Recent Advances in Model-Order Reduction for Radiation Transport Simulations

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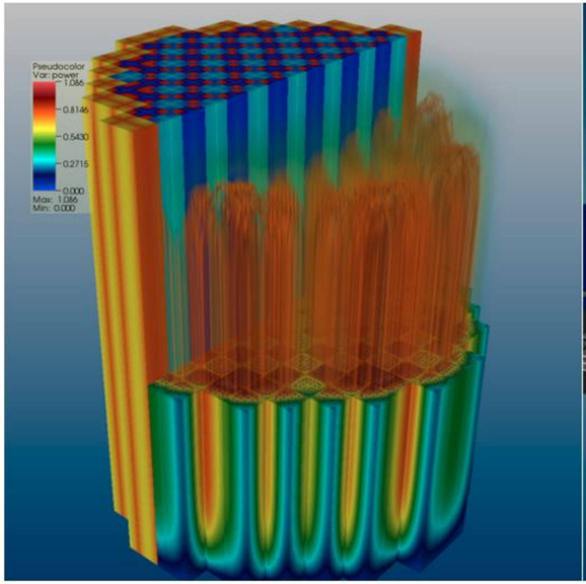
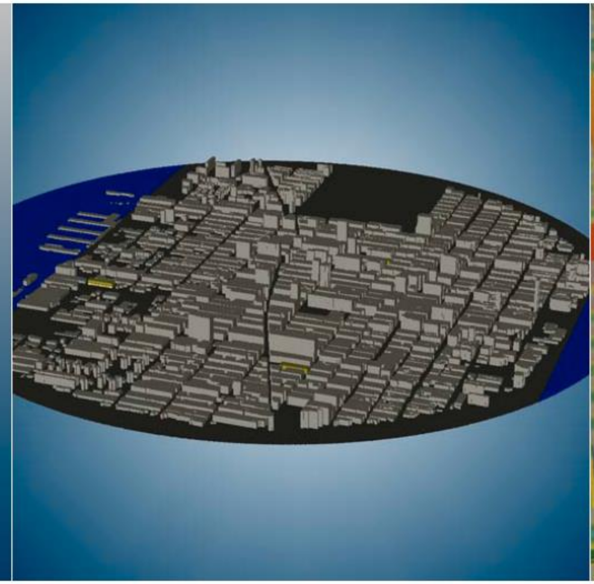
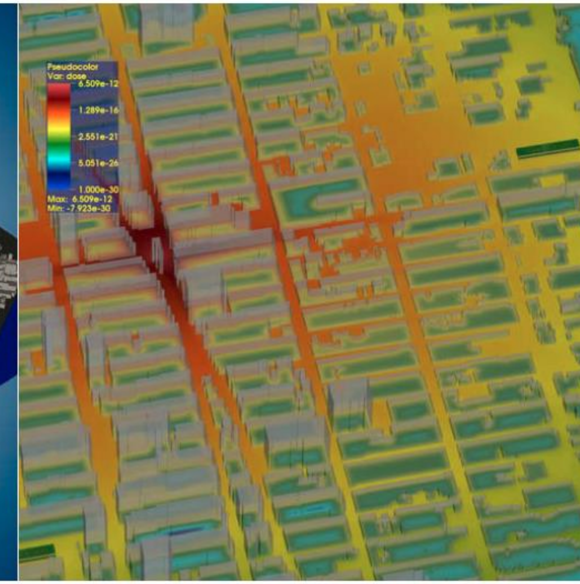
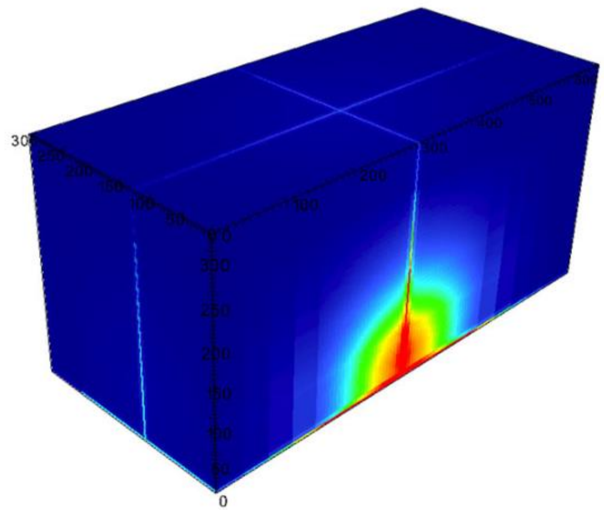
Brown Univ., ICERM Computational Learning for Model Reduction, Jan. 6-10, 2025

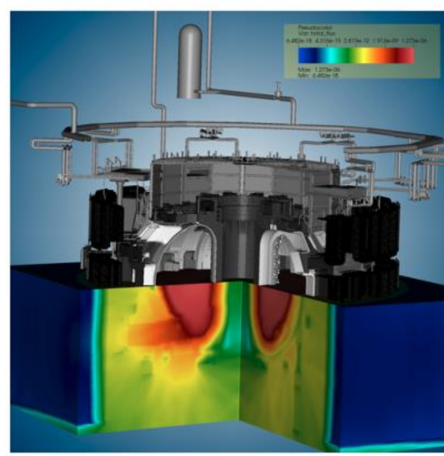
Radiation Transport Is Ubiquitous

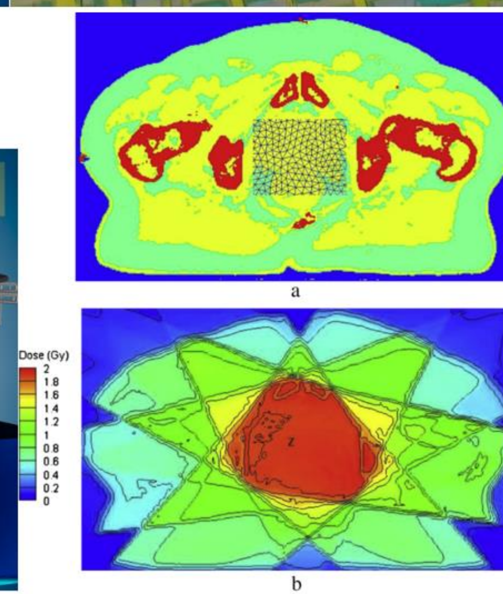












Outline

1. **Background on Radiation Transport**
   - A. *Motivations for (parametric) ROM for Radiation Transport*
   - B. *Crash course on Radiation Transport*

2. **Reduced-Order Models for Radiation Transport**
   - A. *Projection-based pROM:*
     - i. Minimally-invasive approach
     - ii. Affine decomposition of operators
   - B. *Non-intrusive pROM*
     - i. Gaussian process regression, MARS
   - C. *Operator inference for pROM*
     - i. Linear and Nonlinear Frameworks
   - D. *Operator inference for time-dependent ROM (linear manifolds)*
   - E. *Diffusion-based ROM + Discrepancy Emulation (if time permits)*

3. **Conclusions and Outlook**

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3. Conclusions and Outlook

The Linear Boltzmann Transport Equation

- Integro-differential equation

$$\left(\vec{\Omega}\cdot\vec{\nabla}+\sigma_t(\vec{r},E)\right)\Psi(\vec{r},\vec{\Omega},E)=\frac{1}{4\pi}\int_{4\pi}d\Omega'\int dE'\,\sigma_s(\vec{r},E'\to E)\Psi(\vec{r},\vec{\Omega}',E')+S_{\text{fixed}}(\vec{r},\vec{\Omega},E)$$

- Conversation statement in phase space (losses = gains)
- 6-dimensional phase-space: space($\vec{r}$,3)+energy(E,1)+direction($\vec{\Omega}$,2)
- $\Psi(\vec{r},\vec{\Omega},E)$: energy-dependent angular "flux" ("flux" $\rightsquigarrow$ particle/energy density)
- neutral particles = neutrons; photons; coupled neutrons/photons
- can be amended to include time dependence, production from fission

$$\frac{1}{v(E)}\frac{\partial\Psi(t,\vec{r},\vec{\Omega},E)}{\partial t} \qquad \frac{\chi(E)}{4\pi}\int_{4\pi}d\Omega'\int dE'\,\nu\sigma_f(\vec{r},E')\Psi(\vec{r},\vec{\Omega}',E')$$

- can be amended (Boltzmann-Fokker-Planck) for charged particles
- Outcome of particle interactions (cross-section material properties)

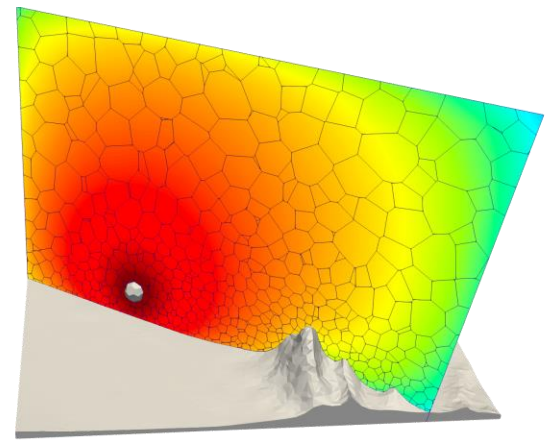
$$\sigma_t(\vec{r},E),\quad \sigma_s(\vec{r},E),\quad \sigma_s(\vec{r},E'\to E)=\sigma_s(\vec{r},E)P_s(E'\to E)$$

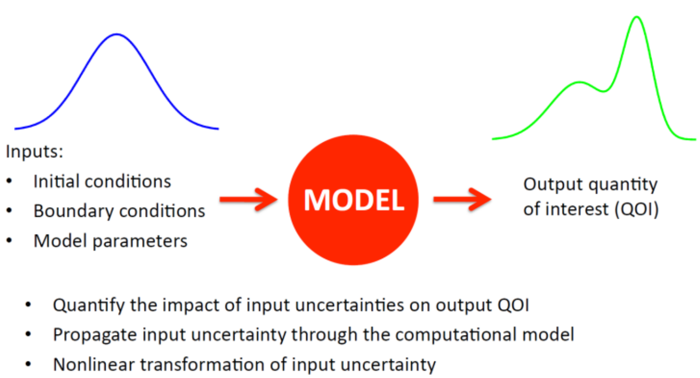
total , scattering, differential scattering = scattering × transfer probability

Parametric Radiation Transport

$$\left(\vec{\Omega}\cdot\vec{\nabla} + \sigma_t(\vec{r},E)\right)\Psi(\vec{r},\vec{\Omega},E) = \frac{1}{4\pi}\int_{4\pi} d\Omega' \int dE'\, \sigma_s(\vec{r},E'\to E)\Psi(\vec{r},\vec{\Omega}',E') + S_{\text{fixed}}(\vec{r},\vec{\Omega},E)$$

- **Parametric full-order model (FOM):**
  - ***Parameters:***
    - **Volumetric + boundary sources**
    - **Material properties (cross sections)**
  - ***Multi-query problems***
    - **Design optimization**
      - *Shielding*
      - *Detection*
      - *Therapeutics*
      - *Power*
    - **Uncertainty Quantification**
      - *Cross-section error*
      - *Manufacturing uncertainty*
    - **Real-time applications**
      - *Reactor monitoring*
      - *Defense applications*
    - **Design of Experiments**
  - ***Ideally suited for parametric ROM (pROM)***





Phase-space Discretization

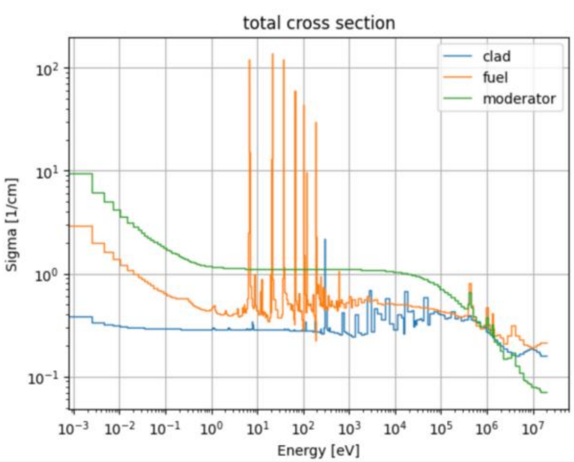
- **Energy variable:** $E \in \mathcal{E} = [0, E_{\max}] = \bigcup_{g=1}^{G} [E_{g+1}, E_g]$
- G: **10's to 100's groups**
- **Introduce** $\Psi^g(\vec{r}, \vec{\Omega}) = \int_{E_{g+1}}^{E_g} dE \; \Psi(\vec{r}, \vec{\Omega}, E)$ **and perform** $\int_{E_{g+1}}^{E_g} dE \; (\text{Transport Eq.})$

$$\left(\vec{\Omega} \cdot \vec{\nabla} + \sigma_t^g(\vec{r})\right) \Psi^g(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi} \sum_{g'=1}^{G} \int_{4\pi} d\Omega' \sigma_s^{g' \to g}(\vec{r}) \Psi^{g'}(\vec{r}, \vec{\Omega}') + S_{\text{fixed}}^g(\vec{r}, \vec{\Omega})$$

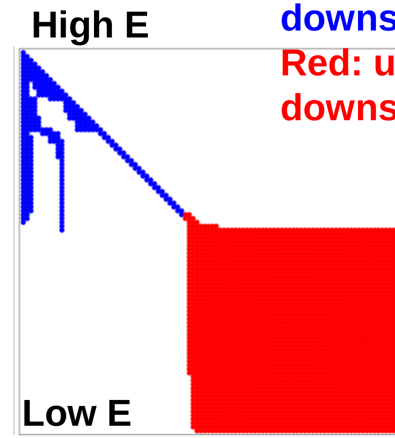
$$1 \leq g \leq G$$

- G **coupled Transport eqs.**
- **Energy coupling occurs on the RHS. LHS is diagonal in groups**

Material properties: log-log scale!



Sparsity pattern of energy transfers:



Blue: only downscatter
Red: up- *and* downscatter

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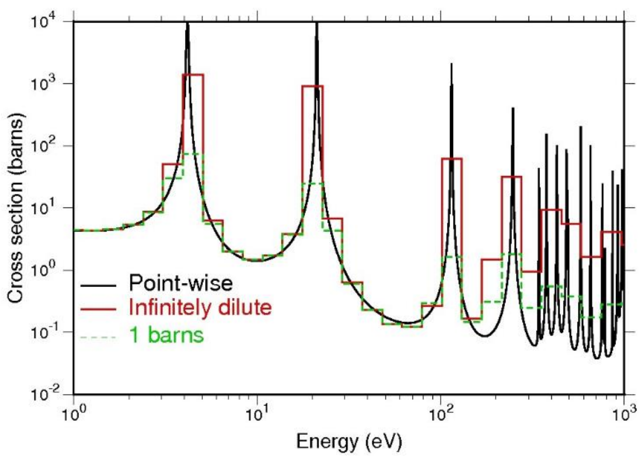

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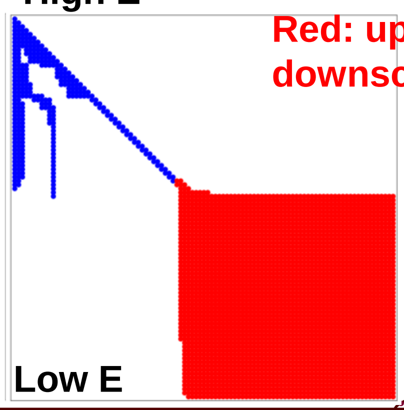

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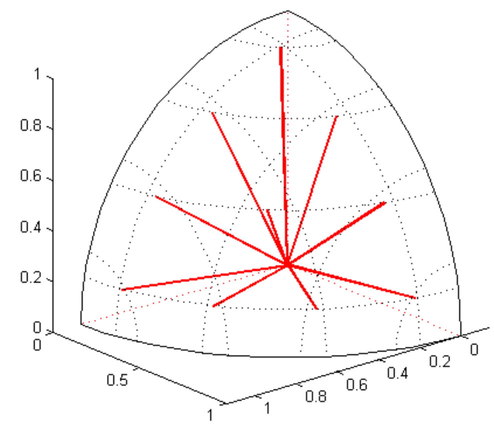
Phase-space Discretization

- **Angular variable:** $\vec{\Omega} \in \mathcal{S}^2$
- **Collocation (angular quadrature)** $\left(w_d, \vec{\Omega}_d\right)_{1\le d\le N_\Omega}$
- N_Ω: **100's to 1000's directions**



- **Solve for** $1 \le g \le G$ **and** $1 \le d \le N_\Omega$

$$\left(\vec{\Omega}_d \cdot \vec{\nabla} + \sigma_t^g(\vec{r})\right)\Psi^g(\vec{r},\vec{\Omega}_d) = \frac{1}{4\pi}\sum_{g'=1}^{G}\sigma_s^{g'\to g}(\vec{r}) \underbrace{\sum_{d'=1}^{N_\Omega} w_{d'}\Psi^{g'}(\vec{r},\vec{\Omega}_{d'})}_{=\Phi^{g'}(\vec{r})} + S^g_{\text{fixed}}(\vec{r},\vec{\Omega}_d)$$

with: $\Psi^g_d(\vec{r}) = \Psi^g(\vec{r},\vec{\Omega}_d)$ **and the angle-integrated solution** $\Phi^g(\vec{r}) = \sum_{d'=1}^{N_\Omega} w_{d'}\Psi^g_{d'}(\vec{r})$

- $G \times N_\Omega$ **coupled Transport eqs.**
- **Angular coupling occurs on the RHS.**
- **LHS is still diagonal in groups and directions**

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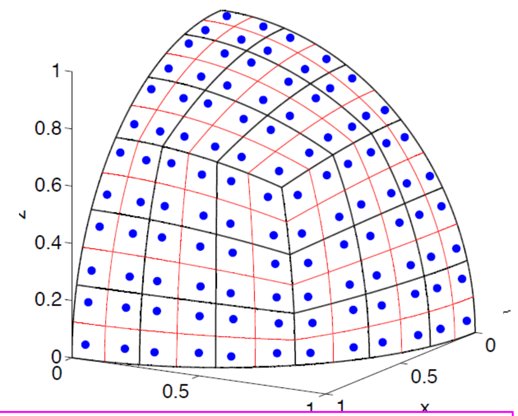

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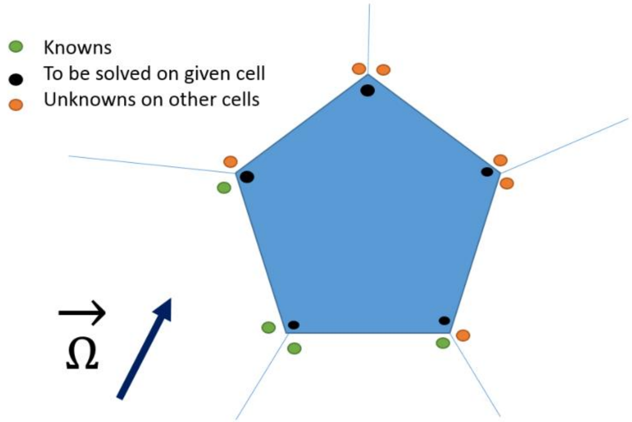
Phase-space Discretization

- Solving for a given group g (omitted below) and a given direction d:

$$\left(\vec{\Omega}_d \cdot \vec{\nabla} + \sigma_t(\vec{r})\right) \Psi_d(\vec{r}) = \frac{\sigma_s(\vec{r})}{4\pi} \Phi(\vec{r}) + S_{\text{fixed+inscattering into } g}$$

- Conundrum: the unknown and its angular integral appear on both sides.
- Lag the angular redistribution (~fixed-point iterative process):
- Spatial variable: DGFEM with upwinding $\uparrow$

$$\left(\Psi_d, -(\vec{\Omega}_d \cdot \vec{\nabla} + \sigma_t) b_i\right)_K + \langle \Psi_d, \vec{\Omega}_d \cdot \vec{n}\ b_i \rangle_{\partial K^+} = (q, b_i)_K + \langle \Psi_d^{\uparrow}, |\vec{\Omega}_d \cdot \vec{n}|\ b_i \rangle_{\partial K^-}$$



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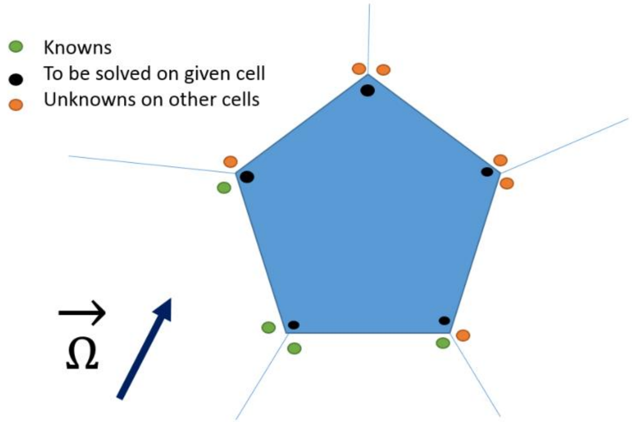

