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Learning Low-Rank Neutron Transport Dynamics on Linear and Nonlinear Manifolds

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Outline

I. Motivation & Problem Setting

- Why ROM for parametric neutron transport?
- The parametric mono-energetic neutron transport problem
- Full order DG- S_N semi-discretization

II. Methodology

- Linear and Nonlinear Manifold ROM
- Proper orthogonal decomposition
- Nonlinear manifolds via quadratic lifting
- Semi-intrusive operator inference

III. Numerical Results

- 1D slab benchmark – projection & inference
- 1D lifting dimension study
- 2D heterogeneous benchmark – scalar flux & convergence

IV. Conclusions & Future Work

Motivation: UQ in Neutron Transport

Physical Setting

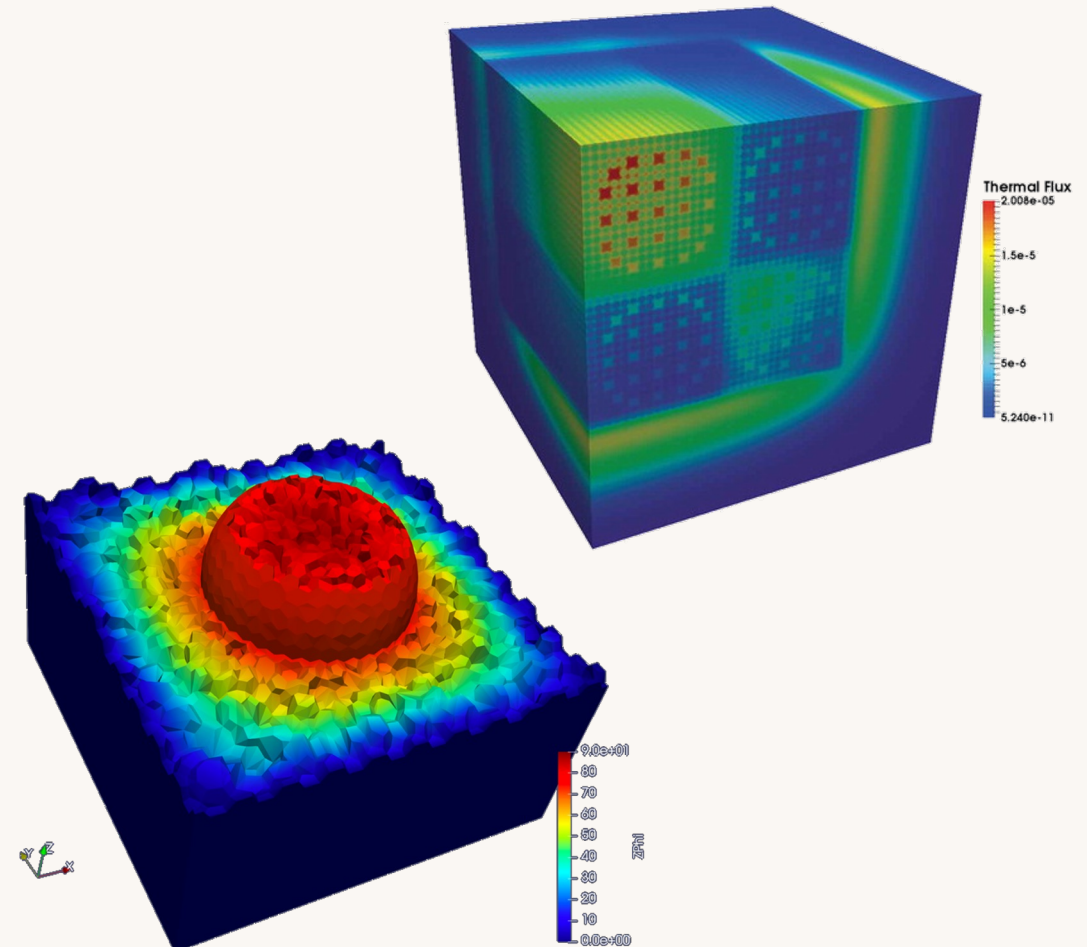
- Time-dependent mono-energetic neutron transport
- Parameter dependent cross sections $\sigma_t(\boldsymbol{\mu})$, $\sigma_s(\boldsymbol{\mu})$
source $Q(t, \boldsymbol{\mu})$, boundary conditions $\Psi^{\text{in}}(\mathbf{x}, \boldsymbol{\Omega}, t; \boldsymbol{\mu})$

The UQ Challenge

- Epistemic uncertainty: $\boldsymbol{\mu}$ not known exactly
- Need statistics of $\Psi(\mathbf{x}, \boldsymbol{\Omega}, t; \boldsymbol{\mu})$ or related QoIs
- Monte Carlo / quadrature requires repeated solves

Computational Bottleneck

- A single FOM solve: 10^5 – 10^9 DOFs, very expensive!
- ROM target: 10^2 – $10^5 \times$ speed-up at certified accuracy





