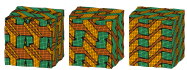
Reduced Order Models Using Non-local Calculus on Unstructured Weighted Graphs



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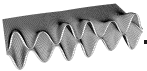
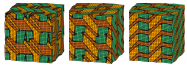
University of Michigan, Ann Arbor

US National Congress on Theoretical and Applied Mechanics

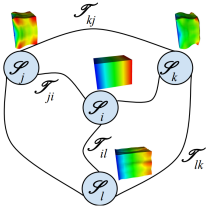
MICDE



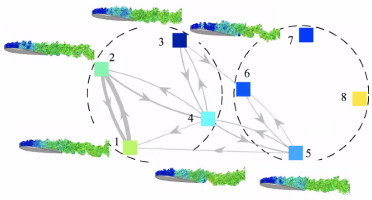
Graphs for Scientific computing



- Representing Physical systems on graph

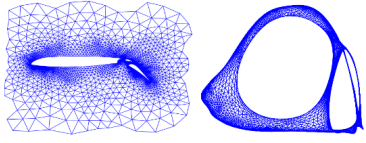


Computational Physics group (UM)

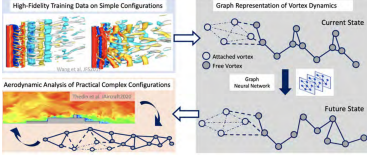


Nair's group (UNevada Reno)

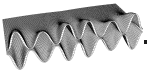
- Computations on graph



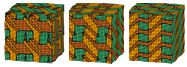
Spielman's group (Yale)



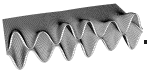
APUS Lab (Penn State)



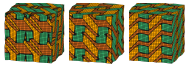
Outline



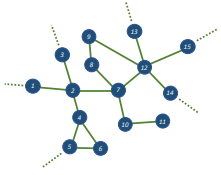
- Representation of physical systems on a graph
- Non-local calculus on a graph
- Reduced order modeling on a graph



Graphs for Scientific computing



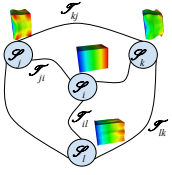
- A mathematical Graph is a collection of a vertices and edges.
- Graph-theoretic representation of physical system involves following abstraction:
  - Physical solution as vertex
  - Transition between solution as edge



Mathematical Graph

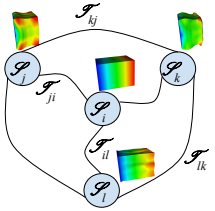
$$
\begin{aligned}
\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{f} &= \boldsymbol{0}, && \text{in} && \Omega \\
\boldsymbol{u} &= \overline{\boldsymbol{u}}(\boldsymbol{p}), && \text{on} && \partial\Omega_u \\
\boldsymbol{\sigma}\boldsymbol{n} &= \boldsymbol{\sigma}_{\boldsymbol{n}}(\boldsymbol{p}), && \text{on} && \partial\Omega_\sigma .
\end{aligned}
$$

Physical System



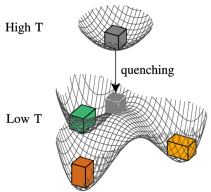
Physical Graph

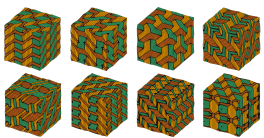
- States $\mathscr{S}_i$, $i = 1, \ldots N$ obtained for parameter sets $\boldsymbol{p}_i$, boundary conditions $\overline{\boldsymbol{u}}_i, \boldsymbol{\sigma}_{n_i}$; (non)linear solution step or change in a "transition quantity" over $\mathscr{S}_j \rightarrow \mathscr{S}_i$ is $\mathscr{T}_{ij}$
- $G(V, E)$ can be constructed s.t. $V = \{\mathscr{S}_i\}_{i=1,\ldots N}$ and $E = \{\mathscr{T}_{ij}\}_{i,j=1,\ldots N}$



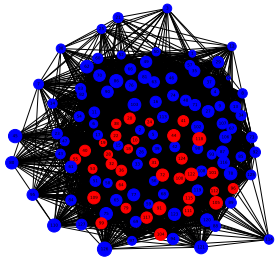
- $G(V, E)$ is connected if every $\mathscr{S}_i$ can be reached from some $\mathscr{S}_j$ along edge $\mathscr{T}_{ij}$; unconnected if solution scheme or transition quantity leaves an isolated state
- Stationary systems as BVPS
  - Reversibility of linear, non-dissipative systems $\implies$ undirected graphs.
  - All admissible states are accessible $\implies$ fully connected graph.