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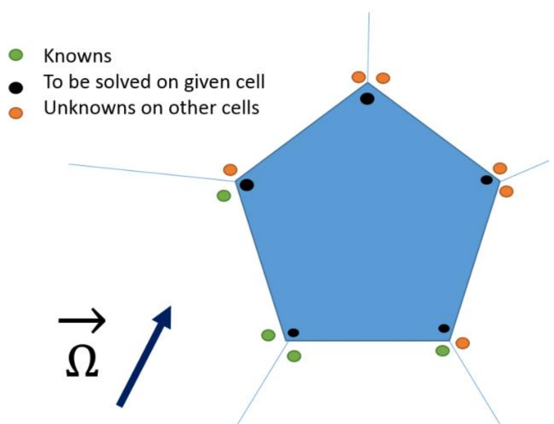

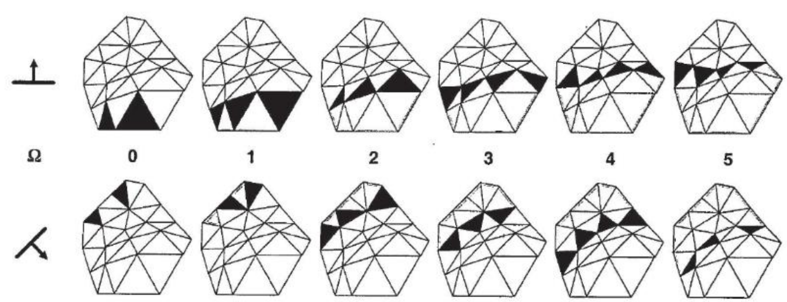

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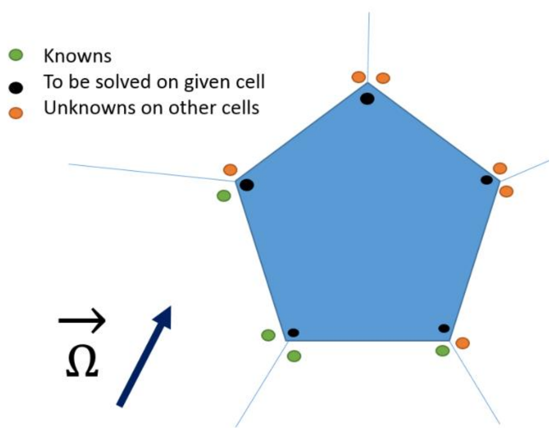
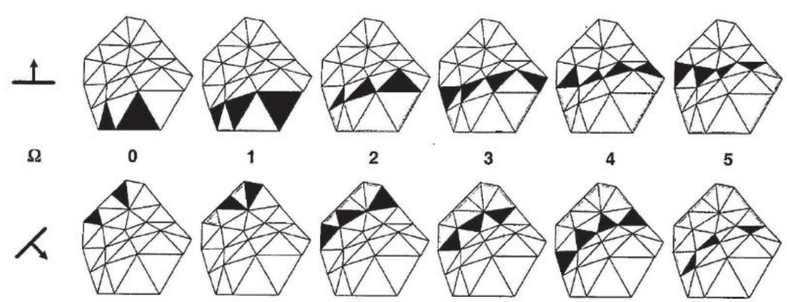
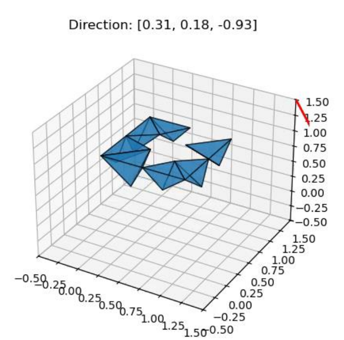
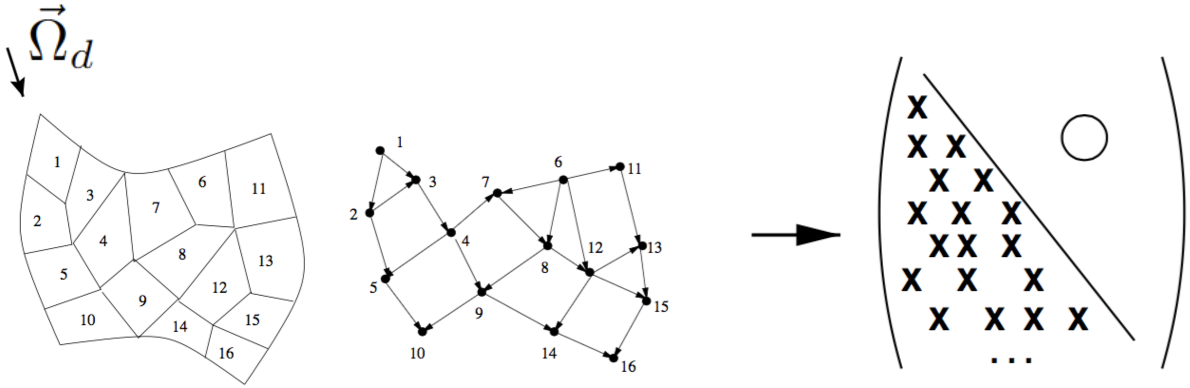


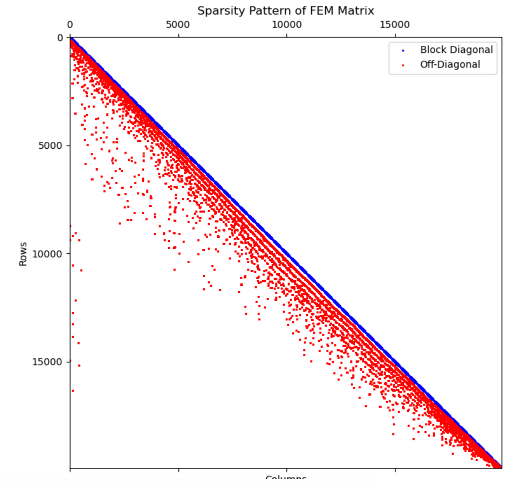




Transport Sweeps: a Matrix-free Process

- The "transport sweep" is a **task-directed graph** that makes the advection-reaction operator block lower triangular





Formidable computational problem:

- Space: $N_x \times N_y \times N_z$ cells (say $100 \times 100 \times 100 = 1$ million spatial cells)
- Angle: 50 - 5,000 directions (say 1,000)
- Groups: several dozens and up (say 100)
- 8 spatial degrees of freedom/cell (discontinuous finite elements)
- Total: about 1 trillion (10^{12}) unknowns, (figures $>$ 1 trillion are not infrequent ...)

Key Points:

- Radiation transport is a linear problem $\boxed{Ax = b}$
- The number of unknowns per vertex of a mesh is gigantic ($> 10,000$)
- Due to the size of the problem, matrix A is not available (not built nor stored)

Transport Sweeps: a Matrix-free Process

- **The "transport sweep" is a task-directed graph that makes the advection-reaction**

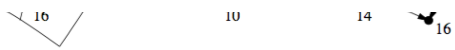
On MIRA (BQ/G):

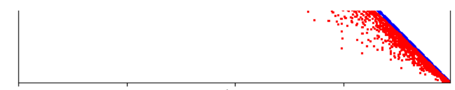
dofs/cells	spatial cells/core	angles	groups	cores	total dofs
8	4,096	80	3	1.5M	12T

dofs/cells	spatial cells/core	angles	groups	cores	total dofs
8	1	31,104	99	768k	19T

Equivalent to U.S. debt

...2018 numbers ...





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Notation

- Parametric Transport Equation

$$\left(\vec{\Omega}\cdot\vec{\nabla} + \sigma_t(\vec{r},E)\right)\Psi(\vec{r},\vec{\Omega},E) = \frac{1}{4\pi}\int_{4\pi} d\Omega' \int dE' \, \sigma_s(\vec{r},E'\to E)\Psi(\vec{r},\vec{\Omega}',E') + S_{\text{fixed}}(\vec{r},\vec{\Omega},E)$$

- Angular integration: $\Phi = D\Psi$
- Hence, the Transport Equation is: $L(\sigma_t)\Psi = \Sigma(\sigma_s)\Phi + q_{\text{fixed}}$

- Where is $Ax = b$?
  - ➢ *Standard solution procedure (radiation codes implement L^{-1} in a **matrix-free** manner):*
    Moment form of the eqs.:

$$\begin{cases} \Psi^{(\ell+1)} = L^{-1}(\Sigma\Phi^{(\ell)} + q_{\text{fixed}}) \\ \Phi^{(\ell+1)} = D\Psi^{(\ell+1)} \end{cases} \Longrightarrow \underbrace{\left(I - DL^{-1}(\sigma_t)\Sigma(\sigma_s)\right)}_{=A(\mu)}\Phi = \underbrace{DL^{-1}q_{\text{fixed}}}_{=b(\mu)}$$

  - ➢ *Another acceptable view for MOR:*
    Angular form of the eqs.:

$$\underbrace{\left(L(\sigma_t) - \Sigma(\sigma_s)D\right)}_{=A(\mu)}\Psi = \underbrace{q_{\text{fixed}}}_{=b(\mu)}$$

Angular Form vs. Moment Form ROM?

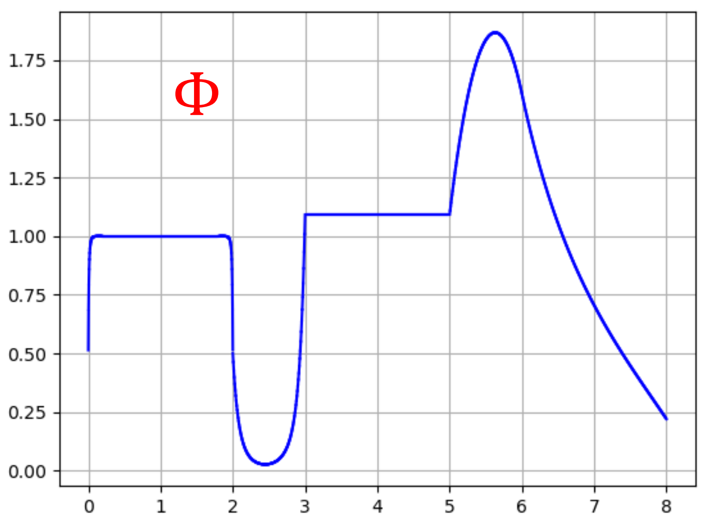
- **Governing law:** $L\Psi = \Sigma \underbrace{D\Psi}_{=\Phi} + q$
- **The FOM solves always involve Ψ:** $\begin{cases} \Psi^{(\ell+1)} = L^{-1}(\Sigma\Phi^{(\ell)} + q) \\ \Phi^{(\ell+1)} = D\Psi^{(\ell+1)} \end{cases} \Longrightarrow (I - DL^{-1}\Sigma)\Phi = DL^{-1}q$
- **However, the ROM is either built considering**

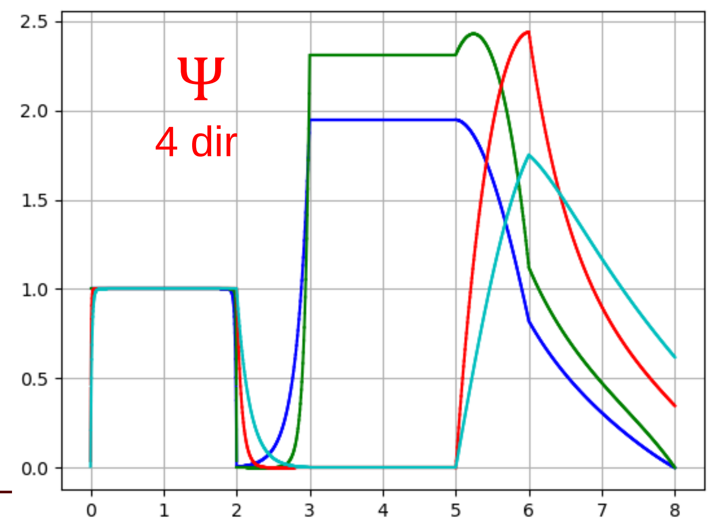
  $L\Psi = \Sigma D\Psi + q$ **(angular form ROM) or** $(I - DL^{-1}\Sigma)\Phi = DL^{-1}q$ **(moment form)**

- **If one only reconstructs Φ, only angle-integrated quantities can be calculated**

$$RR = \int_V d^3 \int dE \int_{4\pi} d\Omega\, \sigma(\vec{r}, E)\Psi(\vec{r}, E, \vec{\Omega}) = \int_V d^3 \int dE\, \sigma(\vec{r}, E)\Phi(\vec{r}, E)$$

- **Ψ and Φ can be vastly different:**





Why Transport and Not Diffusion?

- **Under some circumstances (low absorption, distributed sources, high scattering), a Diffusion approximation is a suitable representation for Φ:**

$$\left(-\vec{\nabla}\cdot D_g\vec{\nabla}+\sigma_t^g-\sigma_s^{g\to g}\right)\Phi^g=\sum_{g'=1,g'\neq g}^{G}\sigma_s^{g'\to g}\Phi^{g'}+S_{\text{fixed}}^g$$

  - *"physics-guided" reduction: 4D problem (space (3) + energy (1)) instead of a 6D problem*
  - *Then perform ROM on the multigroup diffusion eqs.*
    - elliptic operators,
    - affine decomposition

- **But diffusion is not suitable for all transport problems:**
  - *Problems with strong absorption, localized sources, low scattering*
  - *Problems that exhibit a streaming limit (hyperbolic nature)*
    - → low decay of singular values
    - Large Kolmogorov width

Parametric MOR

- Model-order reduction (MOR) reduces the computational complexity of mathematical models in numerical simulations
- Model + input parameters (in) → PDEs → discretization → system with large # unknowns, N (degrees of freedom, DoFs)

Full Order Model (FOM): Solve $$\boldsymbol{A}(in)\vec{x} = \vec{b}(in)\,, \qquad \vec{x} \in \mathbb{R}^N$$

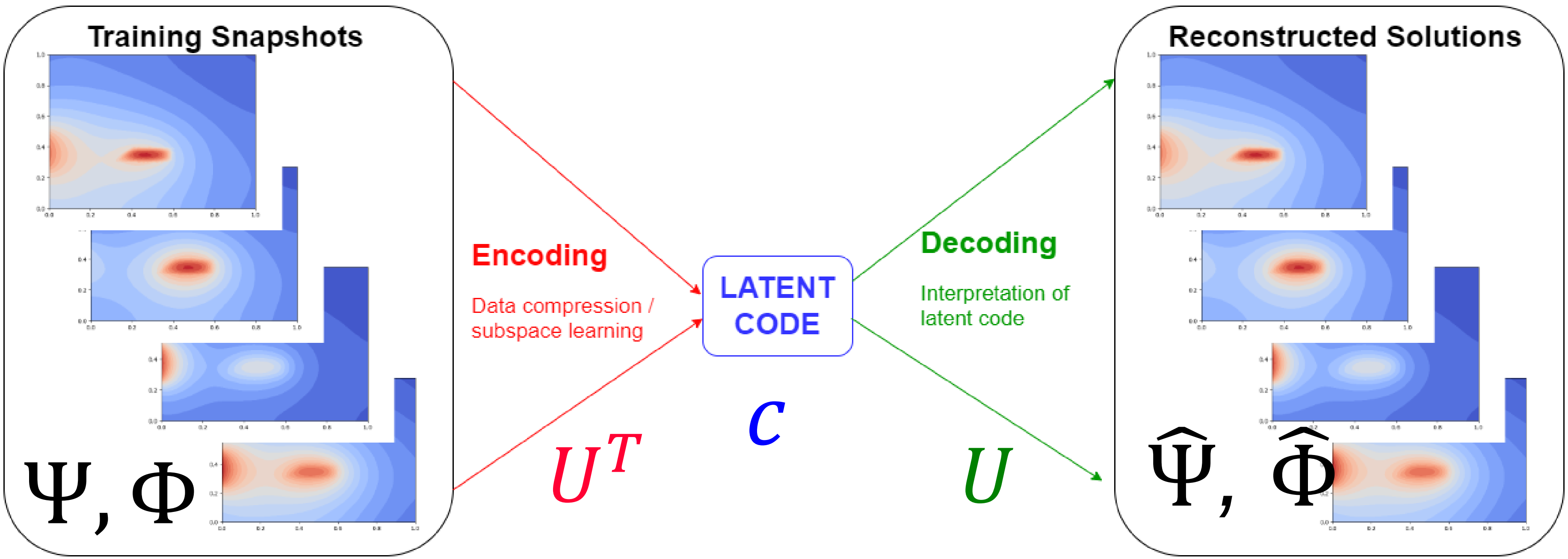
- Model order reduction reduces the computational complexity of a model by reducing the number of DoFs

educed Order Model (ROM): Solve $$\boldsymbol{A}_r(in)\vec{c} = \vec{b}_r(in)\,, \quad \vec{c} \in \mathbb{R}^r\,, \quad (r \ll N)$$

such that $$||\vec{x} - \boldsymbol{U}_r\vec{c}|| \leq C_r(in) \quad \text{with} \quad \lim_{r \to N} C_r = 0\,.$$

- $\boldsymbol{U}_r$ = reconstruction operator
- Data-driven, projection-based ROMs with linear manifolds
  - ROM solution linear combination of r size N basis vectors
  - Offline training phase and online prediction phase

Principle of MOR



$$c = U^T \Phi \qquad \hat{\Phi} = Uc$$

- Linear manifolds: e.g., subspace is obtained via SVD, greedy RB, …
- Nonlinear manifolds: encoding/decoding learning (Willcox, Maday, …)

Data-driven Subspace Learning: Principles

- **Offline phase:**
  - Parameters: $\vec{\mu} = (\sigma_t, \sigma_s, q)$
  - Solve FOM: $\boldsymbol{A}(\vec{\mu}_i)\vec{x}(\vec{\mu}_i) = \vec{b}(\vec{\mu}_i)$
    - $\boldsymbol{X} = (\vec{x}(\vec{\mu}_1), \vec{x}(\vec{\mu}_2), \ldots, \vec{x}(\vec{\mu}_{n_{\text{snap}}}))$
  - Proper orthogonal decomposition (POD)
    - Singular value decomposition (SVD): $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{V}^T$
    - Information content $I(r) = \frac{\sum_{i=1}^{r}\lambda_i^2}{\sum_{i=1}^{n_{\text{snap}}}\lambda_i^2}$
    - Restrict subspace to the first r columns of $\boldsymbol{U}$ as basis vectors $\boldsymbol{U}_r$

- **Online phase:**

Unseen parameter $\vec{\theta}$

- Approximate solution

$$\tilde{\vec{x}}(\vec{\theta}) = \sum_{j=1}^{r} \vec{u}_j c_j(\vec{\theta}) = \boldsymbol{U}_r \vec{c}(\vec{\theta})$$

- Projection

$$\underbrace{\boldsymbol{W}^T(\vec{\theta})\boldsymbol{A}(\vec{\theta})\boldsymbol{U}_r}_{\boldsymbol{A}_r(\vec{\theta})}\vec{c}(\vec{\theta}) = \underbrace{\boldsymbol{W}^T(\vec{\theta})\vec{b}(\vec{\theta})}_{\vec{b}_r(\vec{\theta})}$$

Galerkin: $\boldsymbol{W} = \boldsymbol{U}_r$

Petrov-Galerkin: $\boldsymbol{W}(\vec{\theta}) = \boldsymbol{A}(\vec{\theta})\boldsymbol{U}_r$

- ROM solve

$$\boldsymbol{A}_r(\vec{\theta})\vec{c}(\vec{\theta}) = \vec{b}_r(\vec{\theta})$$

Outline

1. Background on Radiation Transport
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   B. *Crash course on Radiation Transport*

2. Reduced-Order Models for Radiation Transport
   A. *Projection-based pROM:*
      i. Minimally-invasive approach
      ii. Affine decomposition of operators
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3. Conclusions and Outlook

Minimally-invasive Transport ROM: Procedure

- Based on moment form of transport

FOM: $$\underbrace{\left(\boldsymbol{I}-\boldsymbol{D}\boldsymbol{L}(\vec{\theta})^{-1}\boldsymbol{\Sigma}(\vec{\theta})\right)}_{\boldsymbol{A}(\vec{\theta})}\underbrace{\vec{\Phi}(\vec{\theta})}_{\vec{x}(\vec{\theta})}=\underbrace{\boldsymbol{D}\boldsymbol{L}(\vec{\theta})^{-1}\vec{Q}}_{\vec{b}(\vec{\theta})}$$

