ldots\}\ :\ x \in V\}$
- State Transition Edges: $E = \{(x, y)\ :\ x, y \in V\}$
- Edge Weights: $w = \{w(x, y)\ :\ (x, y) \in E\}$
- Neighborhoods of Adjacent Vertices:
  $\delta = \{\delta(x) = \{y \in V\ :\ (x, y) \in E\}\ :\ x \in V\}$



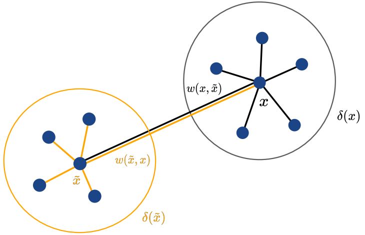

- Derived Quantities (Gilboa and Osher, *Multiscale Model. Simul.*, **7** (2008)):
  *i.e)* $D = \{\{\varphi(x),\ \frac{\delta\Psi}{\delta\varphi_k}(x),\ \frac{\delta\Psi}{\delta\varphi_{\nabla^k}}(x),\ \frac{\delta\Psi}{\delta\varphi_{\nabla_k}}(x), \ldots\}\ :\ x \in V\}$

Partial derivatives, where $z = x - \tilde{x} \sim O(h)$:

$$\frac{\delta \varphi(\tilde{x})}{\delta x^\mu} \equiv \sum_{x \in \delta(\tilde{x})} \frac{\varphi(x) - \varphi(\tilde{x})}{z^\mu} w(\tilde{x}, x) \tag{10}$$

Partial derivatives, where $z = x - \tilde{x} \sim O(h)$:

$$\frac{\delta \varphi(\tilde{x})}{\delta x^{\mu}} \equiv \sum_{x \in \delta(\tilde{x})} \frac{\varphi(x) - \varphi(\tilde{x})}{z^{\mu}} w(\tilde{x}, x) \tag{10}$$

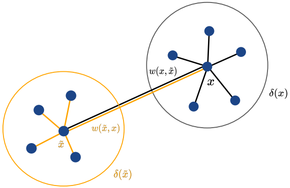


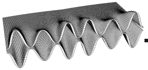
Partial derivatives, where $z = x - \tilde{x} \sim O(h)$:

$$\frac{\delta \varphi(\tilde{x})}{\delta x^{\mu}} \equiv \sum_{x \in \delta(\tilde{x})} \frac{\varphi(x) - \varphi(\tilde{x})}{z^{\mu}} w(\tilde{x}, x) \tag{10}$$

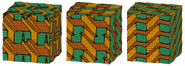
Modified $k$-order Taylor series based at $\tilde{x}$:

$$\begin{aligned} \varphi^{(k)}(x|\tilde{x}) &= \varphi(\tilde{x}) + \sum_{\mu \in \chi} \gamma^{\mu} \frac{\delta \varphi(\tilde{x})}{\delta x^{\mu}} z^{\mu} \\ &\quad + \frac{1}{2!} \sum_{\mu, \nu \in \chi} \gamma^{\mu\nu} \frac{\delta^2 \varphi(\tilde{x})}{\delta x^{\mu} \delta x^{\nu}} z^{\mu\nu} \\ &\quad + \cdots \end{aligned} \tag{11}$$





# Consistency of Modified Taylor Series



Given a $k$-order model, an $r$-order accurate *stencil* yields as $h \to 0$:
The *non-local derivatives* scale as

$$\frac{\delta^l \varphi(\tilde{x})}{\delta x^l} \to \frac{\partial^l \varphi(\tilde{x})}{\partial x^l} + O(h^{r+1-l}) \ , \tag{12}$$

the *linear coefficients* scale as

$$\gamma_l \to 1 + O(h^{\min(k,r)+1-l}) \ , \tag{13}$$

and so the *model error* scales as

$$\varphi^{(k)}(x|\tilde{x}) \to \varphi(x) + O(h^{\min(k,r)+1}) \ , \tag{14}$$

which corresponds with Sobolev interpolation error.