- Numerical computation is facilitated by considering additional structures like **edge weights**. For instance, Low dimensional embeddings (Encoders) can be used to study communities of proximal solutions.

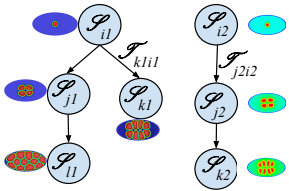




Solutions of a non-convex elastic model



Dissipative dynamical systems represented as graphs



States parameterized by time; *cannot be revisited*; $\mathscr{T}_{ij}$ represents the time step $[t_j, t_i]$ and change in transition quantity

- *Loss of time reversal symmetry* $\implies$ Directed graphs.
- Only one path to a state $\implies$ Graphs are trees
- Second law defines "entropy quantities":
  $\dot{f}(\boldsymbol{u}) \geq 0$, or $\dot{f}(\boldsymbol{u}) \leq 0$, $\dot{\alpha}^B \geq 0$, or $\dot{\alpha}^B \leq 0$. States of dissipative dynamical systems must contain entropy quantities

- Precipitate nucleation and growth driven by Allen-Cahn equation (Teichert & KG, 2018)
- Graph for shape features of precipitate and the free energy.

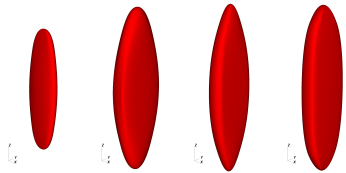
$$\boldsymbol{x}_i = (a_i, b_i, c_i, t_{1_i}, \ldots, t_{8_i}, c_{\mathrm{p}_i}), \quad \mathscr{S}_i = (\boldsymbol{x}_i, \Pi(\boldsymbol{x}_i))$$

a_i, b_i, c_i : bounding box for precipitate

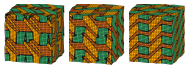
$t_1 \cdots t_8$: Spline control points

c_{p_i} : Alloy concentration

Π : Total free energy of the state



Choices of weights on a graph



$$\boldsymbol{x}_i = (a_i, b_i, c_i, t_{1_i}, \ldots, t_{8_i}, c_{\mathrm{p}_i}), \quad \mathscr{S}_i = (\boldsymbol{x}_i, \Pi(\boldsymbol{x}_i))$$

- Many possibilities for prescribing the graph weights.
- Physical laws induces some choices of weights:

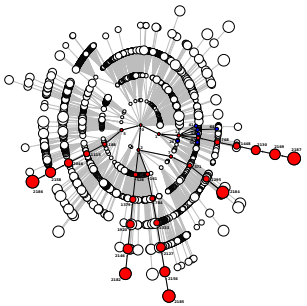
$$\text{Graph chemical potential: } \mu_{i,j} = \frac{\Pi_i - \Pi_j}{\|\boldsymbol{x_i} - \boldsymbol{x_j}\|}$$

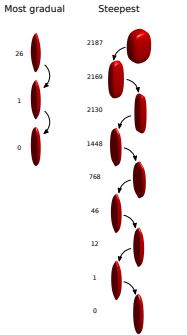
- Graph time of transition

$$\Delta\tau_{ij} \sim \frac{\|\boldsymbol{x_i} - \boldsymbol{x_j}\|}{|\mu_{i,j}|}$$

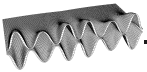
(1) Can we estimate weights in an unsupervised way?
(2) Can we estimate derivatives on graph?

$$\mu = \frac{\partial \Pi}{\partial x}$$

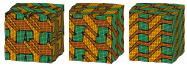




Graph chemical potential induces edges when supplemented by the maximum dissipation principle (alternatively, steepest descent)