ROM: $$\underbrace{\boldsymbol{W}^T(\vec{\theta})(\boldsymbol{I}-\boldsymbol{D}\boldsymbol{L}(\vec{\theta})^{-1}\boldsymbol{\Sigma}(\vec{\theta}))\boldsymbol{U}_r}_{\boldsymbol{A}_r(\vec{\theta})}\vec{c}(\vec{\theta})=\underbrace{\boldsymbol{W}^T(\vec{\theta})\boldsymbol{D}\boldsymbol{L}(\vec{\theta})^{-1}\vec{Q}}_{\vec{b}_r(\vec{\theta})}$$

- Matrix-free $\boldsymbol{L}^{-1}(\vec{\theta})$ contained in $\boldsymbol{A}$ and $\vec{b}$, need transport sweep for each POD mode + one for RHS
  - Repeat for each NEW $\vec{\theta}$; Bottleneck due to full-order operation
  - Minimally intrusive

GMRes: action of mat on vec

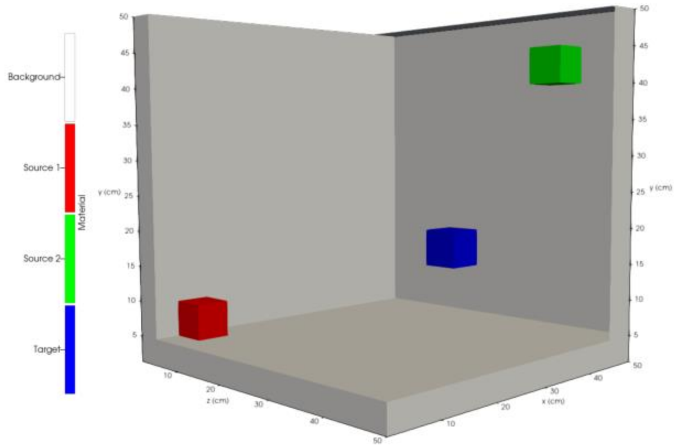
Offline phase

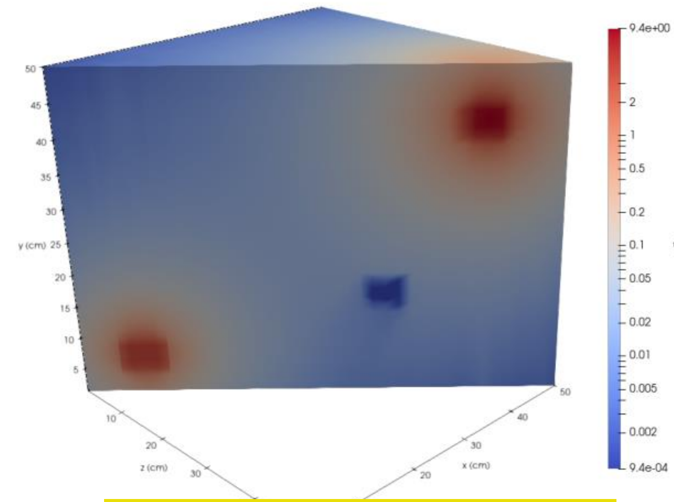
1. Generate $\{\vec{\Phi}(\vec{\mu}_i)\}_{i=1}^{n_{\text{snap}}}$ snapshots
2. Compute SVD, obtain POD modes $\boldsymbol{U}_r$

Online phase; For each $\vec{\theta}$:

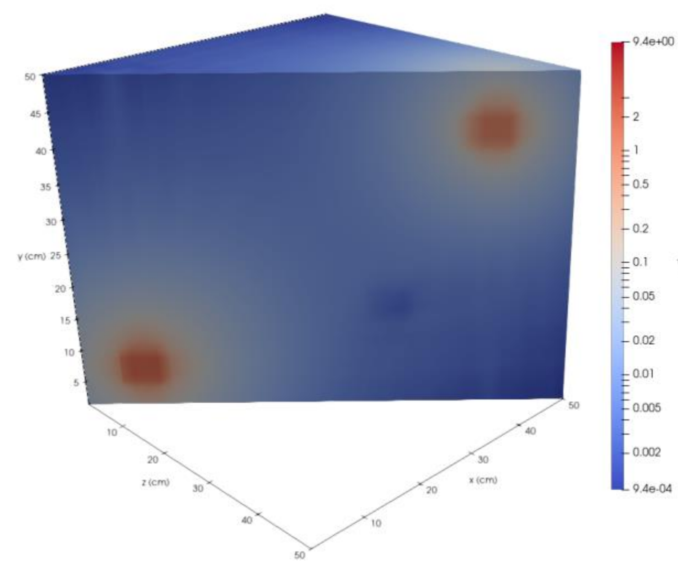
1. Sweep $\boldsymbol{L}^{-1}(\vec{\theta})\boldsymbol{\Sigma}(\vec{\theta})\vec{u}_j$, $j\in[1,r]$, assemble $\boldsymbol{A}(\vec{\theta})\boldsymbol{U}_r$
2. Sweep $\boldsymbol{L}^{-1}(\vec{\theta})\vec{Q}$, assemble $\vec{b}(\vec{\theta})$
3. Define test subspace $\boldsymbol{W}(\vec{\theta})$
   - Galerkin: $\boldsymbol{W}=\boldsymbol{U}_r$
   - Petrov-Galerkin: $\boldsymbol{W}(\vec{\theta})=\boldsymbol{A}(\vec{\theta})\boldsymbol{U}_r$
4. Compute $\boldsymbol{A}_r(\vec{\theta})=\boldsymbol{W}(\vec{\theta})^T\boldsymbol{A}(\vec{\theta})\boldsymbol{U}_r$ and $\vec{b}_r(\vec{\theta})=\boldsymbol{W}(\vec{\theta})^T\vec{b}(\vec{\theta})$
5. Solve reduced system $\boldsymbol{A}_r(\vec{\theta})\vec{c}(\vec{\theta})=\vec{b}_r(\vec{\theta})$
6. Reconstruct full-order solution from reduced coordinate $\vec{\Phi}^{\text{ROM}}(\vec{\theta})=\boldsymbol{U}_r\vec{c}(\vec{\theta})$

Minimally-invasive Transport ROM: Results (1/2)





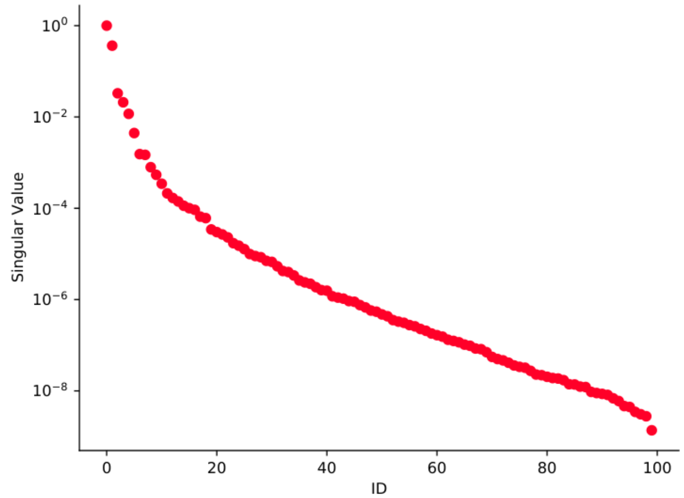
Some snapshots

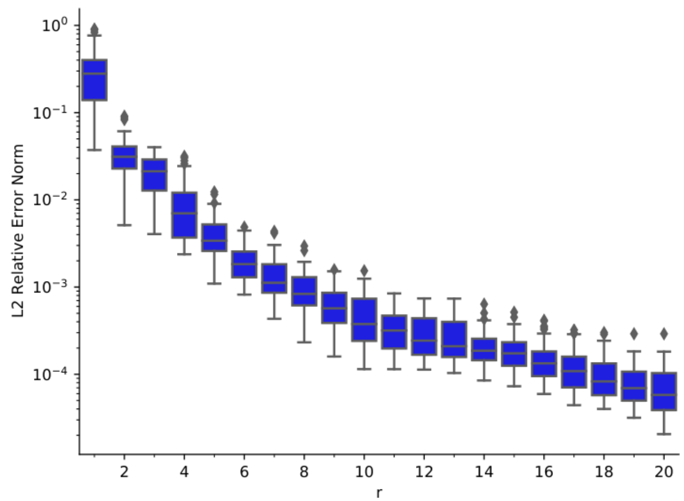


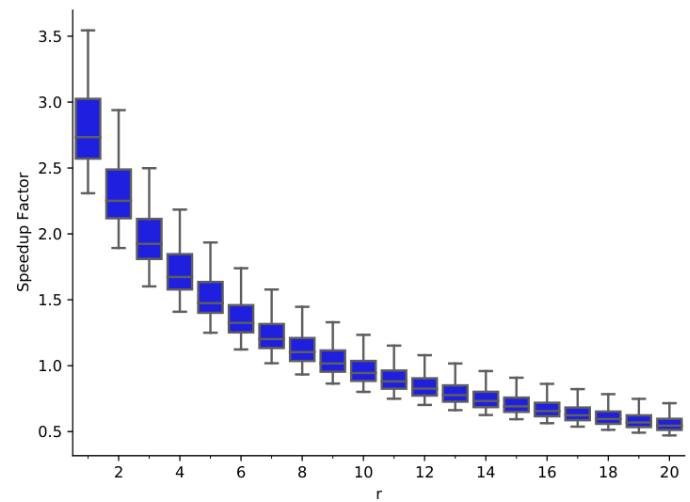
Parameter	Material			
	Background	Target	Source 1	Source 2
Σ_t (cm^{-1})	$\mathcal{U}(0.0, 0.1)$	$\mathcal{U}(0.0, 2.0)$	2.0	0.3
c (cm^{-1})	$\mathcal{U}(0.5, 1.0)$	$\mathcal{U}(0.0, 0.5)$	1.0	0.6
Q $(par\ cm^{-3})$	0.0	0.0	$\mathcal{U}(0.0, 10.0)$	$\mathcal{U}(0.0, 10.0)$

- $N \approx 1.14 \times 10^9$
- 100 snapshots
- 50 test cases

Minimally-invasive Transport ROM: Results (2/2)



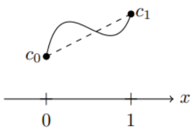


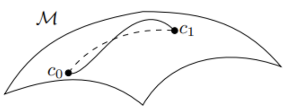


- Minimally invasive but low-speedups due to the need to perform a full-order operation (L^{-1} “transport sweep”) for each new parameter realization

Minimally-invasive Transport ROM: a way forward

- **Interpolate the reduced operator using training data: (OMMI: Offline Maximizing Minimally Invasive)**
- **Linear interpolation vs. Grassmann manifold interpolation**





- **WIP**

Offline phase

1. Generate $\{\vec{\Phi}(\vec{\mu}_i)\}_{i=1}^{n_{\text{snap}}}$ snapshots
2. Compute SVD, obtain POD modes $\boldsymbol{U}_r$
3. Sweep $\boldsymbol{L}^{-1}(\vec{\mu}_i)\boldsymbol{\Sigma}(\vec{\mu}_i)\vec{u}_j$, $i \in [1, n_{\text{snap}}]$ and $j \in [1, r]$, assemble $\boldsymbol{A}(\vec{\mu}_i)\boldsymbol{U}_r$
4. Sweep $\boldsymbol{L}^{-1}(\vec{\mu}_i)\vec{Q}$, $i \in [1, n_{\text{snap}}]$, assemble $\vec{b}(\vec{\mu}_i)$
5. Define test subspace $\boldsymbol{W}(\mu_i)$
   - Galerkin: $\boldsymbol{W} = \boldsymbol{U}_r$
   - Petrov-Galerkin: $\boldsymbol{W}(\mu_i) = \boldsymbol{A}(\vec{\mu}_i)\boldsymbol{U}_r$
6. Compute $\boldsymbol{A}_r(\vec{\mu}_i) = \boldsymbol{W}(\vec{\mu}_i)^T\boldsymbol{A}(\vec{\mu}_i)\boldsymbol{U}_r$ and $\vec{b}_r(\vec{\mu}_i) = \boldsymbol{W}(\vec{\mu}_i)^T\vec{b}(\vec{\mu}_i)$ for $i \in [1, n_{\text{snap}}]$

Online phase; For each $\vec{\theta}$:

1. Interpolate $\boldsymbol{A}_r(\vec{\theta})$ and $\vec{b}_r(\vec{\theta})$ using $\boldsymbol{A}_r(\vec{\mu}_i)$ and $\vec{b}(\vec{\mu}_i)$
2. Solve reduced system $\boldsymbol{A}_r(\vec{\theta})\vec{c}(\vec{\theta}) = \vec{b}_r(\vec{\theta})$
3. Reconstruct full-order solution from reduced coordinate $\vec{\Phi}^{\text{ROM}}(\vec{\theta}) = \boldsymbol{U}_r\vec{c}(\vec{\theta})$

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3. **Conclusions and Outlook**

Affine-decomposed Radiation Transport: 1/3

- **Based on angular form of transport:**

$$\underbrace{\underbrace{(\vec{\Omega}_d \cdot \vec{\nabla}}_{\boldsymbol{G}_d} + \underbrace{\sigma_t^g(\vec{r})}_{\boldsymbol{T}(\vec{\theta})})}_{\boldsymbol{L}(\vec{\theta})} \underbrace{\psi_d^g(\vec{r})}_{\vec{\Psi}} - \frac{1}{4\pi} \sum_{g'=1}^{G} \underbrace{\sigma_s^{g' \to g}(\vec{r})}_{\boldsymbol{\Sigma}(\vec{\theta})} \sum_{d'=1}^{n_\Omega} w_{d'} \underbrace{\psi_{d'}^{g'}(\vec{r})}_{\vec{\Psi}} = \underbrace{Q_d^g(\vec{r})}_{\vec{Q}}$$

$$(\boldsymbol{G} + \boldsymbol{T}(\vec{\theta}) - \boldsymbol{\Sigma}(\vec{\theta})\boldsymbol{D})\vec{\Psi} = \vec{Q}(\vec{\theta})$$

All reaction operators are affine w.r.t parameters. Let k denote material k:

$$\boldsymbol{M}^k = \text{mass matrix}\,, \vec{f}^k = \text{load vector}\,, \qquad \boldsymbol{T}^g(\vec{\theta}) = \sum_{k=1}^{N_{\text{mat}}} \sigma_t^{g,k} \boldsymbol{M}^k\,,$$

$$\boldsymbol{\Sigma}_{g,g'}(\vec{\theta})\boldsymbol{D}_{d'} = \sum_{k=1}^{N_{\text{mat}}} \sigma_s^{g' \to g,k} \boldsymbol{M}^k \boldsymbol{D}_{d'}\,, \qquad \vec{Q}_d^g(\vec{\theta}) = \sum_{k=1}^{N_{\text{mat}}} Q_d^{g,k} \vec{f}^k$$

Affine-decomposed Radiation Transport: 2/3

FOM: $$\underbrace{\left(\boldsymbol{G}+\boldsymbol{T}(\vec{\theta})-\boldsymbol{\Sigma}(\vec{\theta})\boldsymbol{D}\right)}_{\boldsymbol{A}(\vec{\theta})}\underbrace{\vec{\Psi}(\vec{\theta})}_{\vec{x}(\vec{\theta})}=\underbrace{\vec{Q}}_{\vec{b}(\vec{\theta})}$$

Recall:
not solved as is in codes

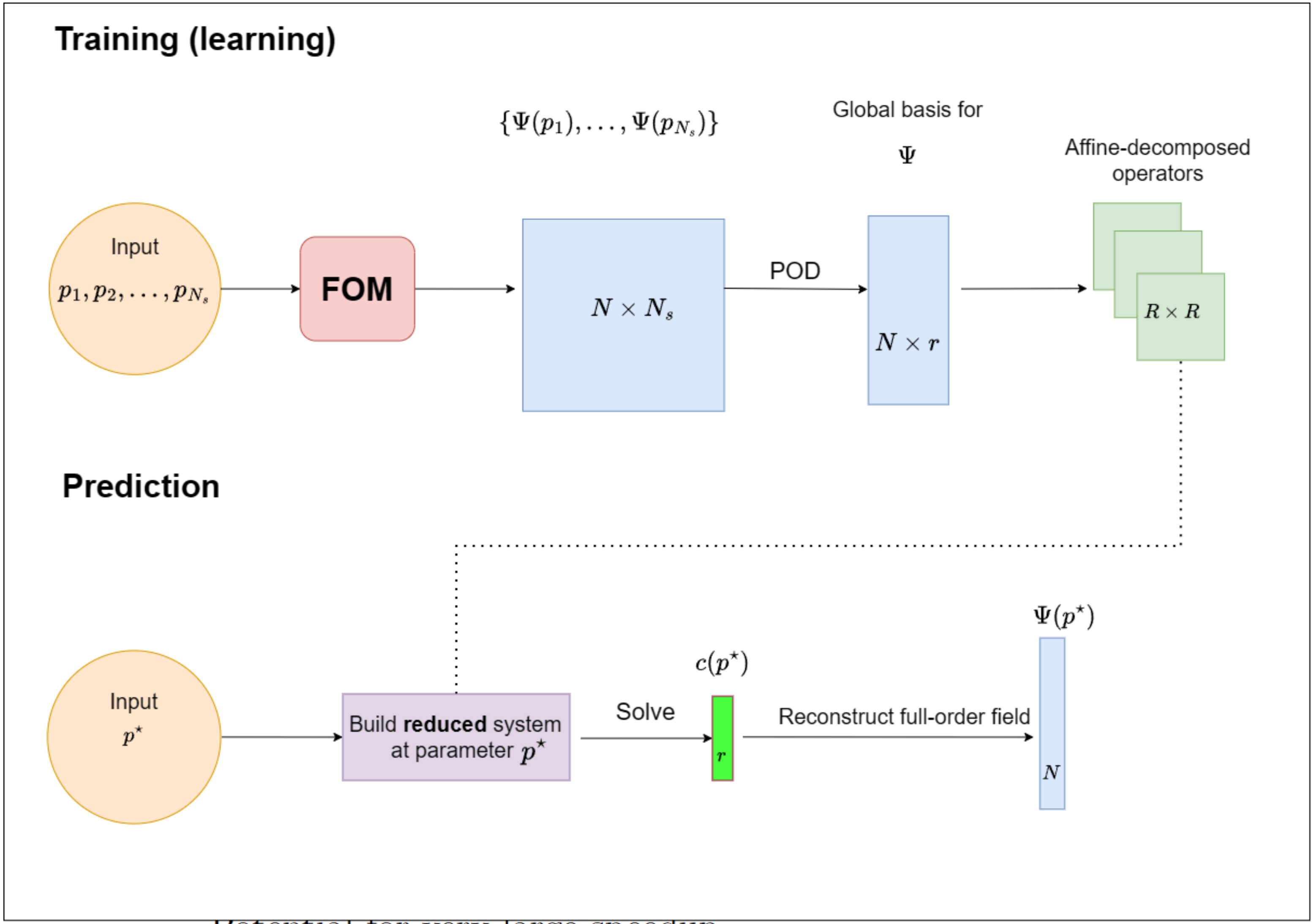
ROM: $$\underbrace{\boldsymbol{W}^T(\vec{\theta})(\boldsymbol{G}+\boldsymbol{T}(\vec{\theta})-\boldsymbol{\Sigma}(\vec{\theta})\boldsymbol{D})\boldsymbol{U}_r}_{\boldsymbol{A}_r(\vec{\theta})}\vec{c}(\vec{\theta})=\underbrace{\boldsymbol{W}^T(\vec{\theta})\vec{Q}}_{\vec{b}_r(\vec{\theta})}$$

$$\boldsymbol{A}(\vec{\theta})=\sum_k \theta_k \boldsymbol{A}^k\,,\qquad \vec{b}(\vec{\theta})=\sum_k \theta_k \vec{b}^k\,,\qquad \boldsymbol{W}(\vec{\theta})=\sum_{k'} \theta_{k'} \boldsymbol{W}^{k'}$$

$$\boldsymbol{A}_r(\vec{\theta})=\sum_k\sum_{k'}(\theta_k\theta_{k'})\underbrace{\left(\boldsymbol{W}_{k'}^T\boldsymbol{A}_k\boldsymbol{U}_r\right)}_{=\boldsymbol{A}_r^{kk'}},\qquad \vec{b}_r(\vec{\theta})=\sum_k\sum_{k'}(\theta_k\theta_{k'})\underbrace{\left(\boldsymbol{W}_{k'}^T\vec{b}_k\right)}_{=\vec{b}_r^{kk'}}$$

- Code-intrusive to precompute components $\boldsymbol{A}_r^{kk'}$ and $\vec{b}_r^{kk'}$ of reduced systems
- Does not required full-order operations
  - Potential for very large speedup