The Parametric Neutron Transport Problem

Strong Form: Find the angular neutron flux $\Psi = \Psi(\mathbf{x}, \boldsymbol{\Omega}, t; \boldsymbol{\mu}) : \mathcal{D} \times \mathcal{S}^2 \times \mathcal{T} \times \mathcal{U} \rightarrow \mathbb{R}$, such that

$$\begin{aligned} \frac{1}{v} \frac{\partial \Psi}{\partial t} + \boldsymbol{\Omega} \cdot \nabla \Psi + \sigma_t(\boldsymbol{\mu}) \Psi - \frac{\sigma_s(\boldsymbol{\mu})}{4\pi} \int_{\mathcal{S}^2} \Psi(\boldsymbol{\Omega}') d\boldsymbol{\Omega}' &= \frac{Q(t, \boldsymbol{\mu})}{4\pi} && \text{in } \mathcal{D} \times \mathcal{S}^2 \times \mathcal{T} \times \mathcal{U}, \\ \Psi(\mathbf{x}, \boldsymbol{\Omega}, t; \boldsymbol{\mu}) &= \Psi^{\text{in}}(\mathbf{x}, \boldsymbol{\Omega}, t; \boldsymbol{\mu}) && \text{on } \Gamma^- \times \mathcal{T} \times \mathcal{U}, \quad (\text{inflow boundary data}) \\ \Psi(\mathbf{x}, \boldsymbol{\Omega}, 0; \boldsymbol{\mu}) &= \Psi_0(\mathbf{x}, \boldsymbol{\Omega}, t; \boldsymbol{\mu}) && \text{on } \mathcal{D} \times \mathcal{S}^2 \times \mathcal{T} \times \mathcal{U}, \quad (\text{initial condition}) \end{aligned}$$

Notation:

- $\mathcal{D} \subset \mathbb{R}^3$ compact Lipschitz domain
- \mathcal{S}^2 is the unit sphere in \mathbb{R}^3 (angle space)
- $\mathcal{T} := [0, T]$ is the integration time horizon
- $\mathcal{U} \subset \mathbb{R}^{N_\mu}$ is the parameters set
- $v \in \mathbb{R}^+$ is the neutron speed
- $\sigma_t, \sigma_s : \mathcal{D} \times \mathcal{U} \rightarrow \mathbb{R}^+$ are heterogeneous macroscopic cross-sections
- $Q : \mathcal{D} \times \mathcal{T} \times \mathcal{U} \rightarrow \mathbb{R}$ is a parametric isotropic volumetric source
- $\mathbf{n}(\mathbf{x}) \in \mathcal{S}^2$ is the unit outward normal to $\partial \mathcal{D}$
- $\Gamma^- := \{(\mathbf{x}, \boldsymbol{\Omega}) \in \partial \mathcal{D} \times \mathcal{S}^2 \mid \boldsymbol{\Omega} \cdot \mathbf{n}(\mathbf{x}) < 0\}$ is the inflow boundary



Full-Order Model: DG- S_N Semi-Discretization

Phase-Space Discretization

- S_N angular quadrature: N_Ω discrete directions
- Discontinuous Galerkin (DG) spatial discretization

Monolithic System ODE

$$\mathbb{M} \frac{d\boldsymbol{\psi}}{dt} + (\mathbb{G} + \mathbb{A}_\mu - \mathbb{B}_\mu) \boldsymbol{\psi} = \mathbf{p}_\mu + \mathbf{q}_\mu$$

where:

$\boldsymbol{\psi} \in \mathbb{R}^{\mathcal{N}}$	state vector ($\mathcal{N} = N_\Omega \times N_x$ DOFs)
$\mathbb{M} \in \mathbb{R}^{\mathcal{N} \times \mathcal{N}}$	mass matrix
$\mathbb{G} \in \mathbb{R}^{\mathcal{N} \times \mathcal{N}}$	streaming operator (advection)
$\mathbb{A}_\mu, \mathbb{B}_\mu \in \mathbb{R}^{\mathcal{N} \times \mathcal{N}}$	absorption / scattering operators
$\mathbf{p}_\mu, \mathbf{q}_\mu \in \mathbb{R}^{\mathcal{N}}$	volume and boundary sources



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Linear vs. Nonlinear Manifold ROM



Linear Manifold (POD-Galerkin)

$$\psi(t; \mu) \approx \psi_\infty(t) + \mathbb{U}_r \mathbf{c}_r(t; \mu) \quad \text{with} \quad \mathbb{U}_r \in \mathbb{R}^{N \times N_r}$$



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ROM via Galerkin projection onto $\text{span}(\mathbf{U}_r)$

$$\mathbf{M}_r \frac{d\mathbf{c}_r}{dt} + (\mathbf{G}_r + \mathbf{A}_{\boldsymbol{\mu},r} - \mathbf{B}_{\boldsymbol{\mu},r}) \mathbf{c}_r = \mathbf{r}_{\boldsymbol{\mu},r}$$

where

$$\mathbf{A}_{\boldsymbol{\mu},r} = \mathbf{U}_r^\top \mathbf{A}_\boldsymbol{\mu} \mathbf{U}_r, \quad \mathbf{M}_r = \mathbf{U}_r^\top \mathbf{M} \mathbf{U}_r$$

$$\mathbf{B}_{\boldsymbol{\mu},r} = \mathbf{U}_r^\top \mathbf{B}_\boldsymbol{\mu} \mathbf{U}_r, \quad \mathbf{G}_r = \mathbf{U}_r^\top \mathbf{G} \mathbf{U}_r$$

$$\mathbf{r}_{\boldsymbol{\mu},r} = \mathbf{U}_r^\top \left(\mathbf{p}_\boldsymbol{\mu} + \mathbf{q}_\boldsymbol{\mu} - (\mathbf{G} + \mathbf{A}_\boldsymbol{\mu} - \mathbf{B}_\boldsymbol{\mu}) \boldsymbol{\psi}_\infty - \mathbf{M} \frac{d\boldsymbol{\psi}_\infty}{dt} \right)$$