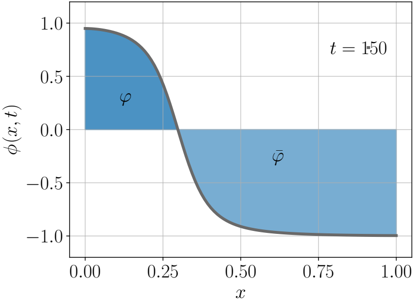
1. Systems of Interest

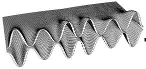
2. Graph Theoretic Approaches

3. Applications

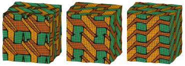
# Evolution of Diffusing Fields

$$\text{Local: } \frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \psi}{\delta \phi} \quad \longrightarrow \quad \text{Global: } \frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$



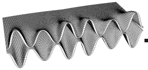


# Evolution of Diffusing Fields

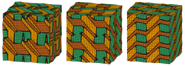


$$\text{Local: } \frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \psi}{\delta \phi} \quad \longrightarrow \quad \text{Global: } \frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

- Specify Landau potential:
  $f(\phi) = -\phi^2(\xi^2 - \phi^2) \;\rightarrow\; \psi = f(\phi) + \lambda|\nabla \phi|^2$
- Specify local material parameters:
  $M_\phi,\ \lambda,\ \xi,$ BCs, ICs, $\ldots$
- Solve system for $N$ trajectories:
  $\mathscr{D}_j = \{\varphi_k, \varphi_{\nabla^2}, \Psi, \frac{\delta \Psi}{\delta \varphi}, \ldots\}^{(j)}$
- Choose global model basis:
  $v = \{\varphi_k, \varphi_{\nabla^2}, F, F',\ \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}'\}$
  $M_\varphi = \sum_\alpha \gamma^\alpha v_\alpha, \qquad \tilde{\mu}_\varphi = \sum_\beta \gamma^\beta v_\beta$



# Evolution of Diffusing Fields



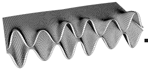
$$\text{Local: } \frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \psi}{\delta \phi} \quad \longrightarrow \quad \text{Global: } \frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

- Specify Landau potential:
  $f(\phi) = -\phi^2(\xi^2 - \phi^2) \;\to\; \psi = f(\phi) + \lambda|\nabla\phi|^2$

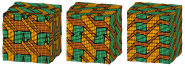
- Specify local material parameters:
  $M_\phi,\ \lambda,\ \xi,$ BCs, ICs, …

- Solve system for $N$ trajectories:
  $\mathscr{D}_j = \{\varphi_k, \varphi_{\nabla^2}, \Psi, \frac{\delta\Psi}{\delta\varphi}, \ldots\}^{(j)}$

- Choose global model basis:
  $v = \{\varphi_k, \varphi_{\nabla^2}, F, F',\ \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}'\}$
  $M_\varphi = \sum_\alpha \gamma^\alpha v_\alpha, \qquad \tilde{\mu}_\varphi = \sum_\beta \gamma^\beta v_\beta$



# Evolution of Diffusing Fields



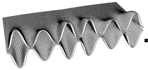
$$\text{Local: } \frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \psi}{\delta \phi} \quad \longrightarrow \quad \text{Global: } \frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

- Specify Landau potential:
  $f(\phi) = -\phi^2(\xi^2 - \phi^2) \ \rightarrow \ \psi = f(\phi) + \lambda|\nabla \phi|^2$

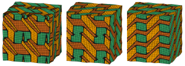
- Specify local material parameters:
  $M_\phi, \ \lambda, \ \xi,$ BCs, ICs, ...