Affine-decomposed Radiation Transport: 2/3



– Potential for very large speedup

Affine-decomposed Radiation Transport: 3/3

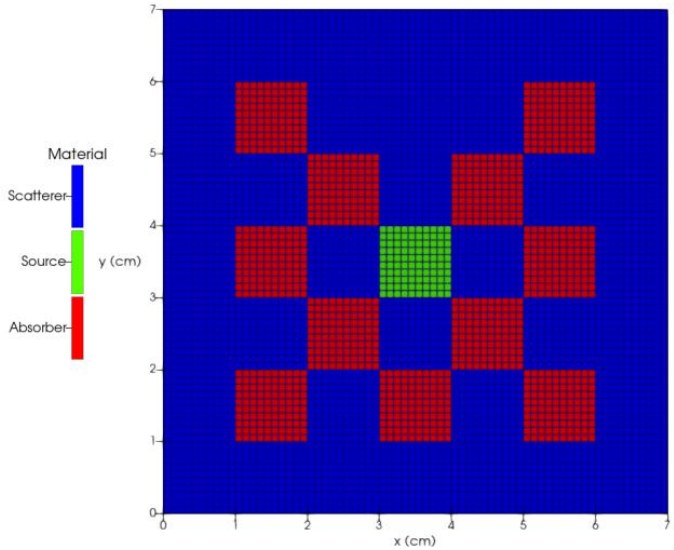
Offline phase

1. Generate snapshots $\{\vec{\Psi}(\vec{\mu}_i)\}_{i=1}^{n_{\text{snap}}}$
2. Compute SVD, get POD modes $\boldsymbol{U}_r$
3. Compute small projection terms $\boldsymbol{A}_r^{kk'} = \boldsymbol{W}_{k'}^T \boldsymbol{A}_k \boldsymbol{U}_r$, $\vec{b}_r^{kk'} = \boldsymbol{W}_{k'}^T \vec{b}_k$ from affine decomposition

Online phase; For each $\vec{\theta}$:

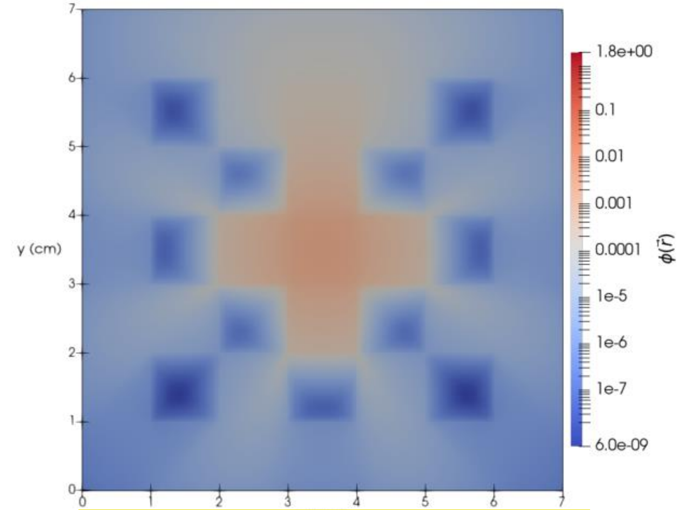
1. Define test subspace $\boldsymbol{W}(\vec{\theta})$
   - Galerkin: $\boldsymbol{W} = \boldsymbol{U}_r$
   - Petrov-Galerkin: $\boldsymbol{W}(\vec{\theta}) = \boldsymbol{A}(\vec{\theta})\boldsymbol{U}_r$
2. Construct $\boldsymbol{A}_r(\vec{\theta}) = \sum_k \sum_{k'} (\theta_k \theta_{k'})\, \boldsymbol{A}_r^{kk'}$
3. Construct $\vec{b}_r(\vec{\theta}) = \sum_k \sum_{k'} (\theta_k \theta_{k'})\, \vec{b}_r^{kk'}$
4. Solve reduced system $\boldsymbol{A}_r(\vec{\theta})\vec{c}(\vec{\theta}) = \vec{b}_r(\vec{\theta})$
5. Reconstruct solution from reduced coordinates $\vec{\Psi}^{\text{ROM}}(\vec{\theta}) = \boldsymbol{U}_r \vec{c}(\vec{\theta})$

Checkerboard bench.: Sweep-based vs. Affine-decomposed ROMs

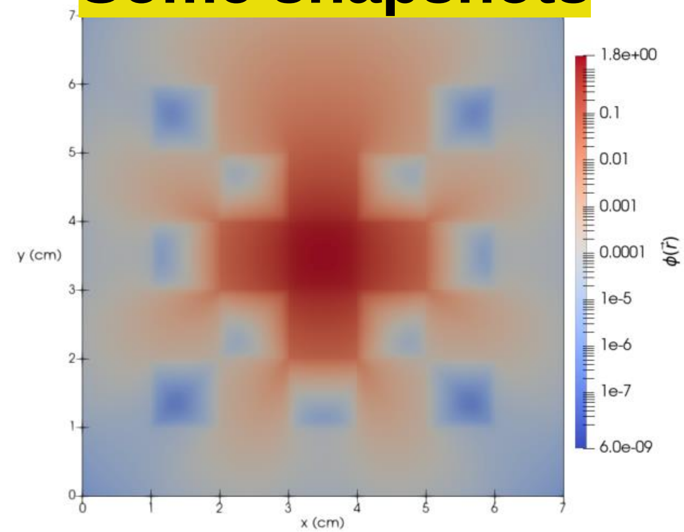


Parameter	Material	
	Absorber	Scatterer
Σ_a (cm^{-1})	$\mathcal{U}(7.5,\ 12.5)$	$\mathcal{U}(0.0,\ 0.5)$
Σ_s (cm^{-1})	$\mathcal{U}(0.0,\ 5.0)$	$\mathcal{U}(0.5,\ 1.5)$
Q $(par\ cm^{-3})$	0	$\mathcal{U}(0.0,\ 2.0)$

- $N \approx 2.01 \times 10^7$
- 300 snapshots
- 50 test cases



Some snapshots



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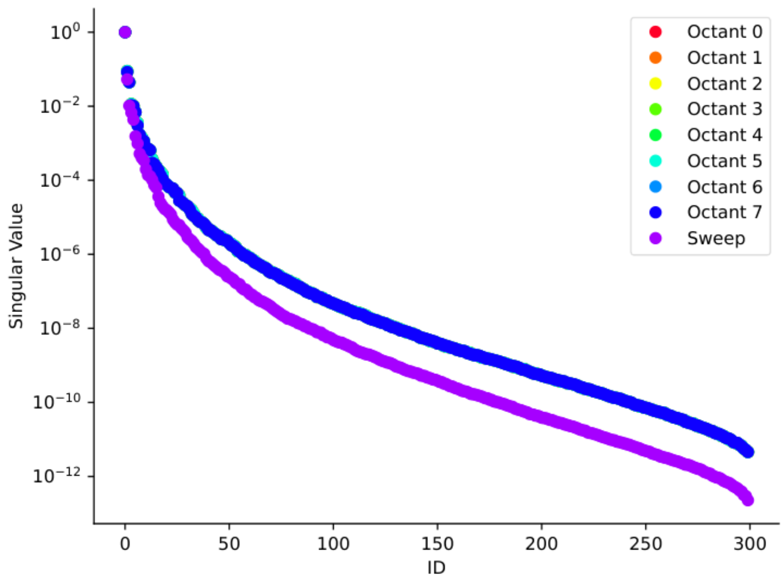
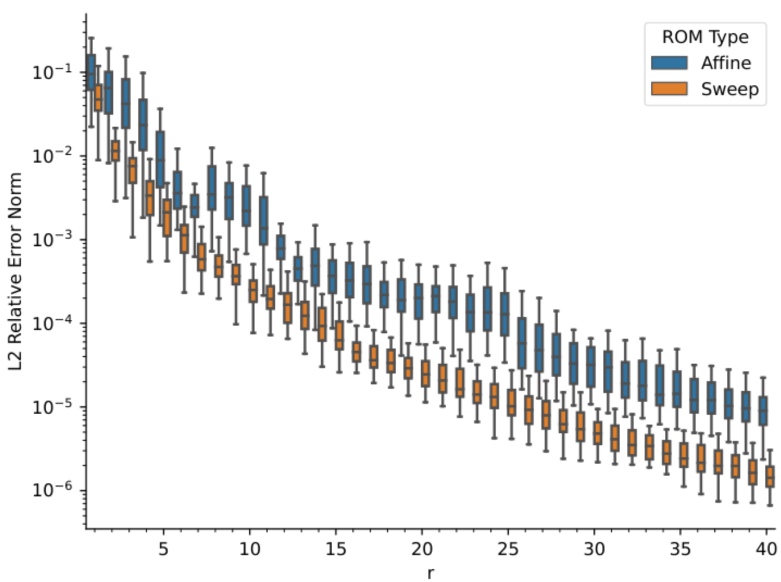
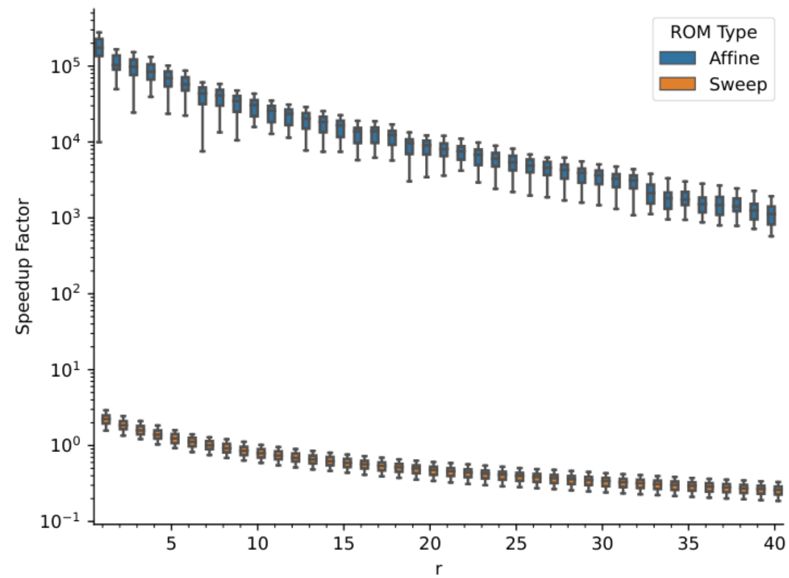
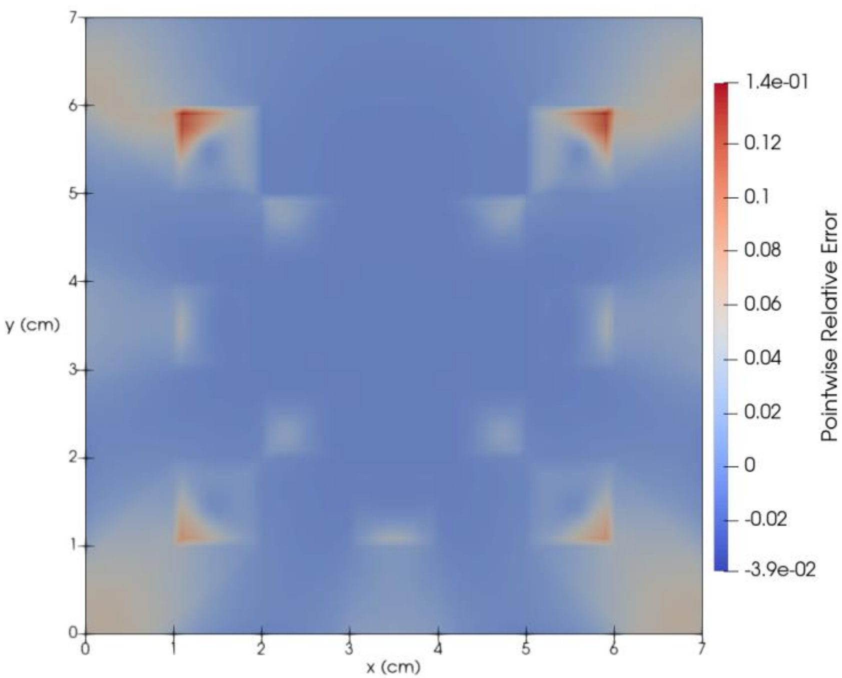




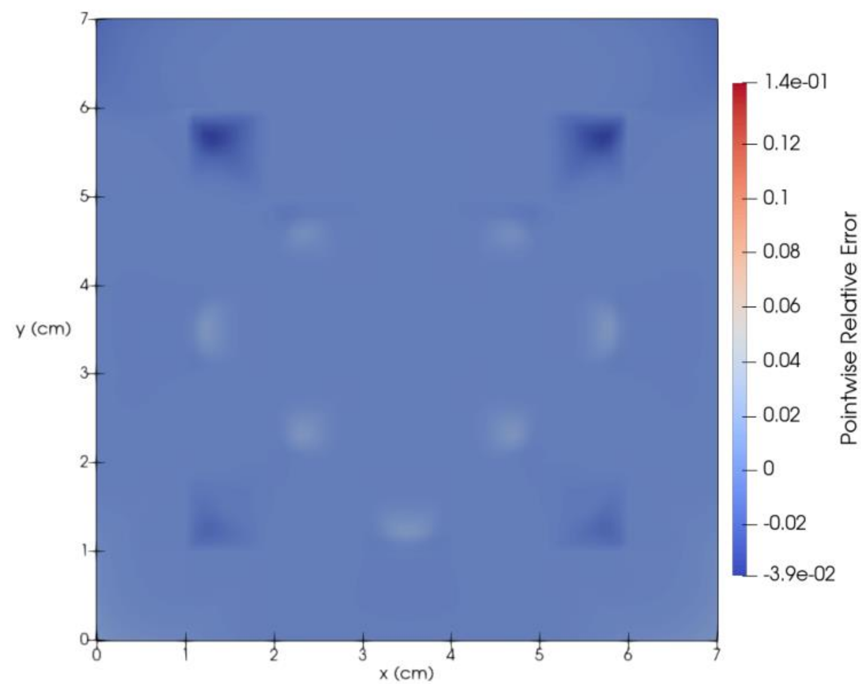


Checkerboard bench.: Sweep-based vs. Affine-decomposed ROMs

Pointwise errors

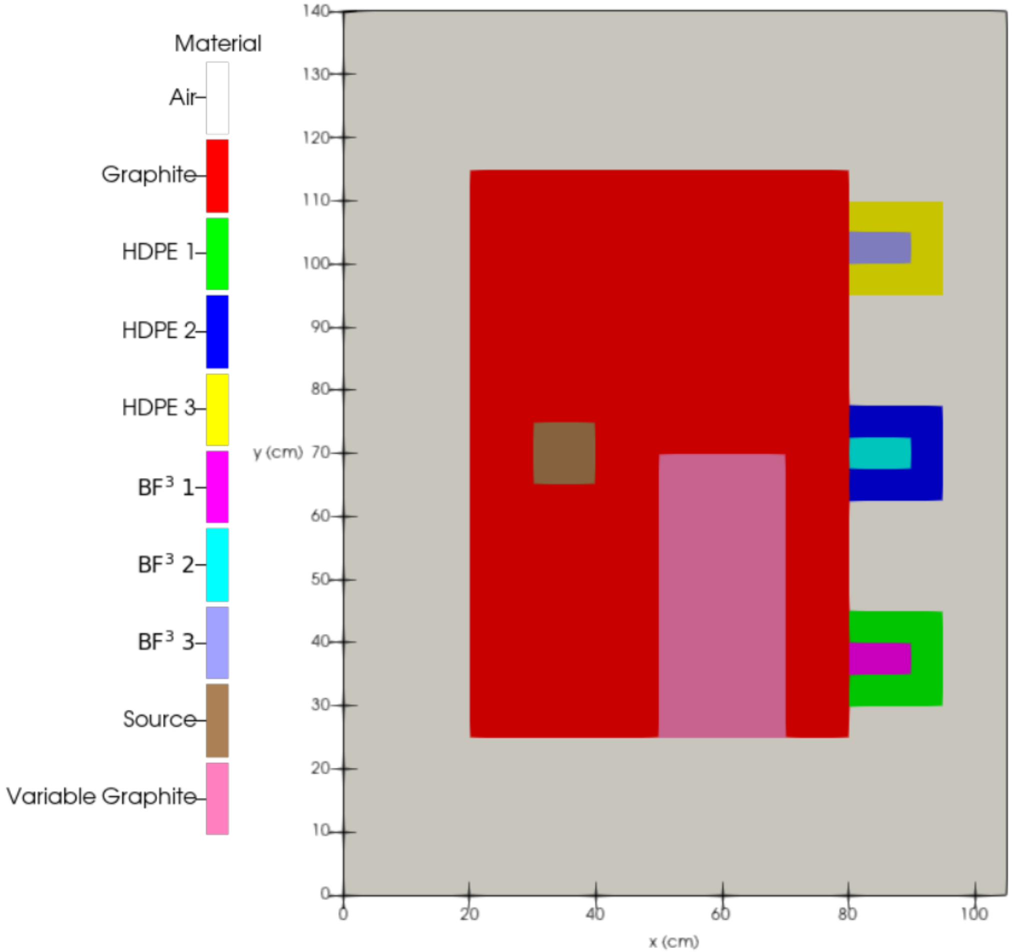


26 POD modes (affine)



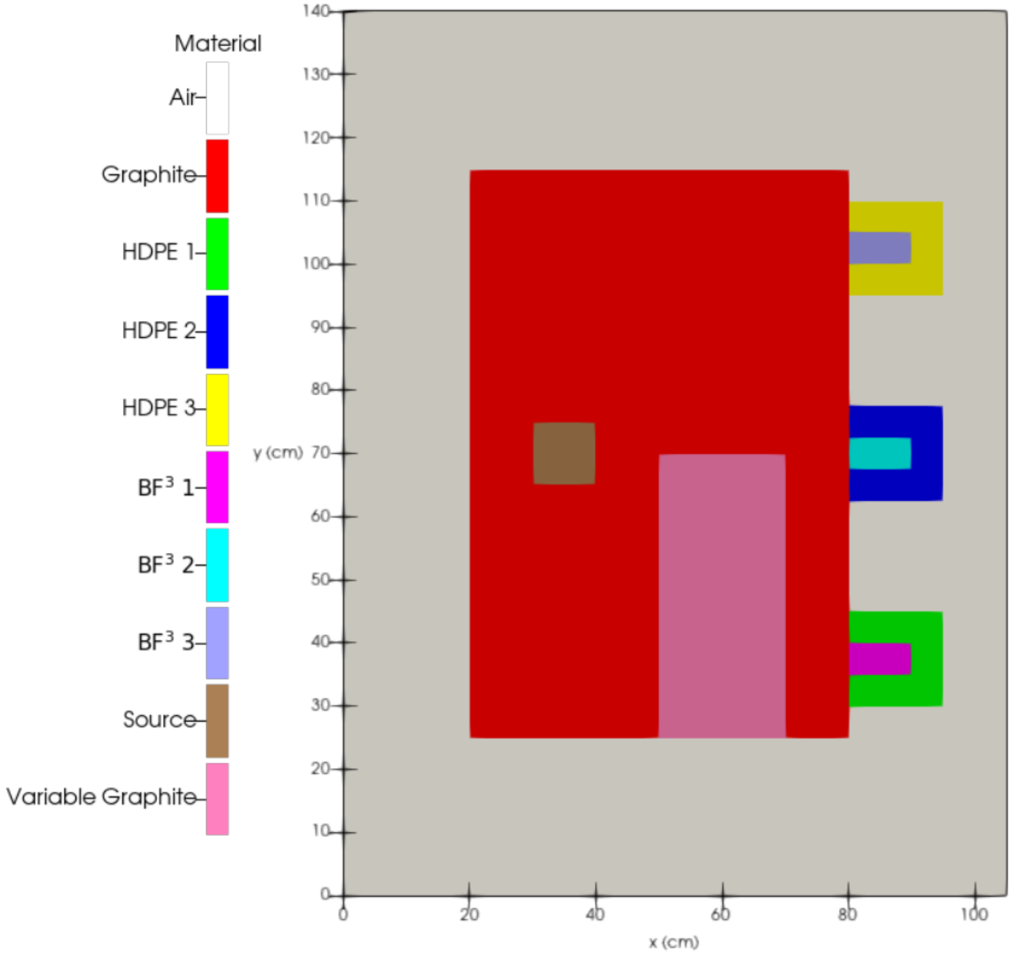
40 POD modes (affine)