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Nonlinear Manifold (Quadratic Lifting)

$$\boldsymbol{\psi}(t; \boldsymbol{\mu}) \approx \boldsymbol{\psi}_\infty(t) + \mathbf{U}_q \mathbf{f}(\mathbf{c}_r(t; \boldsymbol{\mu})) \quad \text{with } \mathbf{U}_q = [\mathbf{U}_r, \bar{\mathbf{U}}_q] \in \mathbb{R}^{\mathcal{N} \times (N_r + N_q)}$$

assuming quadratic lifting

$$\mathbf{f}(\mathbf{c}_r) = [\mathbf{c}_r, \mathbb{X} \text{vec}(\mathbf{c}_r \mathbf{c}_r^T)]^T \in \mathbb{R}^{N_r + N_q}$$

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assuming quadratic lifting

$$\mathbf{f}(\mathbf{c}_r) = [\mathbf{c}_r, \mathbb{X} \text{vec}(\mathbf{c}_r \mathbf{c}_r^\top)]^\top \in \mathbb{R}^{N_r + N_q}$$

ROM via projection onto $\text{span}(\mathbf{U}_r)$ and reconstruction on $\text{span}(\mathbf{U}_q)$

$$\mathbf{M}_r \frac{d\mathbf{c}_r}{dt} + (\mathbf{G}_r + \mathbf{A}_{\boldsymbol{\mu},r} - \mathbf{B}_{\boldsymbol{\mu},r}) \mathbf{c}_r + (\bar{\mathbf{G}}_r + \bar{\mathbf{A}}_{\boldsymbol{\mu},r} - \bar{\mathbf{B}}_{\boldsymbol{\mu},r}) \mathbb{X} \text{vec}(\mathbf{c}_r \mathbf{c}_r^\top) = \mathbf{r}_{\boldsymbol{\mu},r}$$

where

$$\bar{\mathbf{A}}_{\boldsymbol{\mu},r} = \mathbf{U}_r^\top \mathbf{A}_\boldsymbol{\mu} \bar{\mathbf{U}}_q, \quad \mathbf{0} = \mathbf{U}_r^\top \mathbf{M} \bar{\mathbf{U}}_q$$

$$\bar{\mathbf{B}}_{\boldsymbol{\mu},r} = \mathbf{U}_r^\top \mathbf{B}_\boldsymbol{\mu} \bar{\mathbf{U}}_q, \quad \bar{\mathbf{G}}_r = \mathbf{U}_r^\top \mathbf{G} \bar{\mathbf{U}}_q$$



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Why Standard ROMs Struggle

- Slow Kolmogorov n-width decay for transport
- No global assemblage of the matrix \mathbb{G}



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Our Approach

- Nonlinear manifold to overcome slow n-width decay
- Semi-intrusive inference to avoid global \mathbb{G} assembly
- Projection based assemblage of the affine-decomposed operators $\mathbb{A}_\mu, \mathbb{B}_\mu$ and of the vector $\mathbf{p}_\mu, \mathbf{q}_\mu$.



Training Phase: A Three-steps Approach

1) Reduced Basis Space (offline)

- Collect N_S snapshots $\psi(t_i; \mu_i)$ from the full order model
- Compute POD basis $\mathbb{U}_q = [\mathbb{U}_r, \bar{\mathbb{U}}_q] \in \mathbb{R}^{\mathcal{N} \times (N_r + N_q)}$ truncated at relative energy threshold $\varepsilon > 0$

2) Nonlinear Manifold (offline)

- Choose a nonlinear function, $\mathbf{f}(\mathbf{c}_r) = [\mathbf{c}_r, \mathbb{X} \text{vec}(\mathbf{c}_r \mathbf{c}_r^T)]^T$ (N_r latent variables, N_p lifting coordinates)
- Identify the lifting coefficients matrix \mathbb{X} via Tikhonov-regularized least squares

3) Operator Inference (offline)

- Compute the reduced reaction operators $\mathbb{A}_{\mu,r}, \bar{\mathbb{A}}_{\mu,r}$, and $\mathbb{B}_{\mu,r}, \bar{\mathbb{B}}_{\mu,r}$ via direct projection from cell-local data
- Use alternating minimization to infer the nonlinear pair $\mathbb{G}_r, \bar{\mathbb{G}}_r$.