Outline



- Representation of physical systems on a graph
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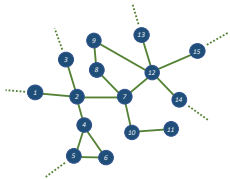
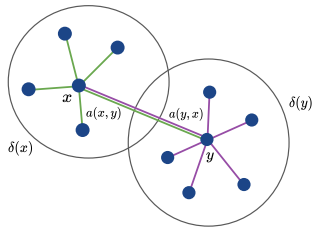
- Representing data on graphs, $G(V, E)$
  - Each vertex has state $(\boldsymbol{x}, \varphi(\boldsymbol{x}))$ representing input/output data.
  - Edges with weights, with possibly multiple edges between vertices.
- G. Gilboa, S. Osher, *Multiscale Modeling & Simulation* (2009), introduced a non-local calculus on Graphs e.g.
  - Non-local gradient operator,
  - Inner product on scalars over vertices,
  - Contraction of vectors on the vertices,
  - Partial derivatives
- First order partial derivatives estimated as:

$$\frac{\delta\varphi}{\delta x^\mu}(x) = \frac{1}{|\mathcal{N}_x|} \sum_{(x,y)\in E} \frac{\varphi(y) - \varphi(x)}{y^\mu - x^\mu} \overline{w}^\mu(x, y)$$

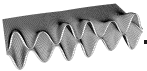
  - $\overline{w}^\mu$ are dimensionless weights
  - Directed Edges: $\overline{w}^\mu(x, y) \neq \overline{w}^\mu(y, x)$
  - Multidimensional edge weights
- Edge Weights prescribed using simple functions like Gaussians[1] and Discrete weights[2]



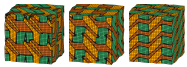


[1] M. Duschenes, K. Garikipati, *arXiv:2105.01740*

[2] M. Duschenes, S. Srivastava, K. Garikipati, *arXiv:2205.02206*



Error in the estimation of derivatives



- Can we find the weights, $\overline{w}^{\mu}$ such that $e \sim \mathcal{O}(h^k)$

$$e(x) = \left| \frac{\delta \varphi}{\delta x} - \frac{\partial \varphi}{\partial x} \right|$$

Yes, with discrete weights[1]. Extendable to higher dimensions and higher order derivatives

Proof by construction – provides an algorithm for estimating these weights

- Key Idea (1D version): Expand non-local derivative definitions in a Taylor series about $\widetilde{x}$:

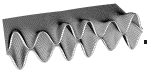
$$\frac{\delta \varphi}{\delta x}(\widetilde{x}) = \frac{1}{|\mathcal{N}_{\widetilde{x}}|} \sum_{(\widetilde{x},x)\in E} \frac{\varphi(x) - \varphi(\widetilde{x})}{x - \widetilde{x}} \overline{w}^{\mu}(\widetilde{x}, x)$$

$$= \sum_{s=0}^{\infty} \frac{1}{(s+1)!} \frac{\partial^{s+1}\varphi}{\partial x^{s+1}}(\widetilde{x}) \sum_{x\in\mathcal{N}(\widetilde{x})} (x - \widetilde{x})^s \overline{w}(x - \widetilde{x}).$$

Then the weights can be found from solving the linear system of equations of the first k moments:

$$\sum_{\mathcal{N}(\widetilde{x})} (x - \widetilde{x})^s \overline{w}(x - \widetilde{x}) = \delta_{0s} \quad s = \{0, \ldots, k-1\} \implies \frac{\delta \varphi}{\delta x} - \frac{\partial \varphi}{\partial x} = \underbrace{\sum_{s=k}^{\infty} \frac{1}{(s+1)!} \frac{\partial^{s+1}\varphi}{\partial x^{s+1}}(\widetilde{x}) \sum_{x\in\mathcal{N}(\widetilde{x})} (x - \widetilde{x})^s \overline{w}(x - \widetilde{x})}_{\mathcal{O}(h^k)}.$$

[1] M. Duschenes, S. Srivastava, K. Garikipati, *arXiv:2205.02206*



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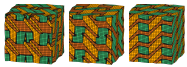


- Key idea continued: Can these constraints be solved ?

$$\sum_{\mathcal{N}(\widetilde{x})} (x-\widetilde{x})^s \overline{w}(x-\widetilde{x}) = \delta_{0s} \quad s = \{0,\ldots,k-1\}$$

- Yes! Rewriting in matrix form:

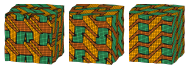
$$\underbrace{\begin{bmatrix} \uparrow & \uparrow & \cdots & \uparrow \\ 1 & (x-\widetilde{x}) & \cdots & (x-\widetilde{x})^{k-1} \\ \downarrow & \downarrow & \cdots & \downarrow \end{bmatrix}_{|\mathcal{N}(\widetilde{x})|\times k}}_{\mathbf{V}}{}^{T} \underbrace{\begin{bmatrix} \uparrow \\ \overline{w}(x,\widetilde{x}) \\ \downarrow \end{bmatrix}_{|\mathcal{N}(\widetilde{x})|\times 1}}_{\overline{\mathbf{w}}} = \underbrace{\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}_{k\times 1}}_{\mathbf{e}_1}$$

$$\boxed{\overline{\mathbf{w}} = (\mathbf{V}\mathbf{V}^T)^{-1}\mathbf{V}\mathbf{e}_1}$$

Pseudo-inverse is well-defined as long as points, $(\widetilde{x}, x_1, \cdots, x_{|\mathcal{N}|})$ are distinct.

- Same idea (with some more tricks) can be applied for higher derivatives in a multidimensional setting.

Numerical results: Error analysis



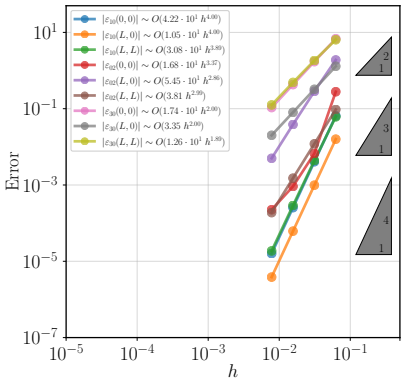
- Error in derivatives as a function of data length scale h
- Interpolation study with data from 2d polynomial of order 6 on a 2D grid.
- Modeled using a 3^{rd} order **Taylor-like expansion** about training points based on non-local derivatives.

$$\varphi(x,y) = \varphi(\mathbf{0}) + \frac{\delta\varphi}{\delta x}(\mathbf{0})x + \frac{\delta\varphi}{\delta y}(\mathbf{0})y + \frac{1}{2}\frac{\delta^2\varphi}{\delta x^2}(\mathbf{0})x^2 + \cdots$$

- Desired accuracy of $\mathcal{O}(h^4)$ is imposed in the pointwise model error.
- The model is required to be trained with stencils corresponding to following errors in partial derivatives.

$$e_{lm}(x,y) \sim \mathcal{O}(h^{5-l-m}), \quad l+m = \{1,2,3\}$$

for derivatives of order l, m with respect to $\{x, y\}$



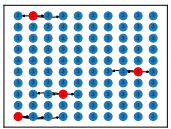
- Provided data $(x, \varphi(x))$, and an order k:
  - Construct a graph (define edges)
  - Estimate weights

  such that the non local derivative:

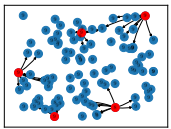
$$\frac{\delta\varphi}{\delta x^\mu}(x) = \frac{1}{|\mathcal{N}_x|} \sum_{(x,y)\in E} \frac{\varphi(y) - \varphi(x)}{y^\mu - x^\mu} \overline{w}^\mu(x, y)$$

  has the property

$$\left| \frac{\delta\varphi}{\delta x} - \frac{\partial\varphi}{\partial x} \right| \longrightarrow \mathcal{O}(h^k)$$

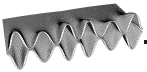


(a) Uniform data with constant integer spacing.



(b) Unstructured data with random spacing.

Figure: 2D graph with 3 order accurate scheme for derivative along horizontal direction



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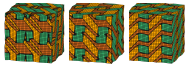

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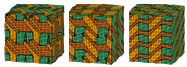
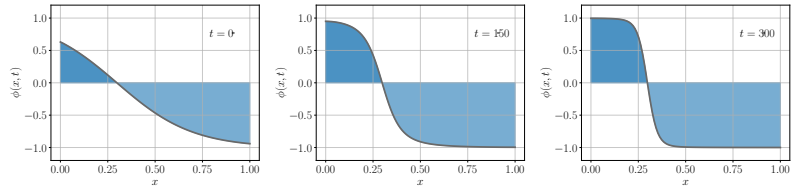
- Reduced order modeling on a graph