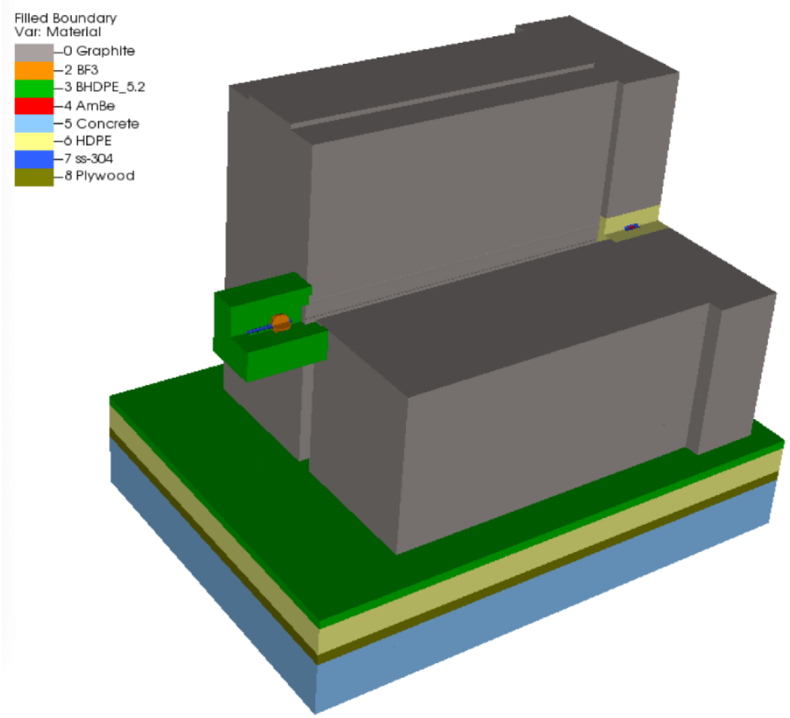
3-D graphite matrix with HDPE shrouds (affine ROM only)



- 4 parameters
  - Mass fraction of boron in HDPE 1-3 ($\mathcal{U}(0, 7.2)\%$)
  - Variable graphite density ($\mathcal{U}(0,\ 2.26)$ g/cm^3)
- 13 energy groups
- $N \approx 2.46 \times 10^8$
- 200 snapshots
- 100 test cases

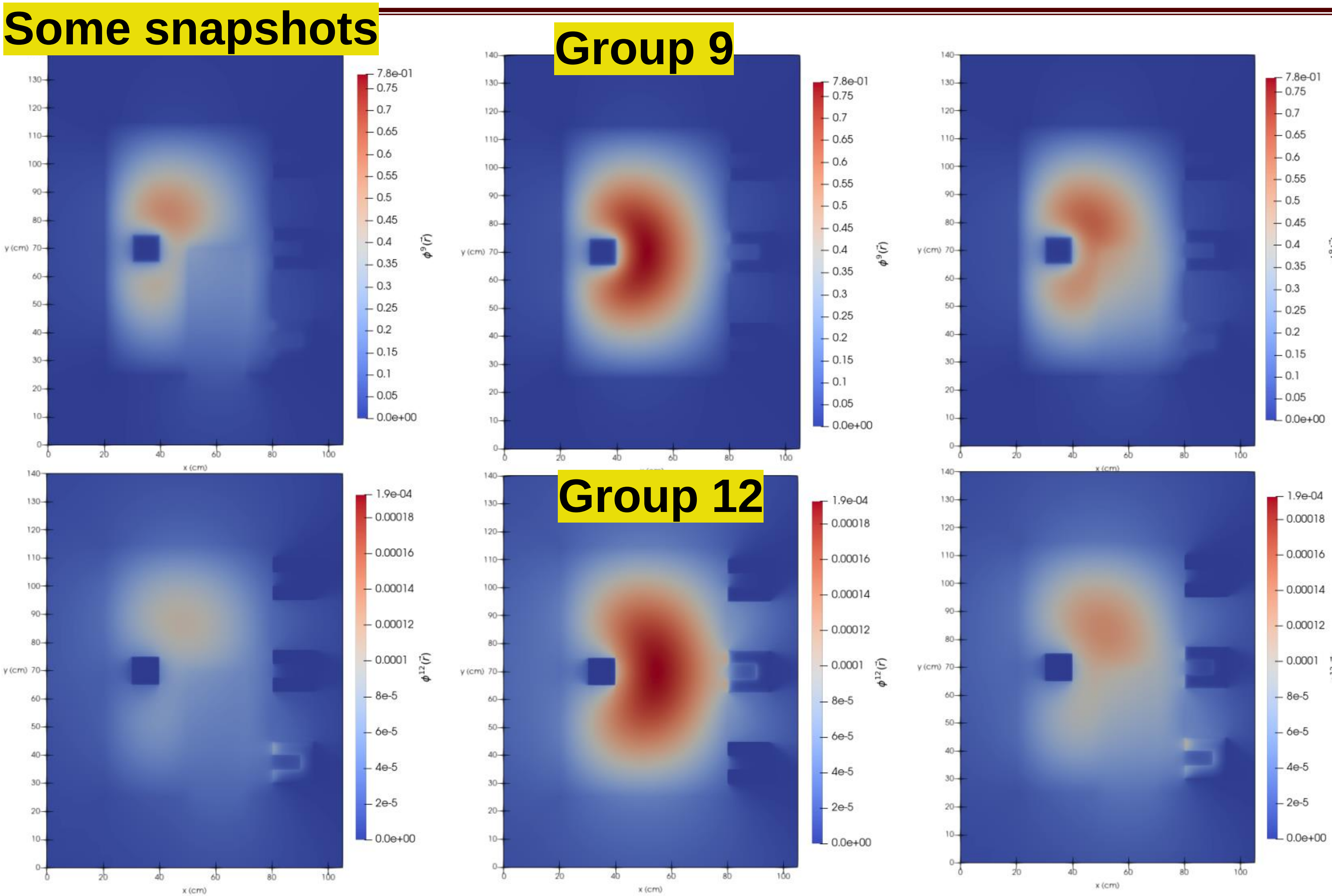
3-D graphite matrix with HDPE shrouds (affine ROM only)



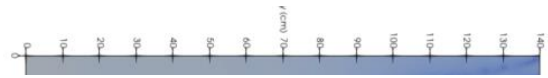


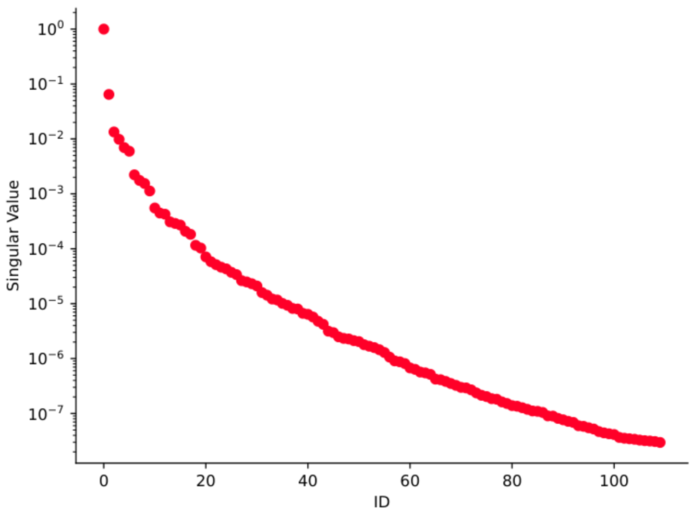
3-D graphite matrix with HDPE shrouds (affine ROM only)

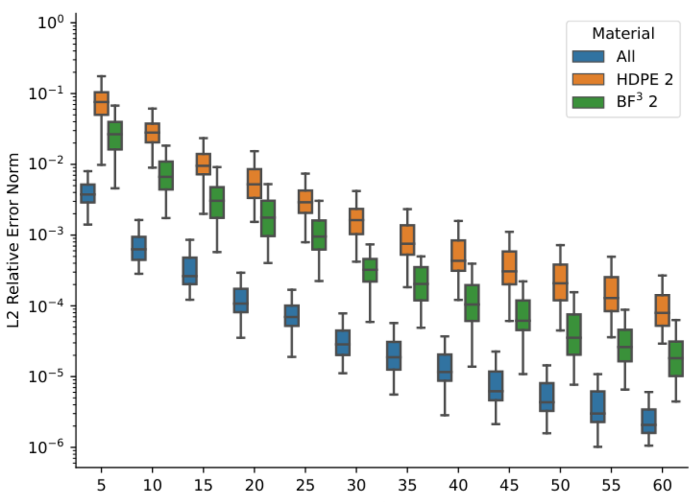
Some snapshots

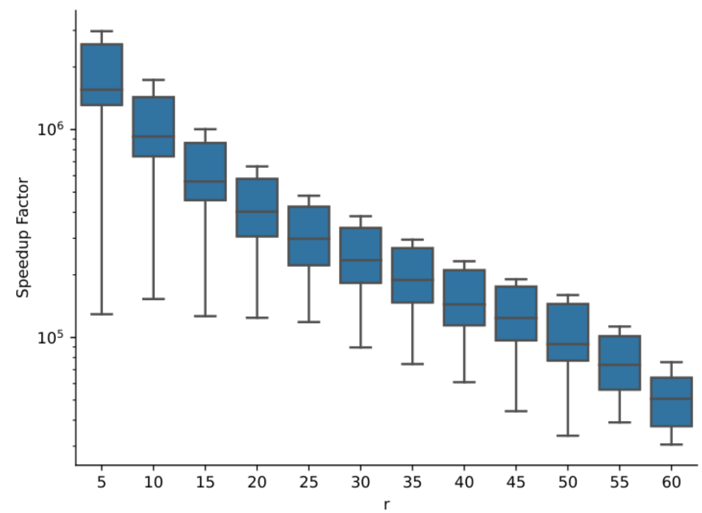


3-D graphite matrix with HDPE shrouds (affine ROM only)









60 POD modes

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3. **Conclusions and Outlook**

Motivation for Operator Inference

- Minimally-invasive ☺ ROM based on the moment form of the TE requires L^{-1}, a full-order operation ☹.
- Affine-decomposition of the angular form of the TE is very code-invasive ☹ but very effective ☺.
- Non-intrusive ☺ black-box schemes

  such as POD + coefficient interpolation / regression / kriging

  Only uses snapshot data and bypasses projection of the PDE.

  Are we still adequately encoding the physics? 😐

- Can we effectively infer the reduced operator from snapshot data without code intrusiveness?

  → Operator inference [Willcox/Peherstorfer/Geelen/…]

Operator inference, with linear manifolds

- **Start with the angular form, seen previously:**

$$\underbrace{\underbrace{(\vec{\Omega}_d \cdot \vec{\nabla}}_{\boldsymbol{G}_d} + \underbrace{\sigma_t^g(\vec{r}))}_{\boldsymbol{T}(\vec{\theta})}}_{\boldsymbol{L}(\vec{\theta})} \underbrace{\psi_d^g(\vec{r})}_{\vec{\Psi}} - \frac{1}{4\pi} \sum_{g'=1}^{G} \underbrace{\sigma_s^{g' \to g}(\vec{r})}_{\boldsymbol{\Sigma}(\vec{\theta})} \sum_{d'=1}^{n_\Omega} w_{d'} \underbrace{\psi_{d'}^{g'}(\vec{r})}_{\vec{\Psi}} = \underbrace{Q_d^g(\vec{r})}_{\vec{Q}}$$

$$(\boldsymbol{G} + \boldsymbol{T}(\vec{\theta}) - \boldsymbol{\Sigma}(\vec{\theta})\boldsymbol{D})\vec{\Psi} = \vec{Q}(\vec{\theta})$$

- **Recognize reaction terms (T and Σ) are affine in the parameters:**

$$\boldsymbol{T}^g(\vec{\theta}) = \sum_{k=1}^{N_{\text{mat}}} \sigma_t^{g,k} \boldsymbol{M}^k , \quad \boldsymbol{\Sigma}_{g,g'}(\vec{\theta})\boldsymbol{D}_{d'} = \sum_{k=1}^{N_{\text{mat}}} \sigma_s^{g' \to g,k} \boldsymbol{M}^k \boldsymbol{D}_{d'} , \quad \vec{Q}_d^g(\vec{\theta}) = \sum_{k=1}^{N_{\text{mat}}} Q_d^{g,k} \vec{f}^k$$

- **Recall that we use DGFEM, so the reaction terms are also block diagonal matrices**
  - ➢ ***Terms are computable, even without access to source code***
    - Need: Mesh (connectivity, material block IDs), and elemental mass matrices/load vectors
  - ➢ ***Material-independent FOM matrices/vectors do not depend on groups or directions***
    - But their small ROM counterparts (because of the POD modes) will be group- and direction-dependent

- **Seek solution as:** $\psi_d^g(\vec{\theta}) = \boldsymbol{U}_r^{g,d} c_d^g(\vec{\theta})$ **(recall, snapshots often are centered)**

Operator inference, with linear manifolds

- **Start with the angular form, seen previously:**

$$\underbrace{\underbrace{(\vec{\Omega}_d \cdot \vec{\nabla}}_{\boldsymbol{G}_d} + \underbrace{\sigma_t^g(\vec{r}))}_{\boldsymbol{T}(\vec{\theta})}}_{\boldsymbol{L}(\vec{\theta})} \underbrace{\psi_d^g(\vec{r})}_{\vec{\Psi}} - \frac{1}{4\pi}\sum_{g'=1}^{G} \underbrace{\sigma_s^{g'\to g}(\vec{r})}_{\boldsymbol{\Sigma}(\vec{\theta})} \sum_{d'=1}^{n_\Omega} w_{d'} \underbrace{\psi_{d'}^{g'}(\vec{r})}_{\vec{\Psi}} = \underbrace{Q_d^g(\vec{r})}_{\vec{Q}}$$

$$(\boldsymbol{G} + \boldsymbol{T}(\vec{\theta}) - \boldsymbol{\Sigma}(\vec{\theta})\boldsymbol{D})\vec{\Psi} = \vec{Q}(\vec{\theta})$$

- **Recognize reaction terms (T and Σ) are affine in the parameters:**

$$\boldsymbol{T}^g(\vec{\theta}) = \sum_{k=1}^{N_{\text{mat}}} \sigma_t^{g,k}\boldsymbol{M}^k\,, \qquad \boldsymbol{\Sigma}_{g,g'}(\vec{\theta})\boldsymbol{D}_{d'} = \sum_{k=1}^{N_{\text{mat}}} \sigma_s^{g'\to g,k}\boldsymbol{M}^k\boldsymbol{D}_{d'}\,, \qquad \vec{Q}_d^g(\vec{\theta}) = \sum_{k=1}^{N_{\text{mat}}} Q_d^{g,k}\vec{f}^k$$

- **Recall that we use DGFEM, so the reaction terms are also block diagonal matrices**
  - ➢ ***Terms are computable, even without access to source code***
    - **Need: Mesh (connectivity, material block IDs), and elemental mass matrices/load vectors**
  - ➢ ***Material-independent FOM matrices/vectors do not depend on groups or directions***
    - **But their small ROM counterparts (because of the POD modes) will be group- and direction-dependent**

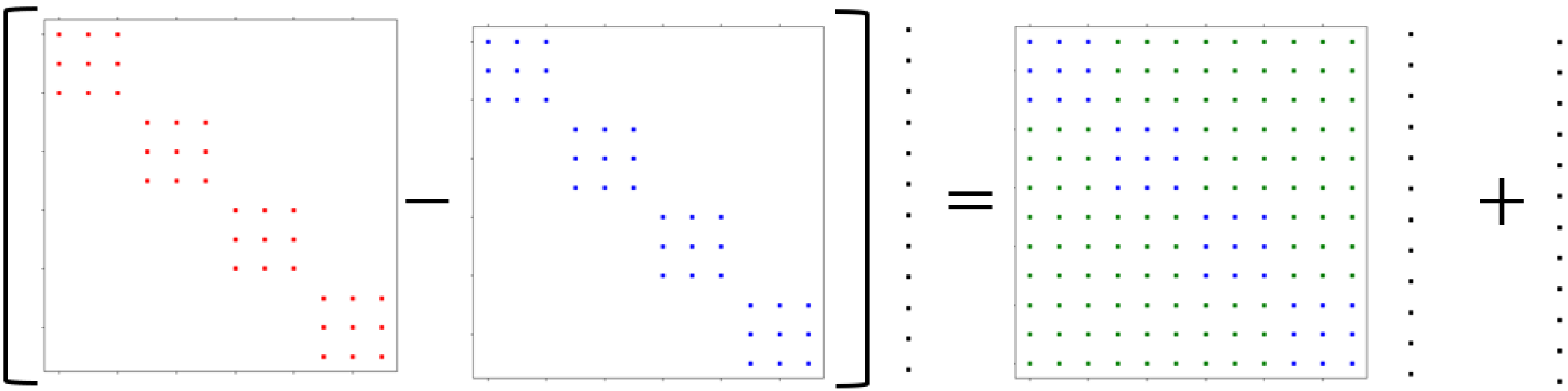
- **Seek solution as:** $\psi_d^g(\vec{\theta}) = \boldsymbol{U}_r^{g,d} c_d^g(\vec{\theta})$ **(recall, snapshots often are centered)**

Operator inference, with linear manifolds

- **After Galerkin projection, the reduced-order system is:**

$$(\boldsymbol{G}_r + \boldsymbol{T}_r(\vec{\mu}) - \boldsymbol{\Sigma}_r(\vec{\mu}))\vec{c}(\vec{\mu})) = \vec{Q}_r(\vec{\mu})$$

  - ***where only $\boldsymbol{G}_r$ is unknown***



Note: can $\boldsymbol{G}_r$ be inferred per group and per direction independently

Operator inference, with linear manifolds

- **After Galerkin projection, the reduced-order system is:**

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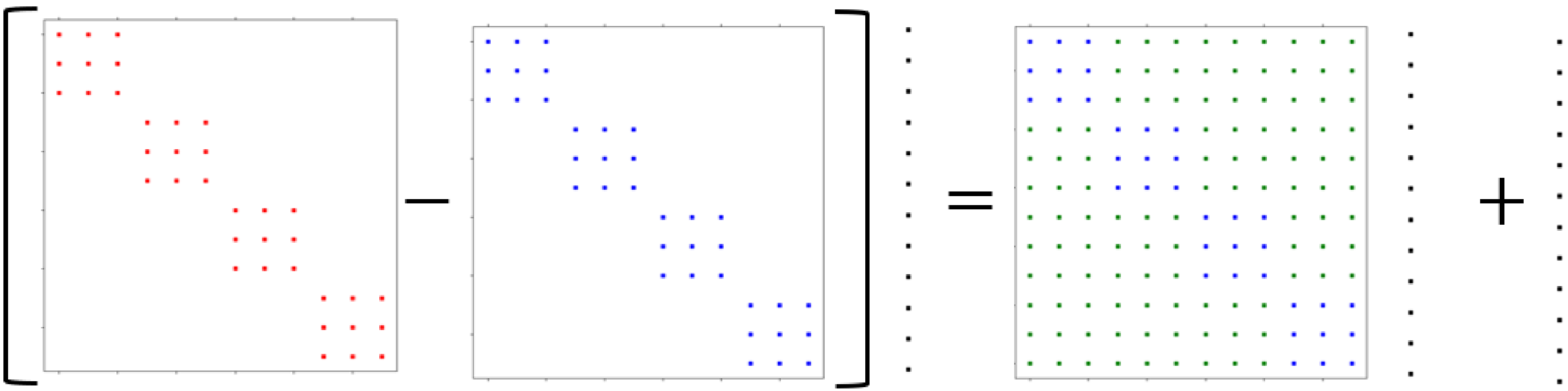

Note: can $\boldsymbol{G}_r$ **be inferred per group and per direction independently**

with

$$\boldsymbol{C} = \begin{bmatrix} \vdots & & \vdots \\ \vec{c}(\mu_1), & \ldots, & \vec{c}(\mu_{N_{\text{snap}}}) \\ \vdots & & \vdots \end{bmatrix} \qquad \boldsymbol{R} = \begin{bmatrix} \vdots & & \vdots \\ \vec{r}(\mu_1), & \ldots, & \vec{r}(\mu_{N_{\text{snap}}}) \\ \vdots & & \vdots \end{bmatrix}$$

and

$$\vec{r}(\mu_i) = \vec{Q}_r(\mu_i) - \left(\boldsymbol{T}_r(\vec{\mu}_i) - \boldsymbol{\Sigma}_r(\vec{\mu}_i)\right)\vec{c}_i$$

Operator Inference, with nonlinear manifolds

$$\psi_d^g = \underbrace{\boldsymbol{U}_r^{g,d} c_d^g}_{=\text{linear}} + \underbrace{\overline{\boldsymbol{U}}_q^{g,d} \mathbf{X}^{g,d} f_p(c_d^g)}_{=\text{nonlinear}}$$

with

- $\boldsymbol{U}_r^{g,d} \in \mathbb{R}^{N\times r}$: linear subspace of dimension r
- c_d^g: reduced coordinates
- $f_p(c) = [c^2, \ldots, c^p]$: polynomial representation from degree 2 up to p
- $\overline{\boldsymbol{U}}_q^{g,d} \in \mathbb{R}^{N\times q}$: q-dimensional subspace. Requiring $[\boldsymbol{U}_r, \overline{\boldsymbol{U}}_q]^T [\boldsymbol{U}_r, \overline{\boldsymbol{U}}_q] = \boldsymbol{I}_{r+q}$ suggests an easy choice for $\overline{\boldsymbol{U}}_q$: the next q POD modes.
- $\mathbf{X}^{g,d} \in \mathbb{R}^{q\times(p-1)r}$: a mapping of the polynomial expansion of the reduced state vector onto $\overline{\boldsymbol{U}}_q$