Proper Orthogonal Decomposition

Snapshot matrix

- Center snapshots: $\mathbf{s}^{(i)} = \boldsymbol{\psi}(t_i; \boldsymbol{\mu}_i) - \boldsymbol{\psi}_\infty(t_i)$
- Build snapshot matrix: $\mathbb{S} = [\mathbf{s}^{(1)}, \dots, \mathbf{s}^{(N_S)}] \in \mathbb{R}^{\mathcal{N} \times N_S}$

Thin SVD and truncation

- Compute: $\mathbb{M}^{1/2} \mathbb{S} = \check{\mathbb{U}} \Sigma \mathbb{V}^\top$, $\sigma_1 \geq \dots \geq \sigma_{N_S} \geq 0$
- Retain $N_r + N_q$ leading modes at energy threshold $\varepsilon > 0$
- Augmented POD basis: $\mathbb{M}^{-\frac{1}{2}} \check{\mathbb{U}}_q = [\mathbb{U}_r, \bar{\mathbb{U}}_q] \in \mathbb{R}^{\mathcal{N} \times (N_r + N_q)}$
- Orthogonal components: $\mathbb{U}_r^\top \mathbb{M} \bar{\mathbb{U}}_q = \mathbf{0}$

Latent and lifting coordinates

- Latent coords: $\mathbf{c}_r = \mathbb{U}_r^\top \mathbf{s} \in \mathbb{R}^{N_r}$
- Lifting coords: $\bar{\mathbf{c}}_q = \bar{\mathbb{U}}_q^\top \mathbf{s} \in \mathbb{R}^{N_q}$



Nonlinear Manifold Learning

Quadratic approximation

- POD residual: $\mathbf{s}^{(i)} - \mathbb{U}_r \mathbf{c}_r^{(i)} \approx \bar{\mathbb{U}}_q \bar{\mathbf{c}}_q^{(i)}$
- Quadratic ansatz: $\mathbf{s}^{(i)} - \mathbb{U}_r \mathbf{c}_r^{(i)} \approx \bar{\mathbb{U}}_q \mathbb{X} \text{vec}(\mathbf{c}_r^{(i)} \mathbf{c}_r^{(i)\top})$

Tikhonov regularized least squares

Estimate the coefficient matrix $\mathbb{X} \in \mathbb{R}^{N_q \times N_r^2}$ by solving the minimization problem

$$\mathbb{X} = \mathbb{Y} \mathbb{L} \quad \text{with} \quad \mathbb{Y} = \arg \min_{\tilde{\mathbb{Y}}} \sum_{i=1}^{N_S} \left\| \tilde{\mathbb{Y}} \mathbb{L} \text{vec}(\mathbf{c}_r^{(i)} \mathbf{c}_r^{(i)\top}) - \bar{\mathbf{c}}_q^{(i)} \right\|^2 + \gamma \|\tilde{\mathbb{Y}}\|^2$$

Where we have introduced the structure matrix $\mathbb{L} \in \mathbb{R}^{N_\ell \times N_r^2}$, and the unknowns' matrix $\mathbb{Y} \in \mathbb{R}^{N_q \times N_\ell}$.



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Two variations for \mathbb{L}

- **Tensorial:** $\mathbb{L} \in \mathbb{R}^{N_r(N_r+1)/2 \times N_r^2}$, $N_\ell = N_r(N_r + 1)/2$, captures all pairwise mode interactions
- **Element-wise quadratic:** $\mathbb{L} \in \mathbb{R}^{N_r/2 \times N_r^2}$, $N_\ell = N_r$, captures only the independent quadratic terms

Notice that \mathbb{X} is computed once offline from snapshot data alone.



Semi-Intrusive Operator Inference

Projected (Intrusive) Operators

- Reaction operator projection requires no global assembly: exploit cell-local structure of DG

$$\mathbb{M}_r \frac{d\mathbf{c}_r}{dt} + (\mathbb{G}_r + \mathbb{A}_{\mu,r} - \mathbb{B}_{\mu,r})\mathbf{c}_r + (\bar{\mathbb{G}}_r + \bar{\mathbb{A}}_{\mu,r} - \bar{\mathbb{B}}_{\mu,r})\mathbb{X} \text{vec}(\mathbf{c}_r \mathbf{c}_r^T) = \mathbf{r}_{\mu,r}$$



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Operator Inference (Linear Case)

- Residual formulation from snapshot data:

$$\mathbb{G}_r \mathbf{c}_r^{(i)} = \mathbf{r}_{\mu_i,r} - (\mathbb{A}_{\mu_i,r} - \mathbb{B}_{\mu_i,r})\mathbf{c}_r^{(i)} - \mathbb{M}_r \frac{d\mathbf{c}_r^{(i)}}{dt} = \mathbf{g}_r^{(i)}$$
$$\mathbf{c}_r^{(i)} = \mathbb{U}_r^T \mathbf{s}(t_i; \mu_i)$$

- Tikhonov regularized least squares over all snapshots

$$\mathbb{G}_r = \arg \min_{\check{\mathbb{G}}_r} \sum_{i=1}^{N_S} \left\| \check{\mathbb{G}}_r \mathbf{c}_r^{(i)} - \mathbf{g}_r^{(i)} \right\|^2 + \lambda_L \left\| \check{\mathbb{G}}_r \right\|^2$$



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Operator Inference (Nonlinear Case)

- Lifted ROM model:

$$\mathbb{G}_r \mathbf{c}_r^{(i)} + \bar{\mathbb{G}}_r \mathbb{X} \text{vec}(\mathbf{c}_r^{(i)} \mathbf{c}_r^{(i)T})$$

$$= \mathbf{r}_{\mu_i, r} - (\mathbb{A}_{\mu_i, r} - \mathbb{B}_{\mu_i, r}) \mathbf{c}_r^{(i)} - (\bar{\mathbb{A}}_{\mu_i, r} - \bar{\mathbb{B}}_{\mu_i, r}) \mathbb{X} \text{vec}(\mathbf{c}_r^{(i)} \mathbf{c}_r^{(i)T}) - \mathbb{M}_r \frac{d\mathbf{c}_r^{(i)}}{dt}$$