Reduced Order Model: Model of interest

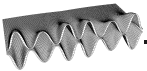


- Gradient flow: $$\frac{\partial \phi}{\partial t} = -M_\phi \frac{D\psi}{D\phi}, \qquad \psi = f(\phi) + \lambda |\nabla \phi|^2$$
- Specify Landau potential: $f(\phi) = -\phi^2(\xi^2 - \phi^2)$
- Specify local material parameters: $M_\phi,\ \lambda,\ \xi,\ \mathrm{BCs},\ \mathrm{ICs}, \ldots$
- Solve system for N trajectories

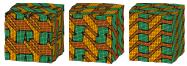


(a) Initial condition. (b) Intermediate solution. (c) Equilibrium solution.

Figure: Field evolution of 1D Allen-Cahn dynamics with $M_\phi = 10^{-3}$ and $\lambda = 1$ at 0, 150, and 300 time steps. A Backward-Euler scheme is used with a time step of $\Delta t = 10^{-2}$.



Reduced Order Model: Global Observables



Guided by the gradient flow of the local quantity ϕ, we expect a global gradient-flow for the observable, $\varphi = \int \phi I_{\phi>0} d\Omega$ to be retained:

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

- Extract global variables from all trajectories: $\mathcal{D}_j = \{\varphi_k, \varphi_{\nabla^2}, \Psi, \frac{\delta \Psi}{\delta \varphi}, \dots\}^{(j)}$
- Global model basis: $M_\varphi, \mathcal{E}_\varphi \in \text{span}\left(\varphi_k, \varphi_{\nabla^2}, F, F',\ \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}', \frac{\delta \Psi}{\delta \varphi_k}, \cdots\right)$

$$\text{Volume averaged quantities: } \Psi = \int_\Omega d\Omega\ \psi\ , \quad F = \int_\Omega d\Omega\ f\ , \cdots$$

$$\text{Phase averaged quantities: } \varphi_k = \frac{1}{\Omega}\int_\Omega d\Omega\ I(\phi)\ \phi^k, \quad \varphi_{\nabla^k} = \frac{1}{\Omega}\int_\Omega d\Omega\ I(\phi)\ \nabla^k \phi\ , \cdots$$

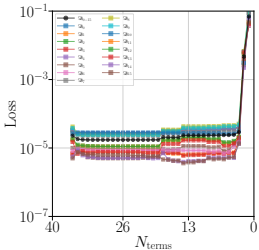
$$\text{Non local derivatives: } \frac{\delta \Psi}{\delta \varphi_k}, \quad \frac{\delta \Psi}{\delta \varphi_{\nabla^k}}, \quad \frac{\delta \Psi}{\delta \varphi_{\nabla_k}}, \quad \cdots$$

Reduced Order Model: Operator Elimination via stepwise regression

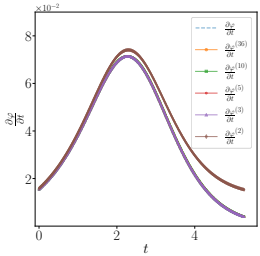
$$\frac{\delta\varphi}{\delta t} = -M_\varphi \frac{\delta \Psi}{\delta \varphi} - \mathcal{E}_\varphi$$

- Train model with a large basis: $M_\varphi, \mathcal{E}_\varphi \in \text{span}\left(\varphi_k, \varphi_{\nabla^2}, F, F', \ \bar{\varphi}_k, \bar{\varphi}_{\nabla^2}, \bar{F}, \bar{F}', \frac{\delta \Psi}{\delta \varphi_k}, \cdots\right)$
- Drop the basis term that causes least change in loss
- Repeat until loss increases drastically.

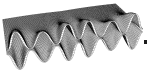
Parameters	M_φ	$\mathcal{E}_\varphi$
4	$\gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2}$	$\gamma^{\varphi}\varphi + \gamma^{\varphi_{3+}}\varphi_{3+} + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2}$
3	0	$\gamma^{\varphi}\varphi + \gamma^{\varphi_{3+}}\varphi_{3+} + \gamma^{\varphi_{\nabla^2}}\varphi_{\nabla^2}$
2	0	$\gamma^{\varphi}\varphi + \gamma^{\varphi_{3+}}\varphi_{3+}$
1	0	$\gamma^{\varphi}\varphi$



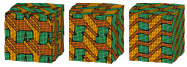
Loss curves



Best fit curve



Conclusion



Representation of Physical System:

- Graph theory offers a framework for representation and analysis of large scale computed solutions.
- The axioms for Physical systems add more mathematical structure to graphs.
- Graph computational techniques can be used to study physical systems.