Operator Inference, with nonlinear manifolds

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- $\mathbf{X}^{g,d} \in \mathbb{R}^{q\times(p-1)r}$: a mapping of the polynomial expansion of the reduced state vector onto $\overline{\boldsymbol{U}}_q$

$$\mathbf{X}^{g,d} = \text{argmin}_{\mathbf{X}\in\mathbb{R}^{q\times(p-1)r}} \left(\frac{1}{2} \sum_{i=1}^{N_{\text{snap}}} \left\| \psi_d^g(\vec{\mu}_i) - \left[\boldsymbol{U}_r^{g,d}, \overline{\boldsymbol{U}}_q^{g,d}\right]^T \begin{bmatrix} c_d^g \\ \mathbf{X} f_p(c_d^g) \end{bmatrix} \right\|_2^2 + \frac{\lambda}{2} \|\mathbf{X}\|_F^2 \right)$$

Operator Inference, with nonlinear manifolds

- **LS solution** $$\mathbf{X}^{g,d} = [\overline{\boldsymbol{U}}_q^{g,d}]^T \underbrace{[\Psi_d^g - \boldsymbol{U}_r^{g,d} c_d^g]}_{=\text{proj.error}} \boldsymbol{F}^T \left(\boldsymbol{F}\boldsymbol{F}^T + \lambda \boldsymbol{I}\right)^{-1}$$

with

$$\boldsymbol{F} = \begin{bmatrix} \vdots & & \vdots \\ f(c_d^g(\mu_1)), & \ldots, & f(c_d^g(\mu_{N_{\text{snap}}})) \\ \vdots & & \vdots \end{bmatrix}$$

Performing OpInf using the nonlinear representation:

$$\boldsymbol{G}_r \vec{c}(\vec{\mu}) + \boldsymbol{P}_r \vec{f}(\vec{\mu}) = \underbrace{\vec{Q}_r(\vec{\mu}) - (\boldsymbol{T}_r(\vec{\mu}) - \boldsymbol{\Sigma}_r(\vec{\mu}))\vec{c}(\vec{\mu})) - (\boldsymbol{T}_r^f(\vec{\mu}) - \boldsymbol{\Sigma}_r^f(\vec{\mu}))\vec{f}(\vec{\mu}))}_{\vec{r}(\mu)}$$

$$\boldsymbol{G}_r = \boldsymbol{U}_r^T \boldsymbol{G} \boldsymbol{U}_r \quad , \quad \boldsymbol{P}_r = \boldsymbol{U}_r^T \boldsymbol{G} \overline{\boldsymbol{U}}_q \mathbf{X} \quad , \quad \boldsymbol{T}_r^f(\vec{\mu}) = \boldsymbol{U}_r^T \boldsymbol{T} \overline{\boldsymbol{U}}_q \mathbf{X} \quad , \quad \boldsymbol{\Sigma}_r^f(\vec{\mu}) = \boldsymbol{U}_r^T \boldsymbol{\Sigma} \overline{\boldsymbol{U}}_q \mathbf{X}$$

Finding $\boldsymbol{G}_r$ and $\boldsymbol{P}_r$ in a least-square sense over all snapshots μ_i

$$(\boldsymbol{G}_r, \boldsymbol{P}_r) = \text{argmin}_{\boldsymbol{G}_r \in \mathbb{R}^{r \times r}, \in \mathbb{R}^{r \times (p-1)r}} \left(\frac{1}{2} \sum_i \left\| \boldsymbol{G}_r \vec{c}(\vec{\mu}_i) + \boldsymbol{P}_r \vec{f}(\vec{\mu}_i) - \vec{r}(\vec{\mu}_i) \right\|_2^2 + \frac{\lambda^G}{2} \|\boldsymbol{G}_r\|_F^2 + \frac{\lambda^P}{2} \|\boldsymbol{P}_r\|_F^2 \right)$$

Coupled system: alternating directions (solve for $\boldsymbol{G}_r$ with old $\boldsymbol{P}_r$, then solve for $\boldsymbol{P}_r$ using updated $\boldsymbol{G}_r$, ...)

Problem Set-up

Source in absorber	Absorber	Void	Source in scatterer	Scatterer
$S_{\text{fixed}}, \sigma_t$	σ_t		$S_{\text{fixed}}, \sigma_t, \sigma_s$	σ_s, σ_t

6 params

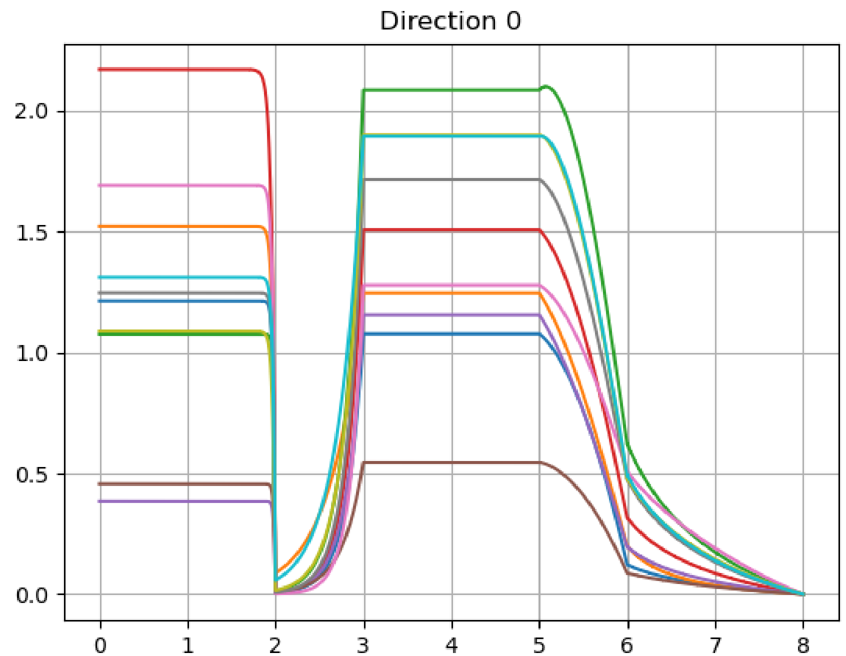
Solution in 8 discrete directions at nominal values of the parameters

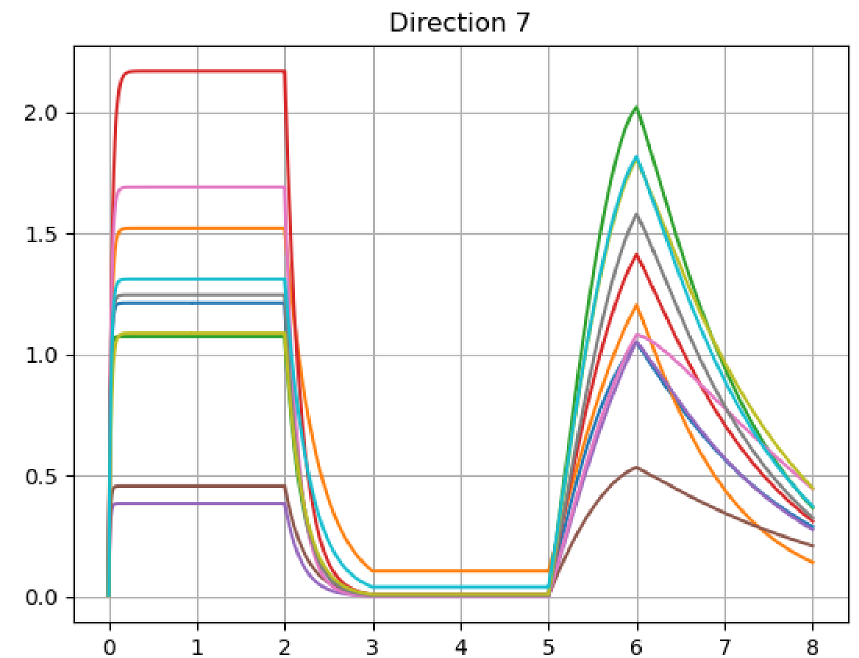
Sample snapshots

Source in absorber	Absorber	Void	Source in scatterer	Scatterer
$S_{\text{fixed}}, \sigma_t$	σ_t		$S_{\text{fixed}}, \sigma_t, \sigma_s$	σ_s, σ_t

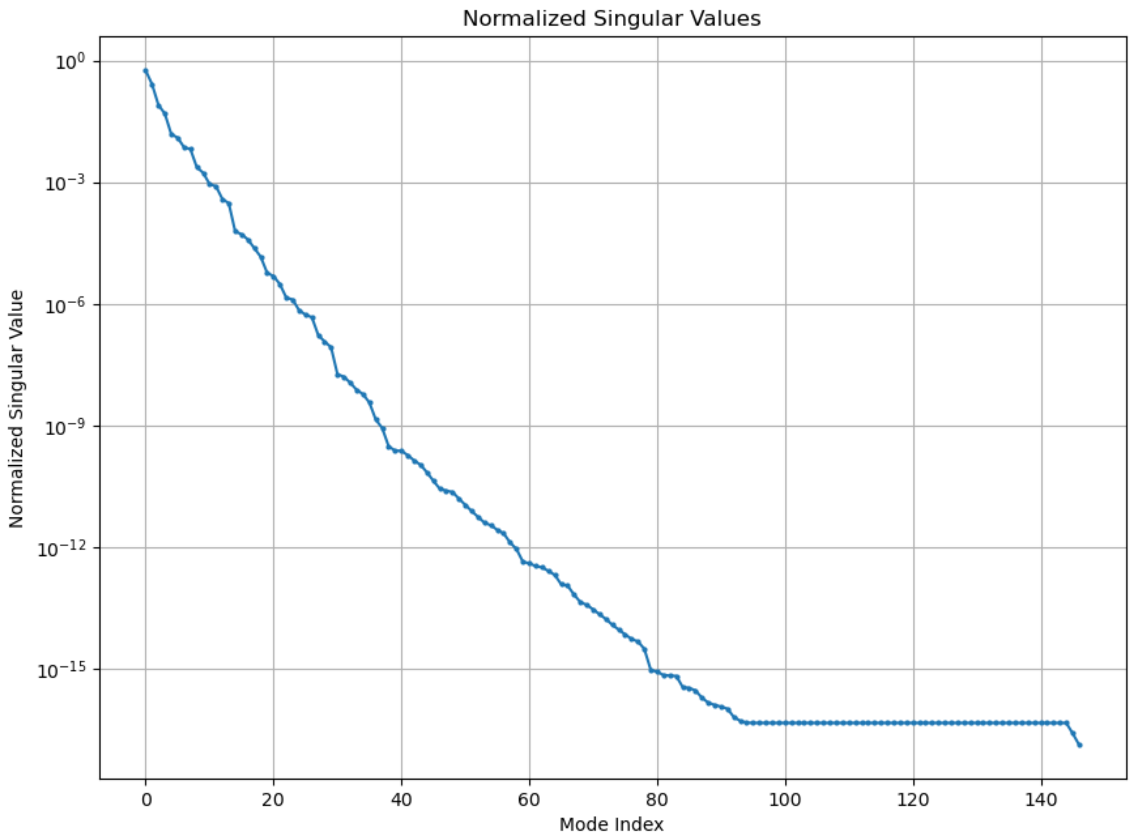
6 params

- **Parametric range +/- 50% of nominal values**
- **Sample snapshots for first and last directions:**



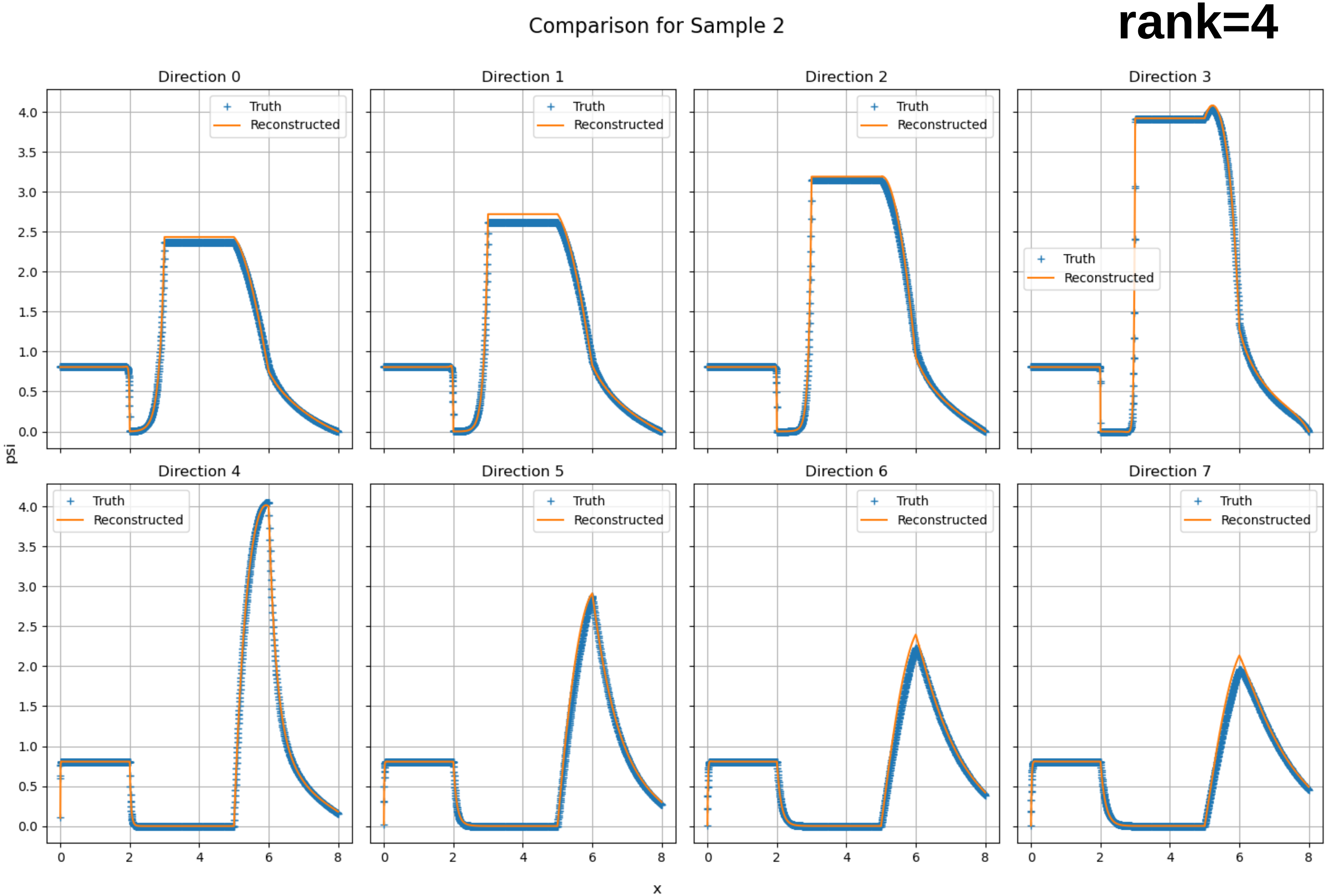


OpInf reconstruction, with linear manifolds



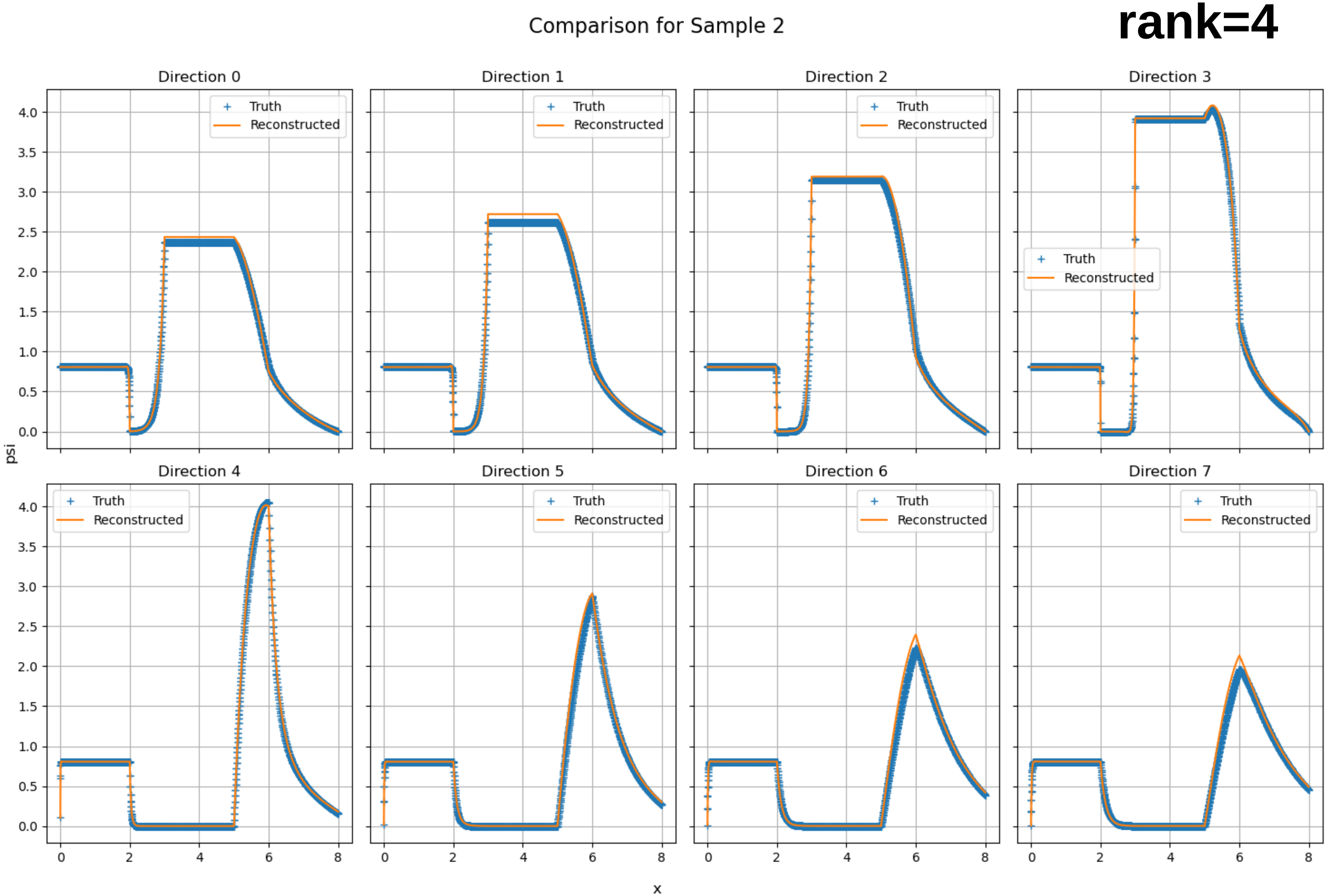
OpInf reconstruction, with linear manifolds