- Alternating minimization:

- Fix $\bar{\mathbb{G}}_r$, solve for \mathbb{G}_r by least squares (λ_L regularization)
- Fix \mathbb{G}_r , solve for $\bar{\mathbb{G}}_r$ by least squares (λ_H regularization)

Repeat until convergence



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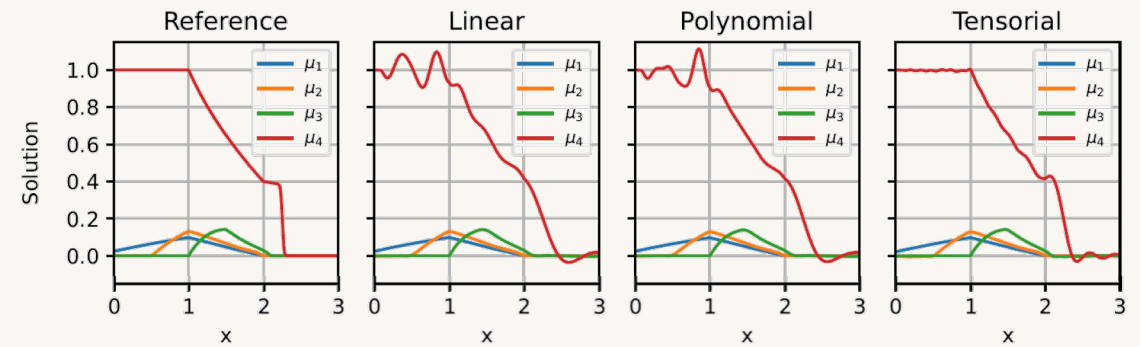
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1D Slab Benchmark



1D Slab Configuration

- Domain: $\mathcal{D} = [0, 3]$
- Scattering ratio: $\sigma_s/\sigma_t = 0.99$ (highly scattering)
- S_N quadrature: $N_\Omega = 4$ angles
- DG spatial: $N_x = 1,500$ cells
- Total DOF: $\mathcal{N} = 6,000$
- Time horizon: $T = 10$, $N_S = 7,501$ snapshots



1D Slab Benchmark

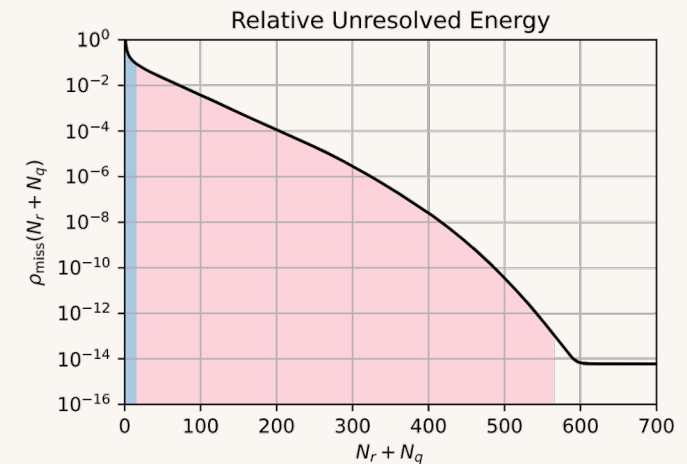
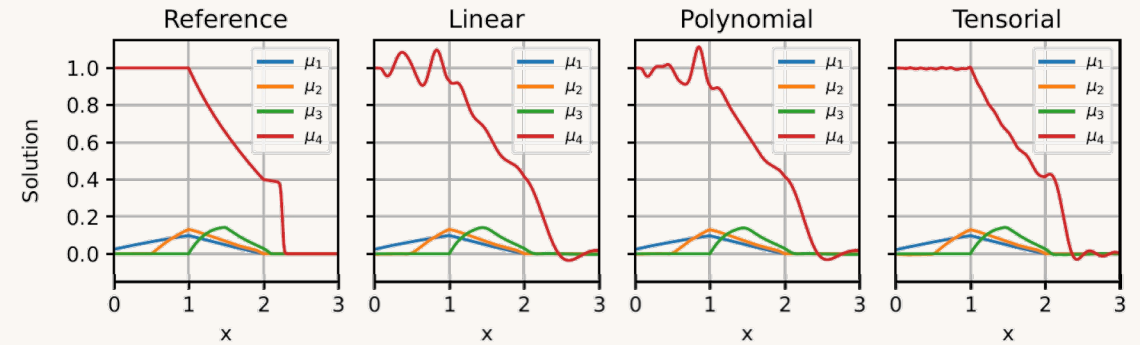


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ROM Configuration

- Latent dimension: $N_r = 16$
- Lifting dimension: $N_q = 548$
- Models tested: Linear, Element-wise, Tensorial
- Intrusive (projected) vs Semi-intrusive (inferred)