- Solve system for $N$ trajectories:
  $\mathscr{D}_j = \{\varphi_k, \varphi_{\nabla^2}, \Psi, \frac{\delta \Psi}{\delta \varphi}, \ldots\}^{(j)}$

- Choose global model basis:
  $v = \{\varphi_k, \varphi_{\nabla^2}, F, F', \ \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}'\}$
  $M_\varphi = \sum_\alpha \gamma^\alpha v_\alpha, \qquad \tilde{\mu}_\varphi = \sum_\beta \gamma^\beta v_\beta$



# Evolution of Diffusing Fields



$$\text{Local: } \frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \psi}{\delta \phi} \quad \longrightarrow \quad \text{Global: } \frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

- Specify Landau potential:
  $f(\phi) = -\phi^2(\xi^2 - \phi^2) \;\rightarrow\; \psi = f(\phi) + \lambda|\nabla\phi|^2$
- Specify local material parameters:
  $M_\phi,\; \lambda,\; \xi,\;$ BCs, ICs, $\ldots$
- Solve system for $N$ trajectories:
  $\mathscr{D}_j = \{\varphi_k, \varphi_{\nabla^2}, \Psi, \frac{\delta\Psi}{\delta\varphi}, \ldots\}^{(j)}$
- Choose global model basis:
  $v = \{\varphi_k, \varphi_{\nabla^2}, F, F',\; \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}'\}$
  $M_\varphi = \sum_\alpha \gamma^\alpha v_\alpha, \qquad \tilde{\mu}_\varphi = \sum_\beta \gamma^\beta v_\beta$

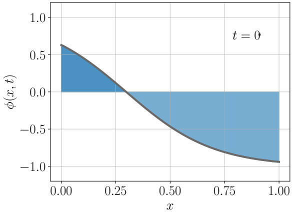



Figure 1: Field evolution for specific material parameters.

# Evolution of Diffusing Fields

$$\text{Local: } \frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \psi}{\delta \phi} \quad \longrightarrow \quad \text{Global: } \frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

- Specify Landau potential:
  $f(\phi) = -\phi^2(\xi^2 - \phi^2) \ \rightarrow \ \psi = f(\phi) + \lambda|\nabla\phi|^2$
- Specify local material parameters:
  $M_\phi,\ \lambda,\ \xi,$ BCs, ICs, …
- Solve system for $N$ trajectories:
  $\mathscr{D}_j = \{\varphi_k, \varphi_{\nabla^2}, \Psi, \frac{\delta\Psi}{\delta\varphi}, \ldots\}^{(j)}$
- Choose global model basis:
  $v = \{\varphi_k, \varphi_{\nabla^2}, F, F',\ \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}'\}$
  $M_\varphi = \sum_\alpha \gamma^\alpha v_\alpha, \qquad \tilde{\mu}_\varphi = \sum_\beta \gamma^\beta v_\beta$

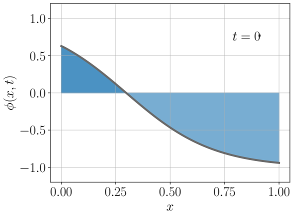



Figure 1: Field evolution for specific material parameters.

# Stepwise Regression

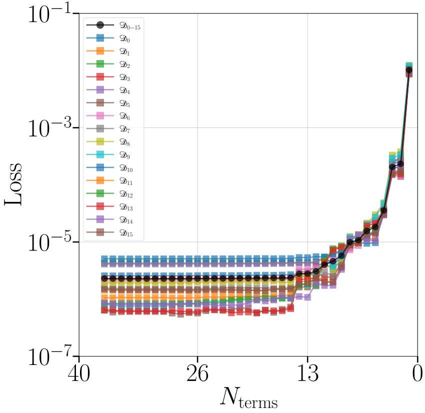



Figure 2: Loss curves as model becomes more parsimonious.

# Stepwise Regression

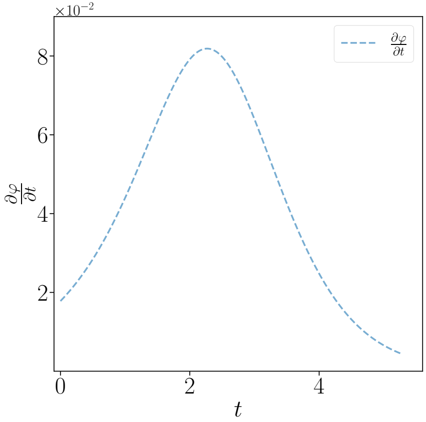



Figure 3: Fitted dynamics for $\mathscr{D}_5$ as model becomes more parsimonious.