rank=4

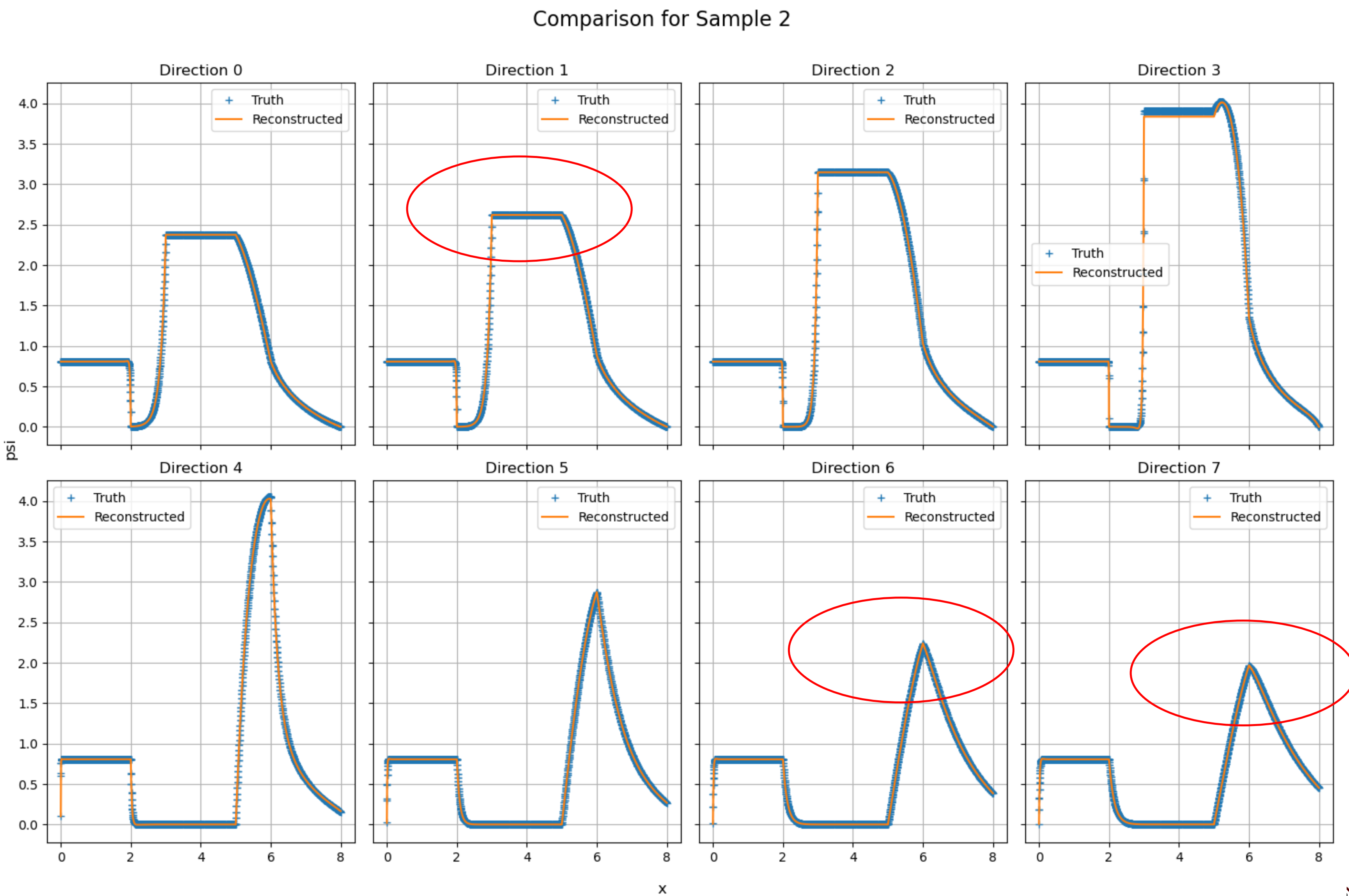


OpInf reconstruction, with linear manifolds

rank=4

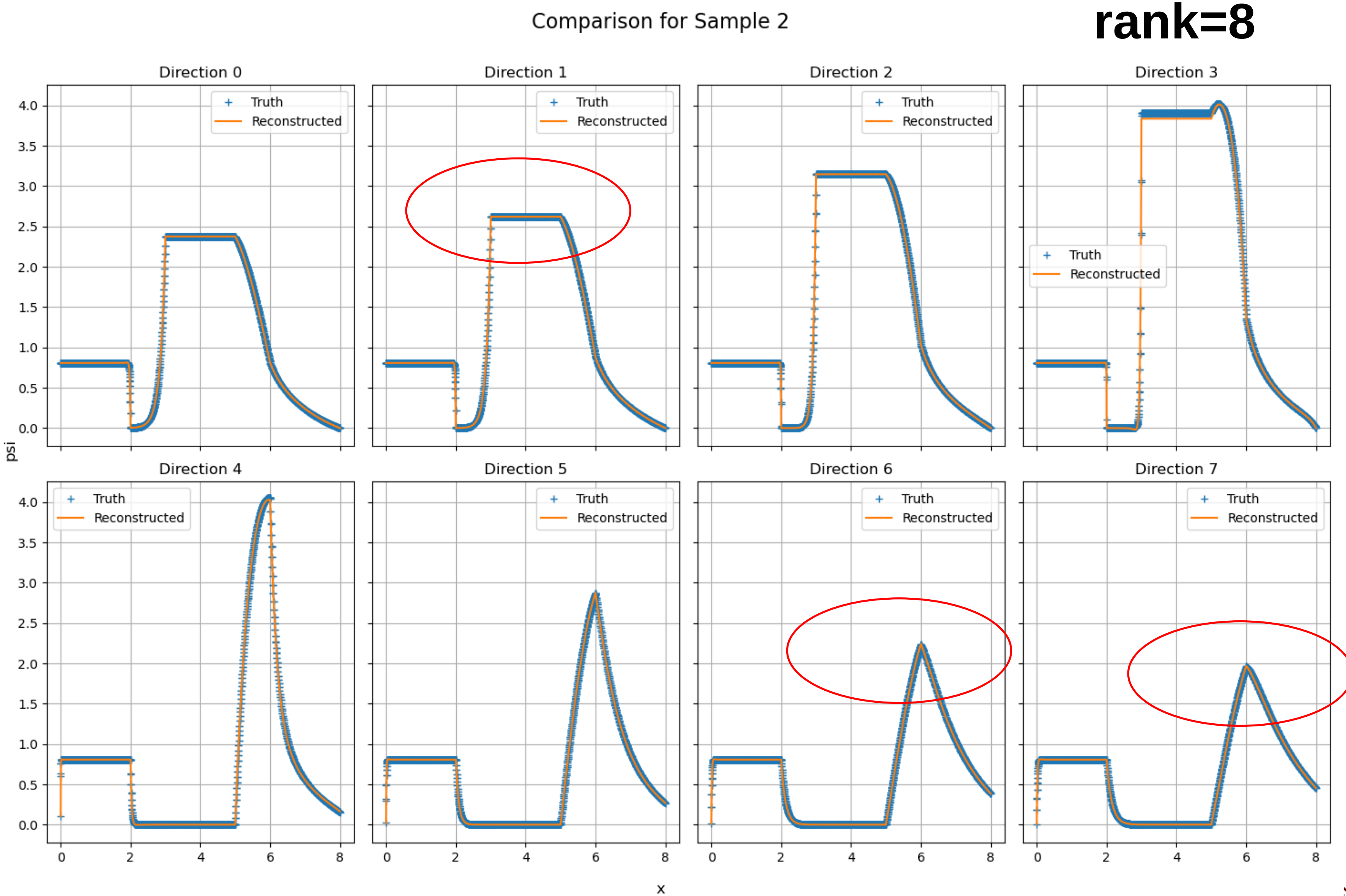


OpInf reconstruction, with linear manifolds

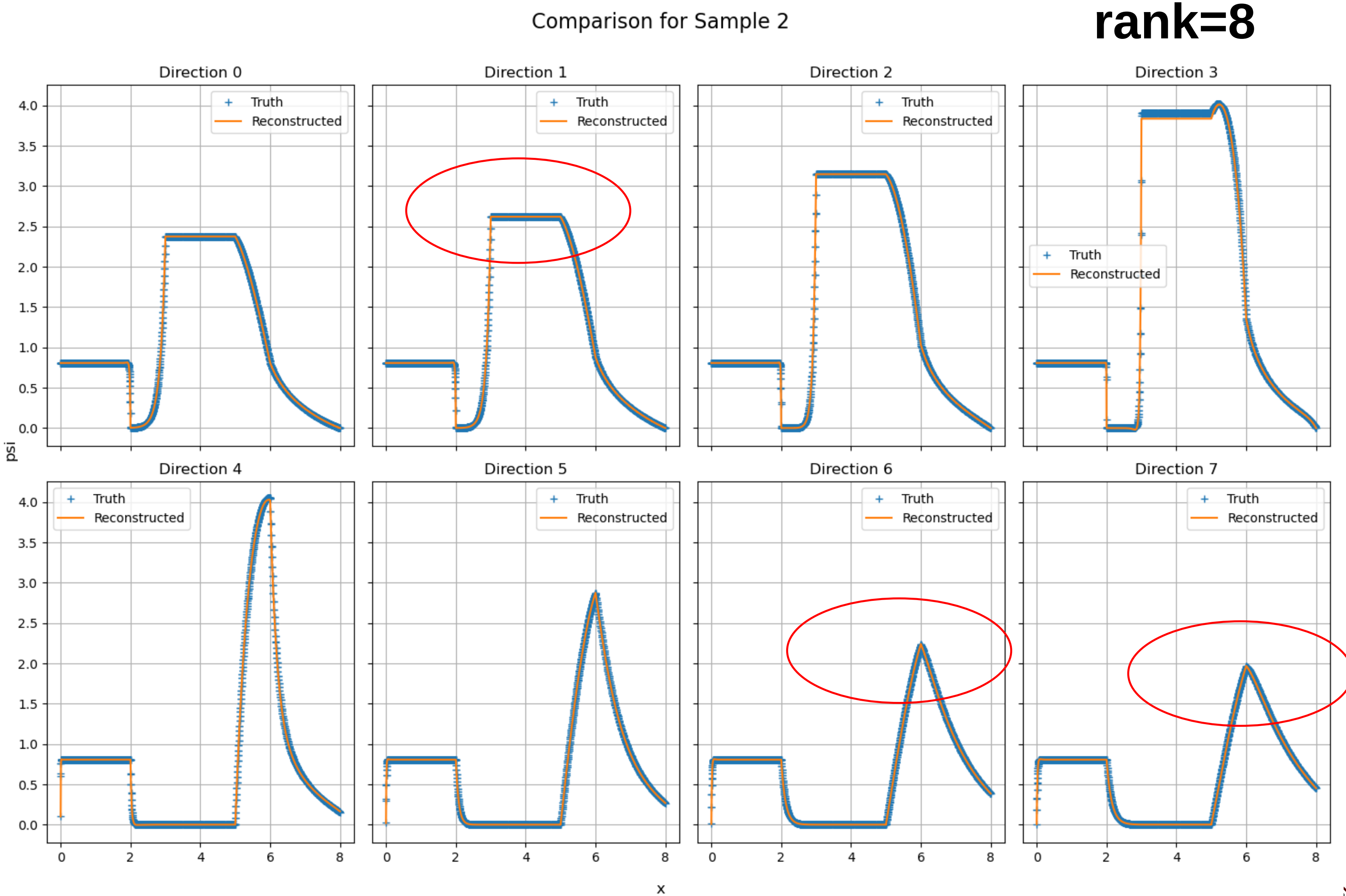


OpInf reconstruction, with linear manifolds

rank=8

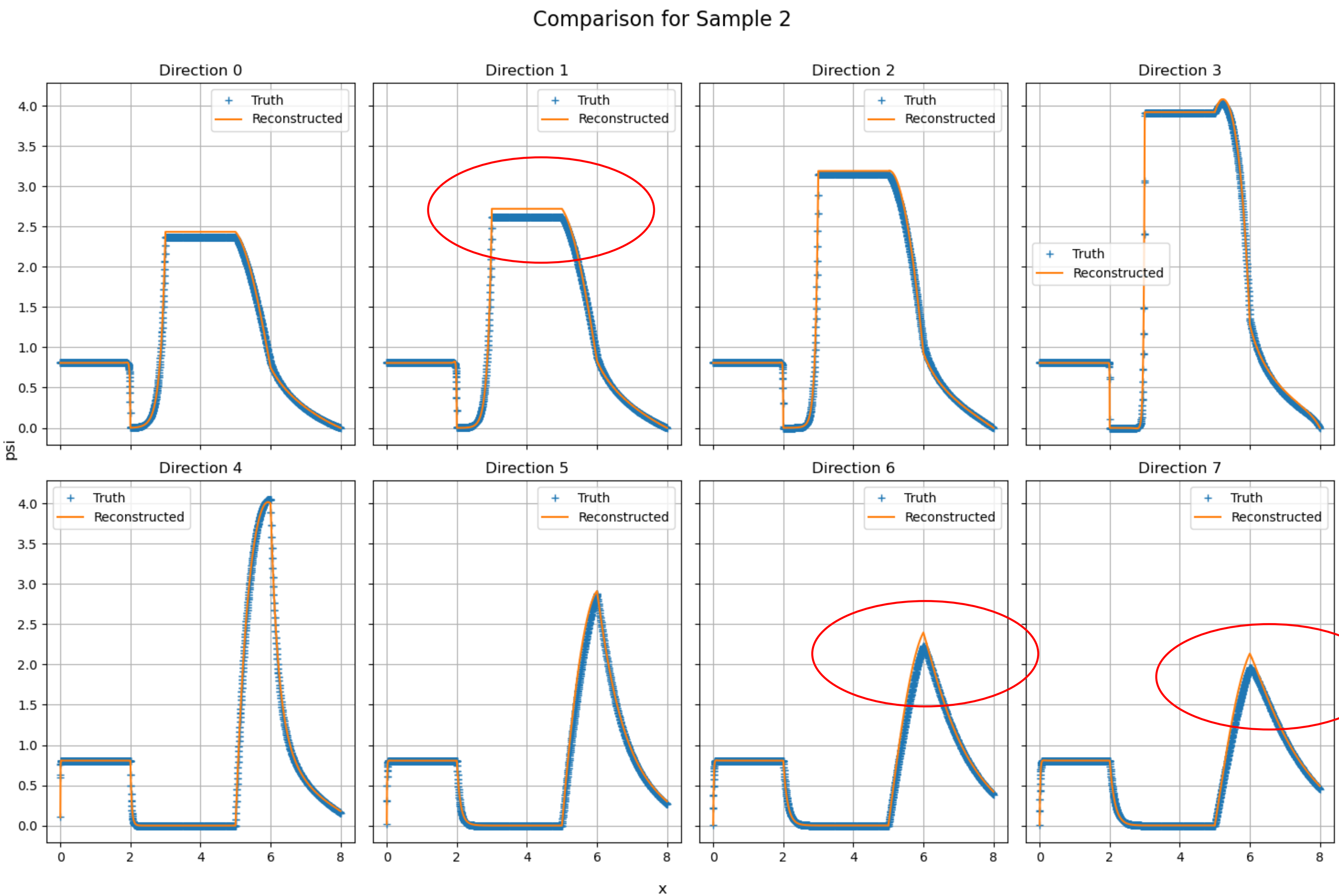


OpInf reconstruction, with linear manifolds



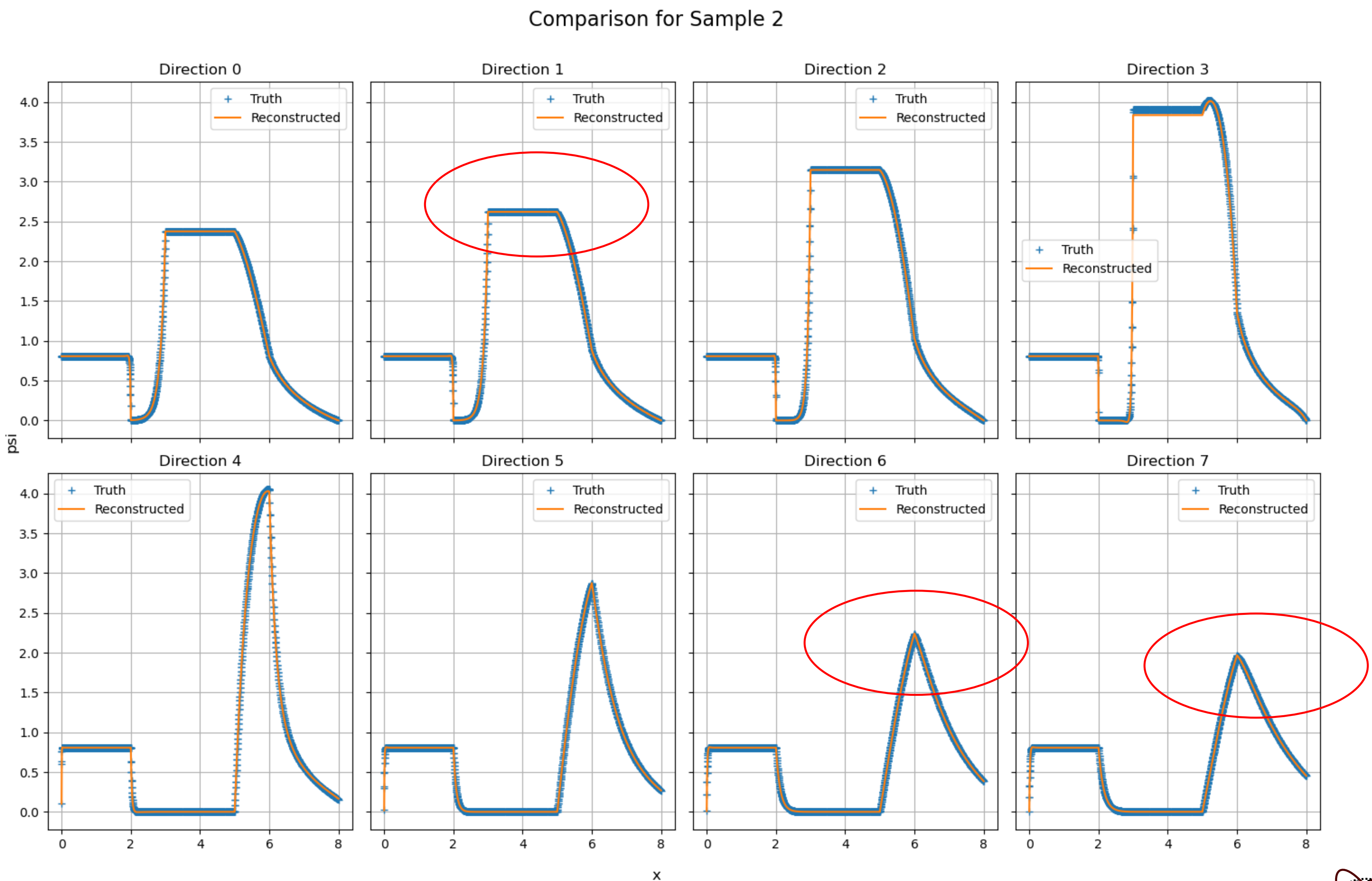
OpInf, with linear and nonlinear manifolds

rank=4



OpInf, with linear and nonlinear manifolds

rank=4



Outline

1. **Background on Radiation Transport**
   - A. *Motivations for (parametric) ROM for Radiation Transport*
   - B. *Crash course on Radiation Transport*

2. **Reduced-Order Models for Radiation Transport**
   - A. *Projection-based pROM:*
     - i. Minimally-invasive approach
     - ii. Affine decomposition of operators
   - B. *Non-intrusive pROM*
     - i. Gaussian process regression, MARS
   - C. *Operator inference for pROM*
     - i. Linear and Nonlinear Frameworks
   - D. *Operator inference for time-dependent ROM (linear manifolds)*
   - E. *Diffusion-based ROM + Discrepancy Emulation (if time permits)*

3. **Conclusions and Outlook**

Operator inference: Time-dependent problems

- **Time-evolution FOM:** $$\frac{\mathbf{1}}{\boldsymbol{v}}\partial_t \Psi + (\boldsymbol{G}+\boldsymbol{T}-\boldsymbol{\Sigma}\boldsymbol{D})\Psi = Q$$
- **Same philosophy:**
  - *All reaction terms are affine-decomposable, hence computable easily*
  - $\boldsymbol{G}_r$ *is the only unknown*
- **Using training data and form a least-square system (with Tikhonov regularization)**

$$\boldsymbol{G}_r = \operatorname{argmin}_{\boldsymbol{G}_r \in \mathbb{R}^{r\times r}} \left(\frac{1}{2}\sum_{n=1}^{N_\tau} \left\| \frac{\mathbf{1}}{\boldsymbol{v}}\frac{d}{dt}\vec{c}_n + \boldsymbol{G}_r\vec{c}_n + (\boldsymbol{T}_r - \boldsymbol{\Sigma}_r)\vec{c}_n - \vec{Q}_r \right\|_2^2 + \frac{\lambda}{2}\|\boldsymbol{G}_r\|_F^2 \right)$$

  - $\frac{d}{dt}\vec{c}_n$*: computed using high-order finite-differences from the collected temporal snapshots*

- **LS solve (same as before):**

$$\boldsymbol{G}_r = \boldsymbol{R}\boldsymbol{C}^T\left(\boldsymbol{C}\boldsymbol{C}^T + \lambda\boldsymbol{I}\right)^{-1}$$

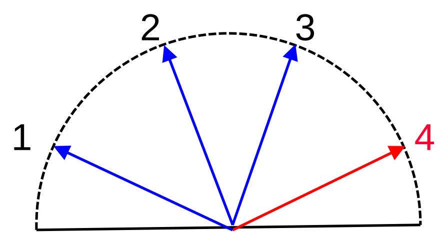
with

$$\boldsymbol{C} = \begin{bmatrix} \vdots & & \vdots \\ \vec{c}(t_1), & \ldots, & \vec{c}(t_{N_\tau}) \\ \vdots & & \vdots \end{bmatrix} \qquad \boldsymbol{R} = \begin{bmatrix} \vdots & & \vdots \\ \vec{r}(t_1), & \ldots, & \vec{r}(t_{N_\tau}) \\ \vdots & & \vdots \end{bmatrix}$$