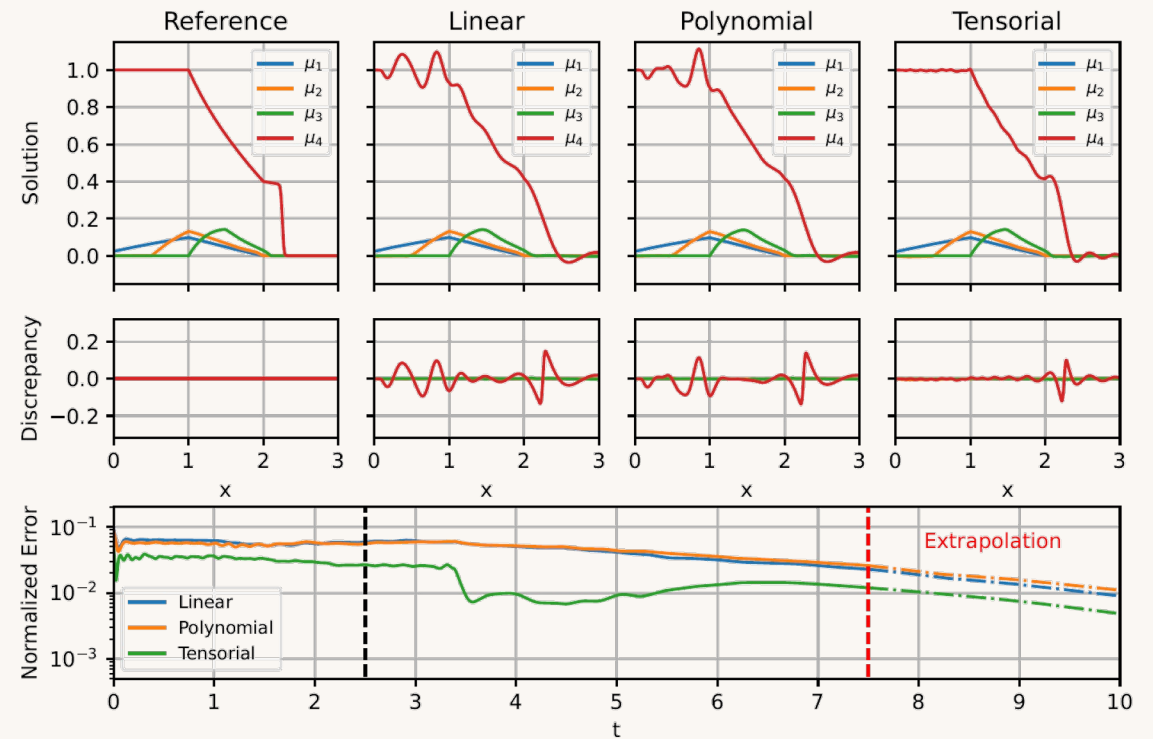


1D Results



Projection-Based (Intrusive) ROM

- Tensorial model achieves lowest $L^2(\mathcal{D} \times \mathcal{S}^2)$ error
- Element-wise \approx Linear: polynomial structure insufficient
- All models stable over full time interval $\mathcal{T} = [0, T]$





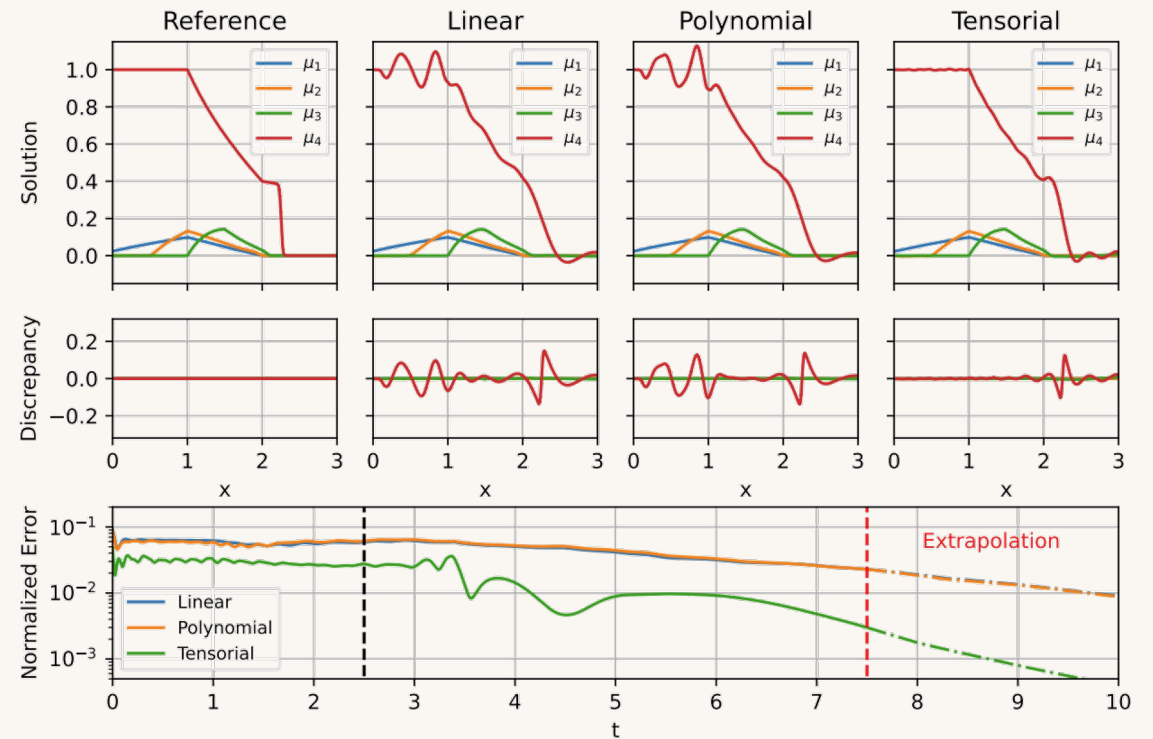
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Semi-Intrusive (Inferred) ROM