Non-local calculus on graphs:

- Constraining non-locality of operators ensures consistency of model.
- Multi-dimensional weights on a directed graph

Reduced-order models:

- Reduced order models can be computed using physical ansatz and a basis of operators enriched with non-local derivatives
- Algorithm available in the open-source package `mechanoChemML`: `https://pypi.org/project/mechanoChemML/`

Relevant Publications:

- Graph representation: R. Banerjee, K. Sagiyama, G.H. Teichert, K. Garikipati, CMAME 2019
- Analysis with simple radial functions as weights: M. Duschenes, K. Garikipati, *arXiv:2105.01740*
- Analysis with discrete weights: M. Duschenes, S. Srivastava, K. Garikipati, *arXiv:2105.01740*

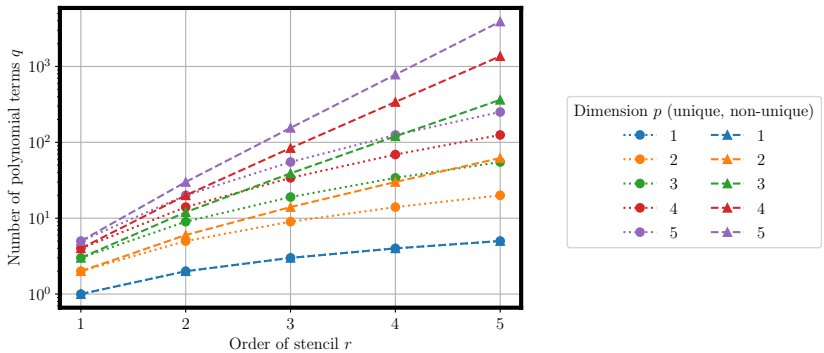
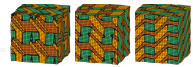


Figure: Number of constraints when considering unique and non-unique terms due to commutativity of multiplication of monomials in each term.

Error in the estimation of higher order derivatives



- Second order derivatives in 1D

$$\frac{\delta^2 u(x)}{\delta x^2} - \frac{\partial^2 u(\widetilde{x})}{\partial x^2} = \sum_{s=r_2}^{\infty} \frac{1}{(s+1)!} \frac{\partial^{s+2} u(\widetilde{x})}{\partial x^{s+2}} \left[\sum_{\mathcal{N}^{(2)}(\widetilde{x})} z(\widetilde{x})^s a^{(2)}(z(\widetilde{x})) \right]$$

$$+ \sum_{s=r_1}^{\infty} \frac{1}{(s+1)!} \frac{\partial^{s+1} u(\widetilde{x})}{\partial x^{s+1}} \left[\sum_{\mathcal{N}^{(2)}(\widetilde{x})} \frac{a^{(2)}(z(\widetilde{x}))}{z(\widetilde{x})} \left[\sum_{\mathcal{N}^{(1)'}(x)} z'(x)^s a^{(1)}(z'(x)) - \sum_{\mathcal{N}^{(1)'}(\widetilde{x})} z'(\widetilde{x})^s a^{(1)}(z'(\widetilde{x})) \right] \right]$$

$$+ \sum_{s=r_1}^{\infty} \sum_{s'=0}^{\infty} \frac{1}{(s+1)!(s'+1)!} \frac{\partial^{s+s'+2} u(\widetilde{x})}{\partial x^{s+s'+2}} \left[\sum_{\mathcal{N}^{(2)}(\widetilde{x})} z(\widetilde{x})^{s'} a^{(2)}(z(\widetilde{x})) \left[\sum_{\mathcal{N}^{(1)'}(x)} z'(x)^s a^{(1)}(z'(x)) \right] \right],$$

Non-commuting second term

M. Duschenes, S. Srivastava, K. Garikipati, *arXiv:2205.02206*