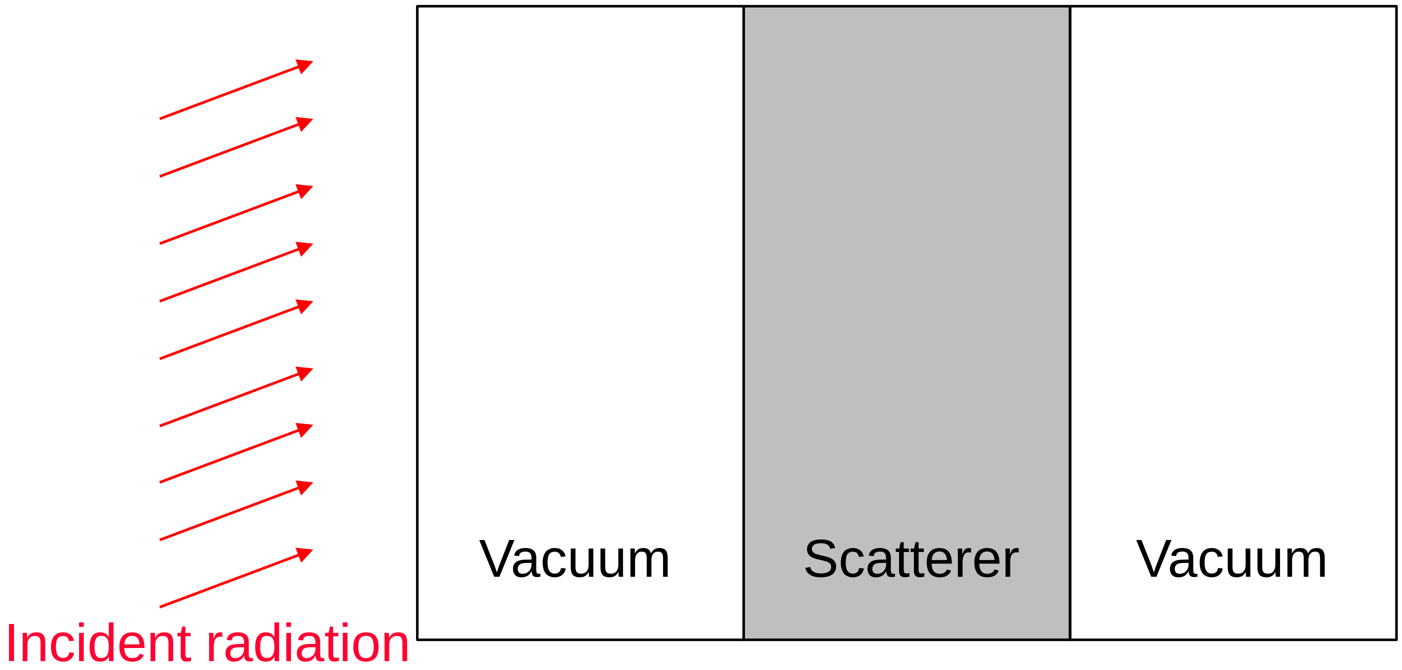
and

$$\vec{r}(t_n) = \vec{Q}_r - (\boldsymbol{T}_r - \boldsymbol{\Sigma}_r)\vec{c}(t_n) - \frac{\mathbf{1}}{\boldsymbol{v}}\frac{d}{dt}\vec{c}(t_n)$$

Problem Set-up



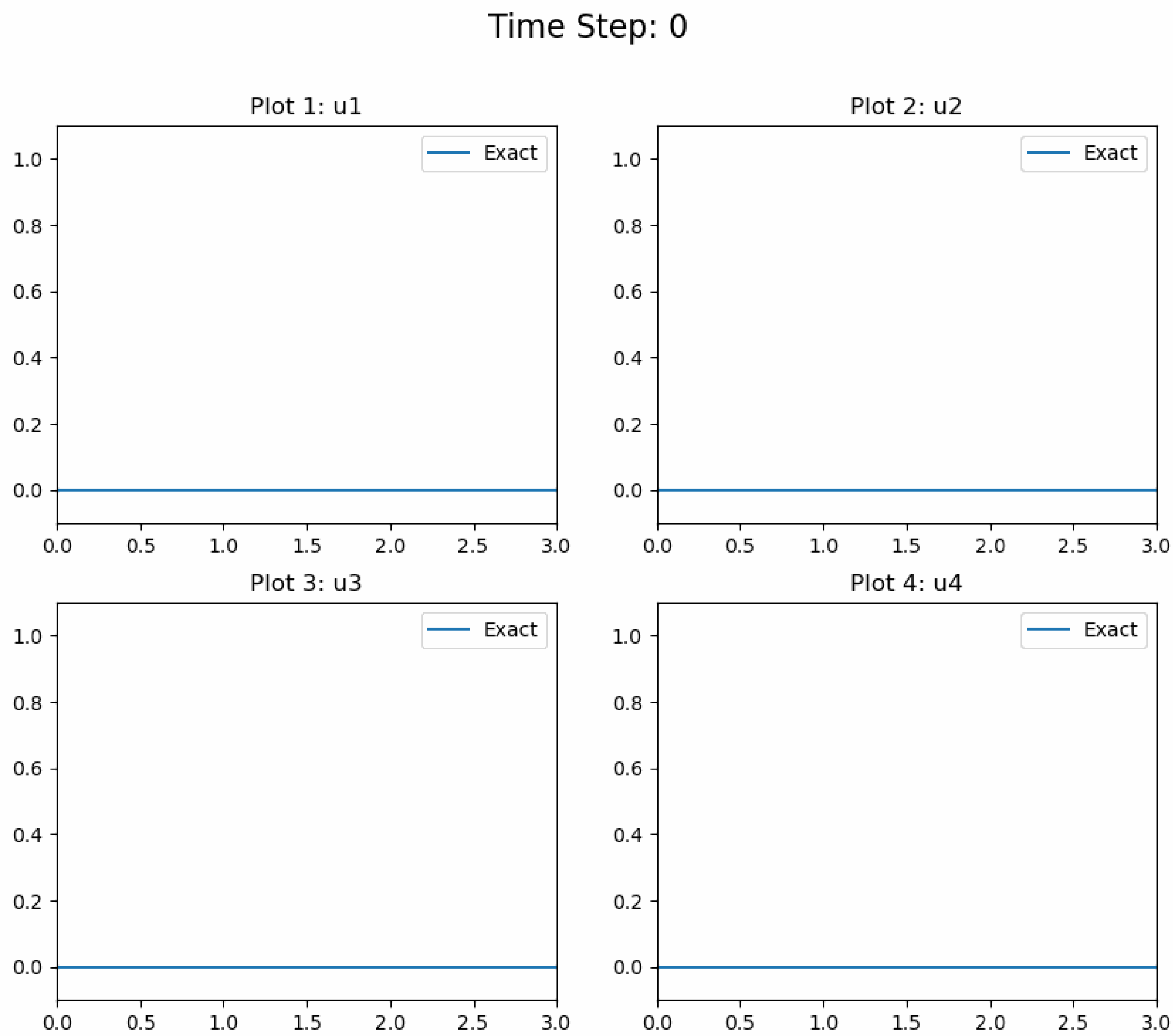
Tracking radiation in 4 directions (cones)



Exact (reference) Solution

d = 1

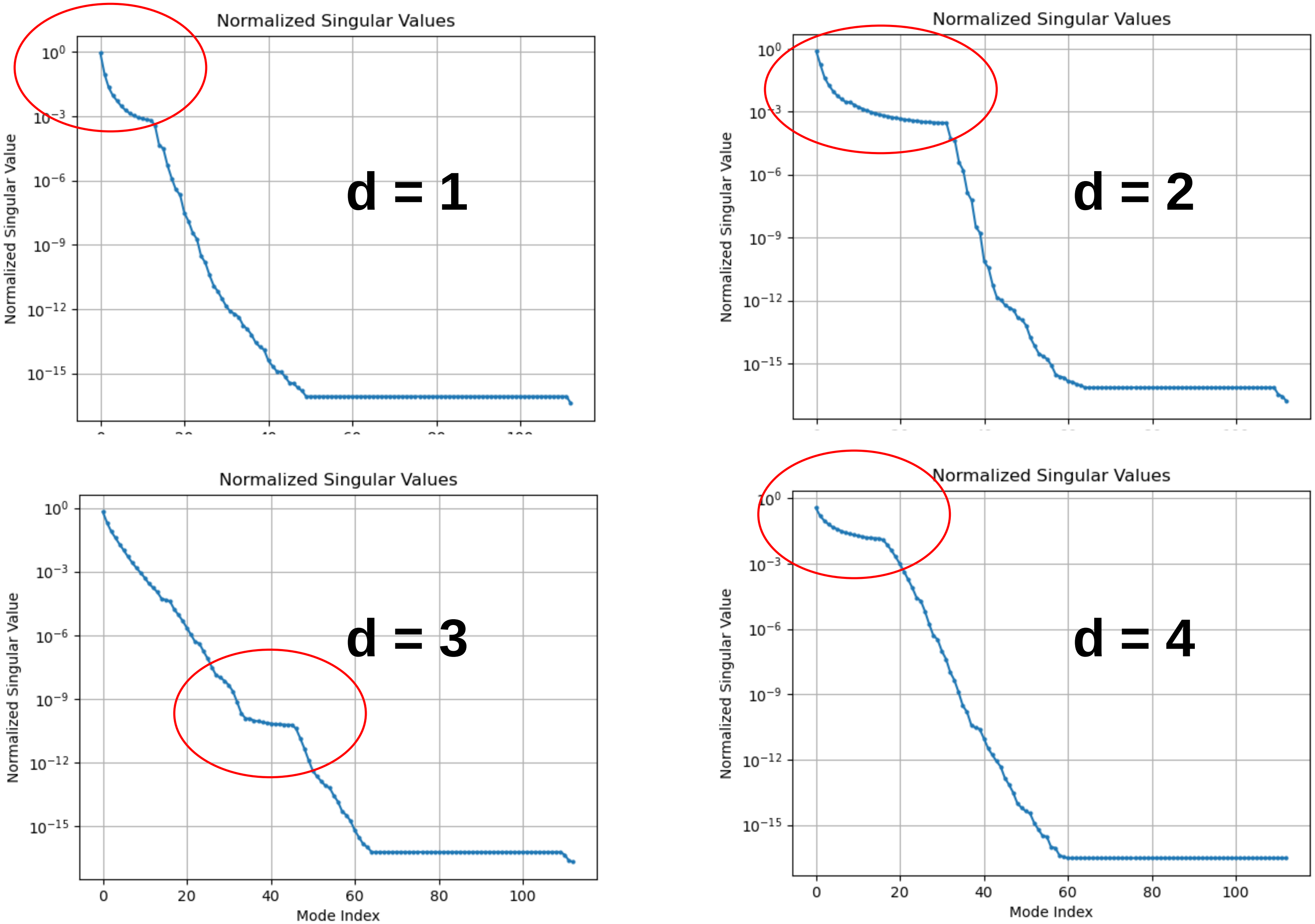
d = 2



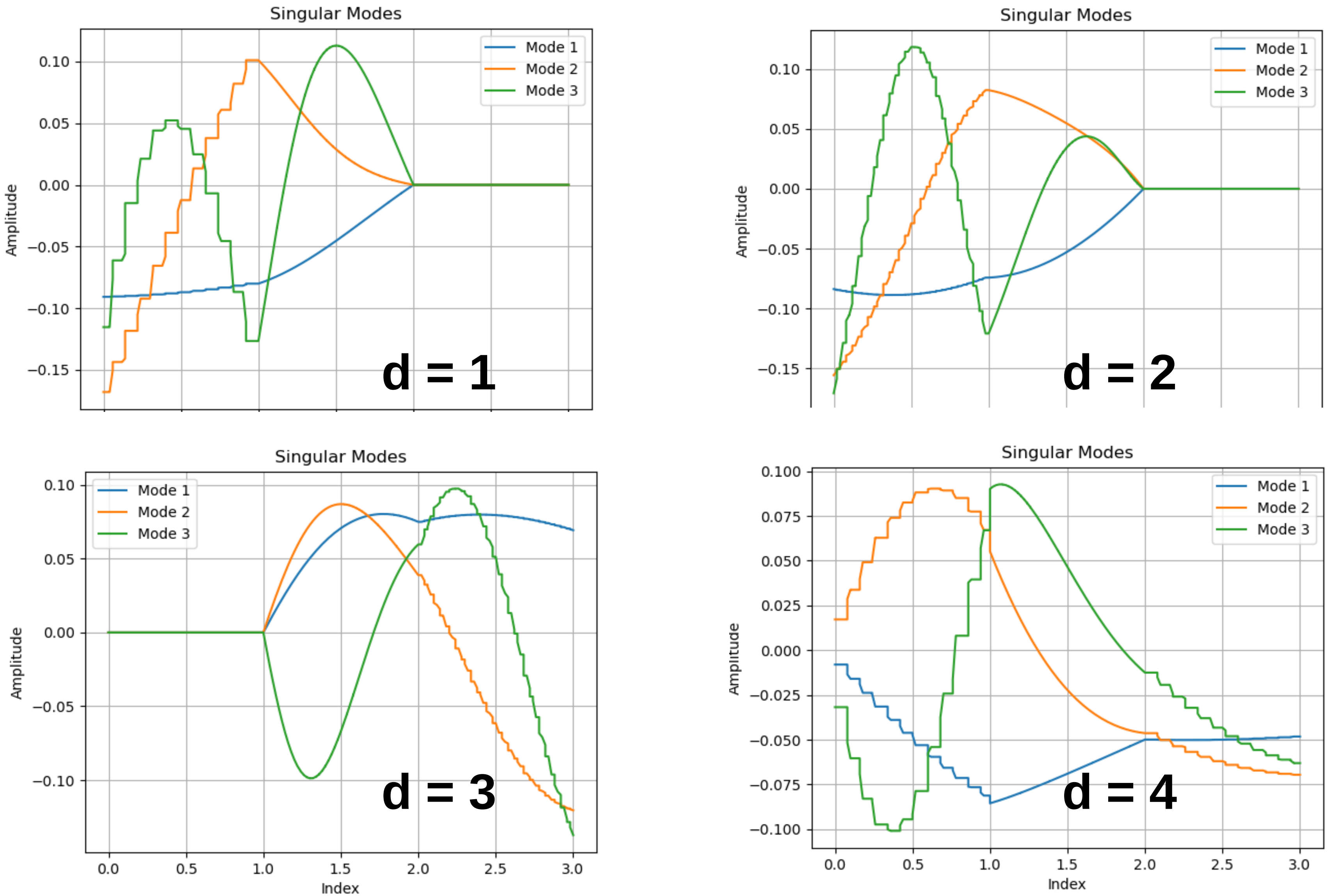
d = 3

d = 4

Singular values plots per direction

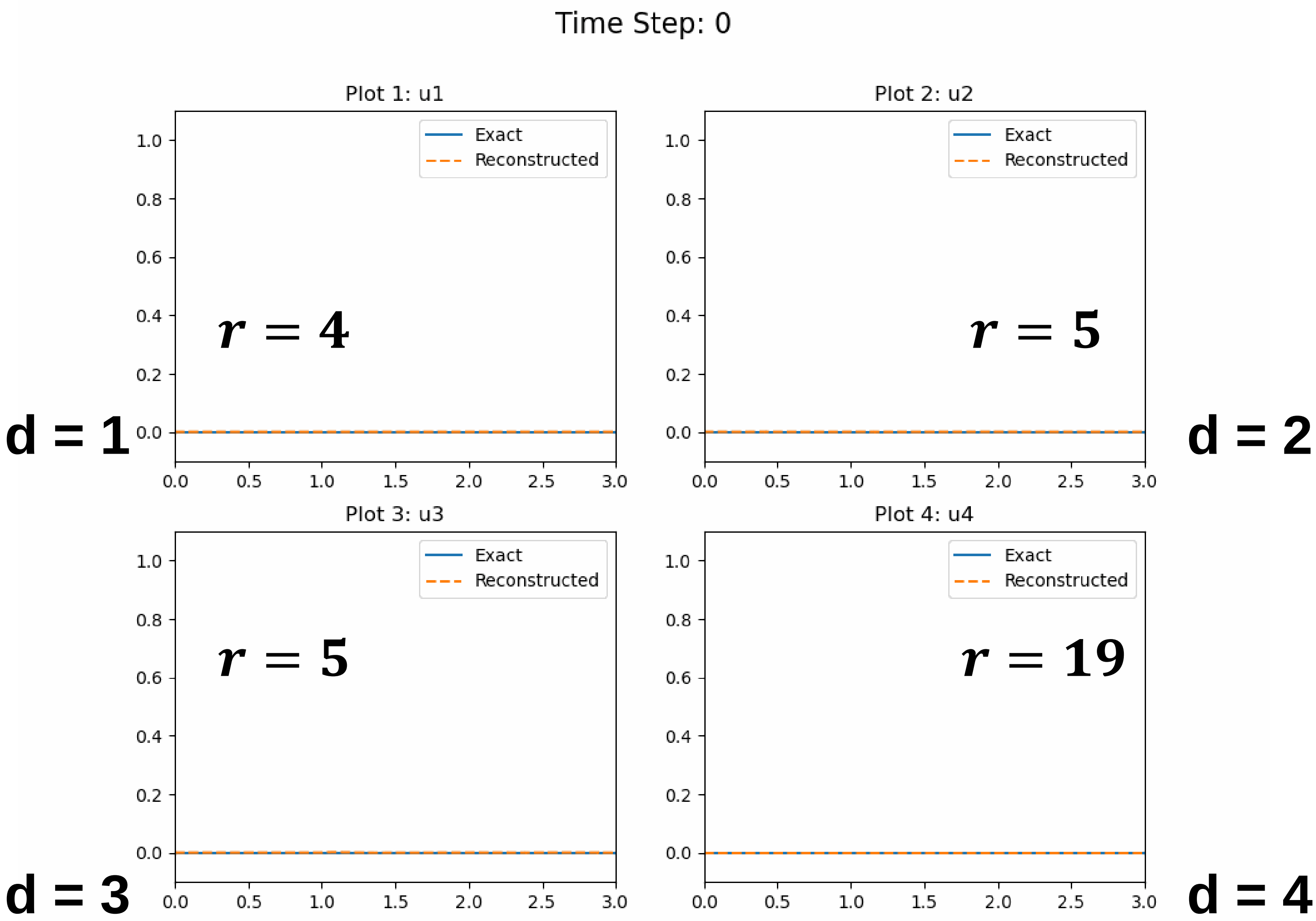


POD modes



Singular Modes
Mode 1
Mode 2
Mode 3
Amplitude
Index
d = 1
d = 2
d = 3
d = 4

Reconstruction with OpInf



Conclusions

- Parametric ROM for radiation transport
  - *Minimally-invasive approach*
  - *Affine Decomposition*
  - *Non-intrusive POD+regression (Gaussian process, sparse-grid interpolant, MARS)*
  - *Operator inference with linear and nonlinear manifolds*
- Operator inference for time-dependent problems (with linear manifolds)

- Next:
  - *Operator inference for TD with nonlinear manifolds*
  - *Low-rank approximation in the 6D phase-space (space+energy+direction)*
    - Tensor decomposition

- Open-source Software: OpenSn
  - https://github.com/Open-Sn/OpenSn
  - Massively parallel Linear Boltzmann solver
  - No physics: user supplies interaction properties σ

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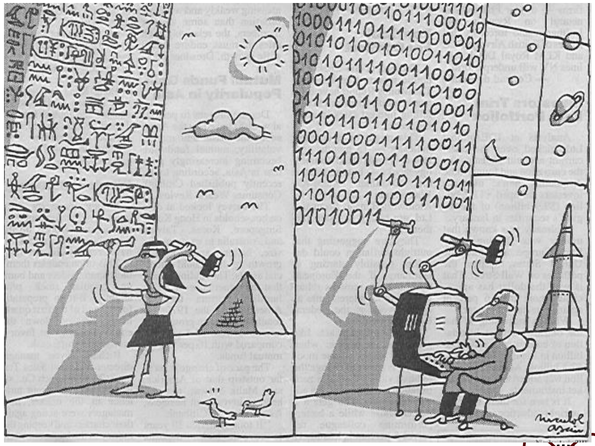

Thanks and EOF

- **Students and Post-docs: Patrick Behne (INL), Ian Halvic (X-energy), Peter German (INL), Dominic Caron (LLNL), Mauricio Tano (INL), Ian Aranda (LANL), Quincy Huhn (2025)**
- **Sponsors:**
  - **DOE/NEUP (Nuclear Energy)**
  - **DOD/DTRA (Defense Thread Reduction Agency)**
  - **LLNL**

10 *20* *50* *100*