- Inferred models match or exceed projected counterparts
- Tensorial inference achieves best accuracy
- Demonstrates semi-intrusive approach viability

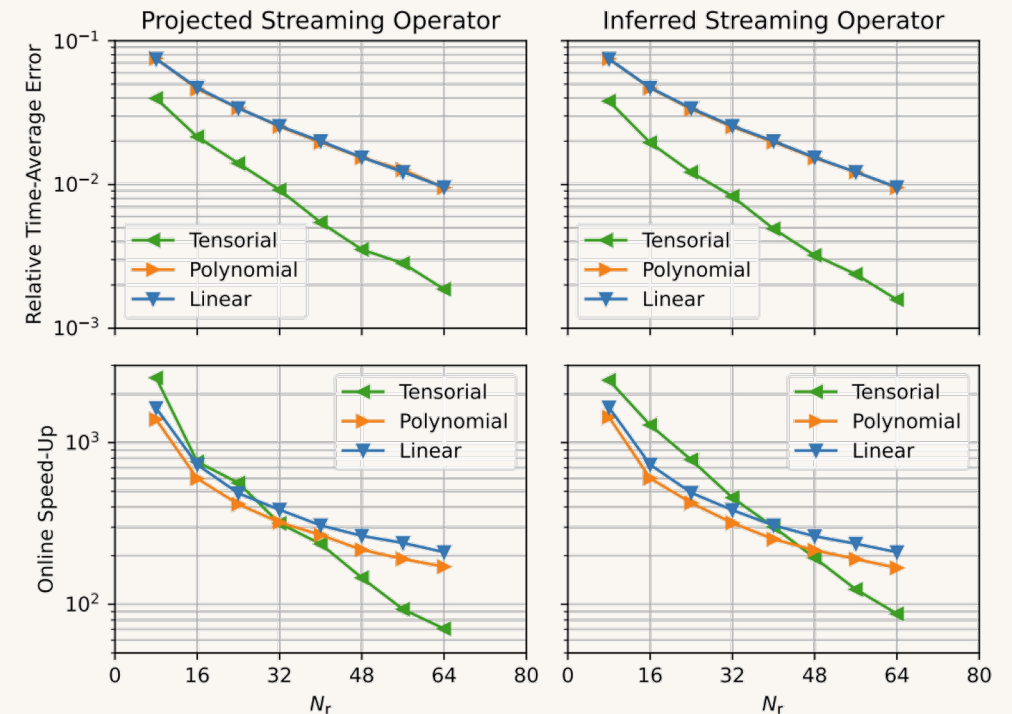




1D Convergence & Efficiency

Convergence vs. Latent Dimension

- Time-averaged $L^2(\mathcal{D} \times \mathcal{S}^2)$ error vs N_r (top): tensorial decays fastest
- Online speed-up vs N_r (bottom): all models achieve $10^2 - 10^3 \times$
- $N_r + N_q = 564$ fixed: trading latent for lifting dimensions
- Semi-intrusive inference \geq projection for all N_r values

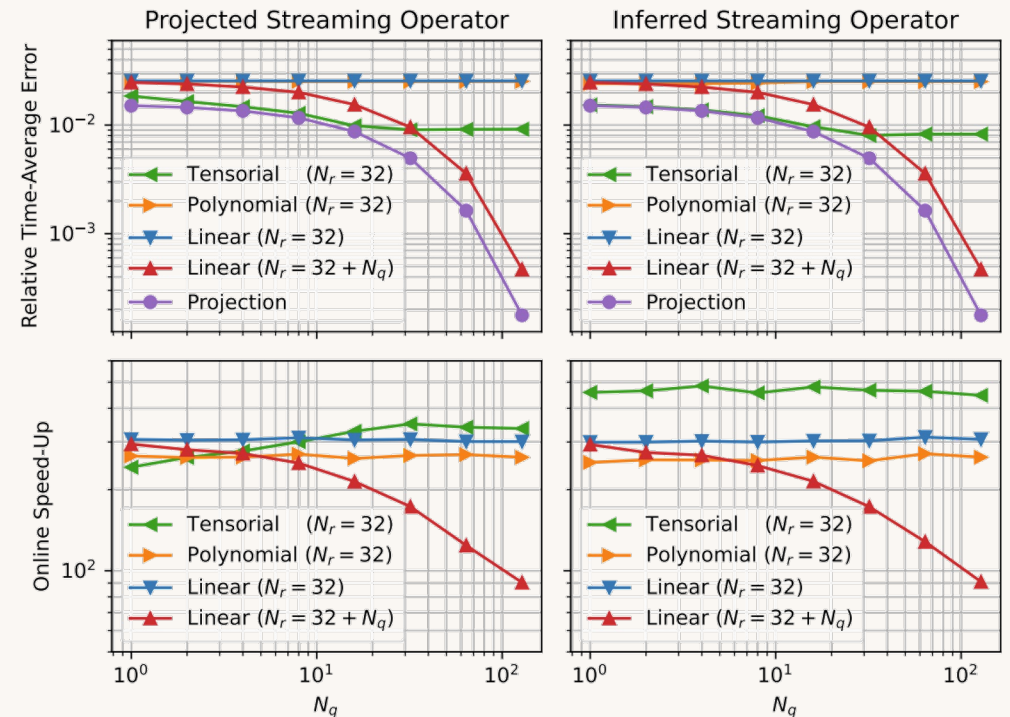




1D Lifting Dimension Study

Effect of Lifting Dimension (Latent Dimension Fixed)