# Stepwise Regression

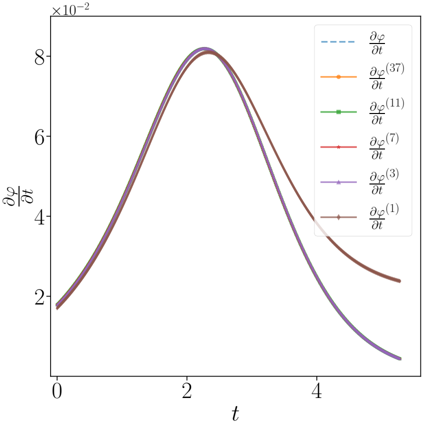



Figure 3: Fitted dynamics for $\mathscr{D}_5$ as model becomes more parsimonious.

# Stepwise Regression

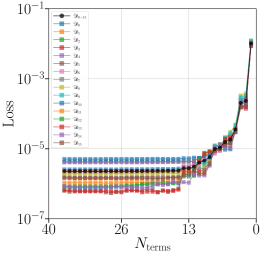



Figure 2: Loss curves.

$$\frac{\partial \varphi}{\partial t} = -M_{\varphi}\frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_{\varphi}$$

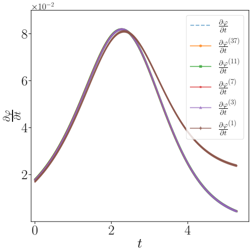



Figure 3: Fitted dynamics for $\mathscr{D}_5$.

# Stepwise Regression

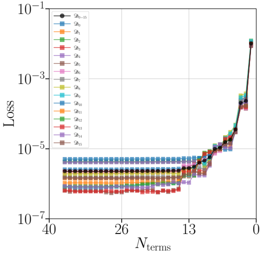



Figure 2: Loss curves.

$$\frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

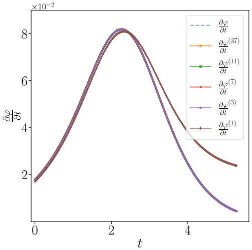
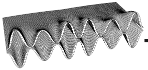


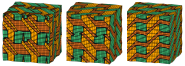

Figure 3: Fitted dynamics for $\mathscr{D}_5$.

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2} + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_{\nabla^2}}\varphi_{\nabla^2}$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$



# Stepwise Regression



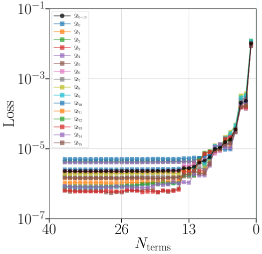



Figure 2: Loss curves.

$$\frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

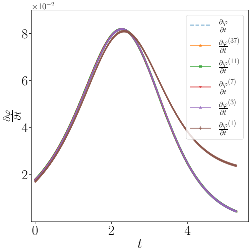



Figure 3: Fitted dynamics for $\mathscr{D}_5$.

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2} + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_{\nabla^2}}\varphi_{\nabla^2}$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2}$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

# Stepwise Regression

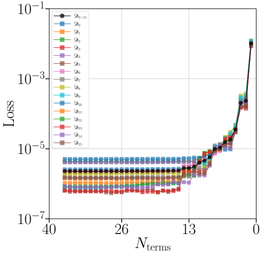



Figure 2: Loss curves.

$$\frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

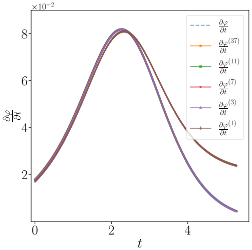



Figure 3: Fitted dynamics for $\mathscr{D}_5$.

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2} + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_{\nabla^2}}\varphi_{\nabla^2}$$

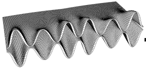
$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2}$$

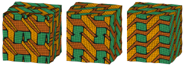
$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$



# Stepwise Regression



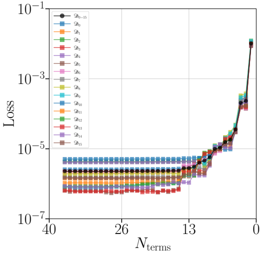



Figure 2: Loss curves.

$$\frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

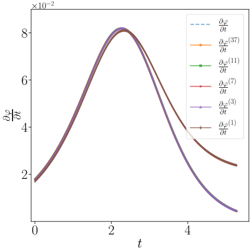



Figure 3: Fitted dynamics for $\mathscr{D}_5$.

$$M_\varphi = \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi}\varphi + \gamma^{\frac{\delta \Psi}{\delta \varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2} + \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi_{\nabla^2}}\varphi_{\nabla^2}$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi}\varphi + \gamma^{\frac{\delta \Psi}{\delta \varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2}$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi}\varphi$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta \Psi}{\delta \varphi}\varphi_3}\varphi_3$$

$$\tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

# Stepwise Regression

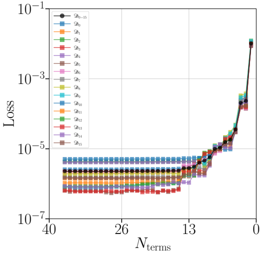



Figure 2: Loss curves.

$$\frac{\partial \varphi}{\partial t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \tilde{\mu}_\varphi$$

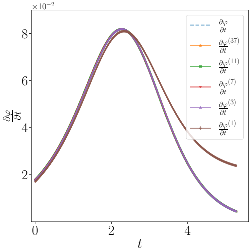



Figure 3: Fitted dynamics for $\mathscr{D}_5$.

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2} + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_{\nabla^2}}\varphi_{\nabla^2} \qquad \tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi + \gamma^{\frac{\delta\Psi}{\delta\varphi}\bar{\varphi}_{\nabla^2}}\bar{\varphi}_{\nabla^2} \qquad \tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 + \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi}\varphi \qquad \tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

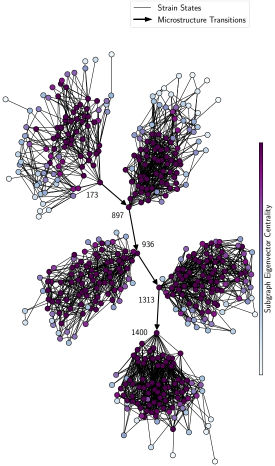
$$M_\varphi = \gamma^{\frac{\delta\Psi}{\delta\varphi}\varphi_3}\varphi_3 \qquad \tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

$$M_\varphi = 0 \qquad \tilde{\mu}_\varphi = \gamma^{F'}F' + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2} + \gamma^{\varphi_3}\varphi_3 + \gamma^{\varphi_4}\varphi_4 + \gamma^{\bar{\varphi}_5}\bar{\varphi}_5 + \gamma^{\bar{\varphi}_2}\bar{\varphi}_2 + \gamma^{\bar{\varphi}_4}\bar{\varphi}_4$$

# Summary

- Taken's theorem shows existence of *embeddings* of high dimensional dynamical systems
- Constraining non-locality of operators ensures *consistency* of model
- Reduced order models can be computed using physical ansatz and a *basis* of operators
- Interpretation of reduced order model is very *basis-dependent*
- Very *general* framework for many physical systems

# Thank you!




Computational Physics Group:

Dr. Krishna Garikipati
Dr. Xiaoxuan Zhang
Dr. Zhenlin Wang
Dr. Greg Teichert
Liz Livingston
Siddhartha Srivastava

Collaborators:

Dr. Brendan Kochunas
Dean Price
Thomas Folk