- Increasing N_q : tensorial error drops orders of magnitude
- Element-wise & linear plateau early: limited by linear subspace quality
- Speed-up remains high ($10^2 - 10^3 \times$) across all N_q values
- Tensorial: best accuracy-efficiency trade-off

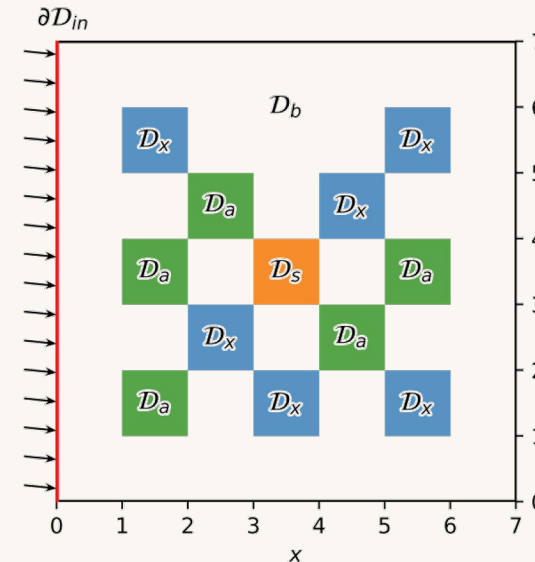




2D Benchmark: Heterogeneous Inclusions

2D Heterogeneous Configuration

- Domain: $\mathcal{D} = [0,7]^2$
- 12 material inclusions, 3 material types + background
- Solver: OpenSn (massively parallel, open-source)
- S_N quadrature: $N_\Omega = 32$ directions (level-symmetric)
- DG spatial: $N_x = 21,840$ triangular cells
- Total DOF: $\mathcal{N} \approx 700,000$
- Time horizon: $T = 5$, $N_S = 1,000$ snapshots
- Full FOM solve: ~ 1 hour



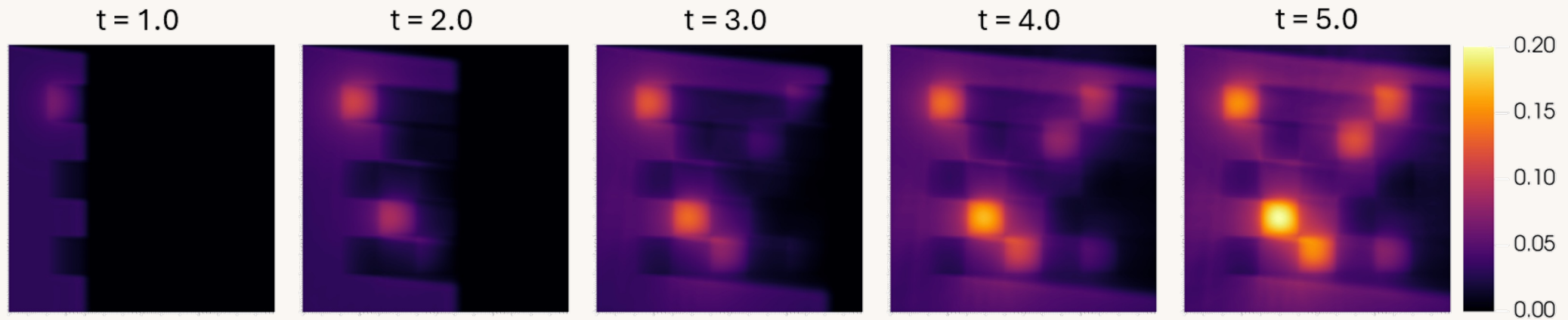
$$\sigma_t(\mathbf{x}) = \begin{cases} 1.00 & \mathbf{x} \in \mathcal{D}_a, \\ 1.00 & \mathbf{x} \in \mathcal{D}_x, \\ 1.00 & \mathbf{x} \in \mathcal{D}_s, \\ 0.00 & \mathbf{x} \in \mathcal{D}_b. \end{cases} \quad \sigma_s(\mathbf{x}) = \begin{cases} 0.00 & \mathbf{x} \in \mathcal{D}_a, \\ 1.96 & \mathbf{x} \in \mathcal{D}_x, \\ 0.75 & \mathbf{x} \in \mathcal{D}_s, \\ 0.00 & \mathbf{x} \in \mathcal{D}_b. \end{cases}$$



2D Scalar Flux Evolution

Scalar Flux: $\Phi(x, t) = \int_{S^2} \Psi(x, \Omega, t) d\Omega$

- Neutron front propagates from left boundary through heterogeneous medium
- Inclusions create scattering and absorption shadows
- Solution is sharply structured in angle and space (challenging for linear ROMs)

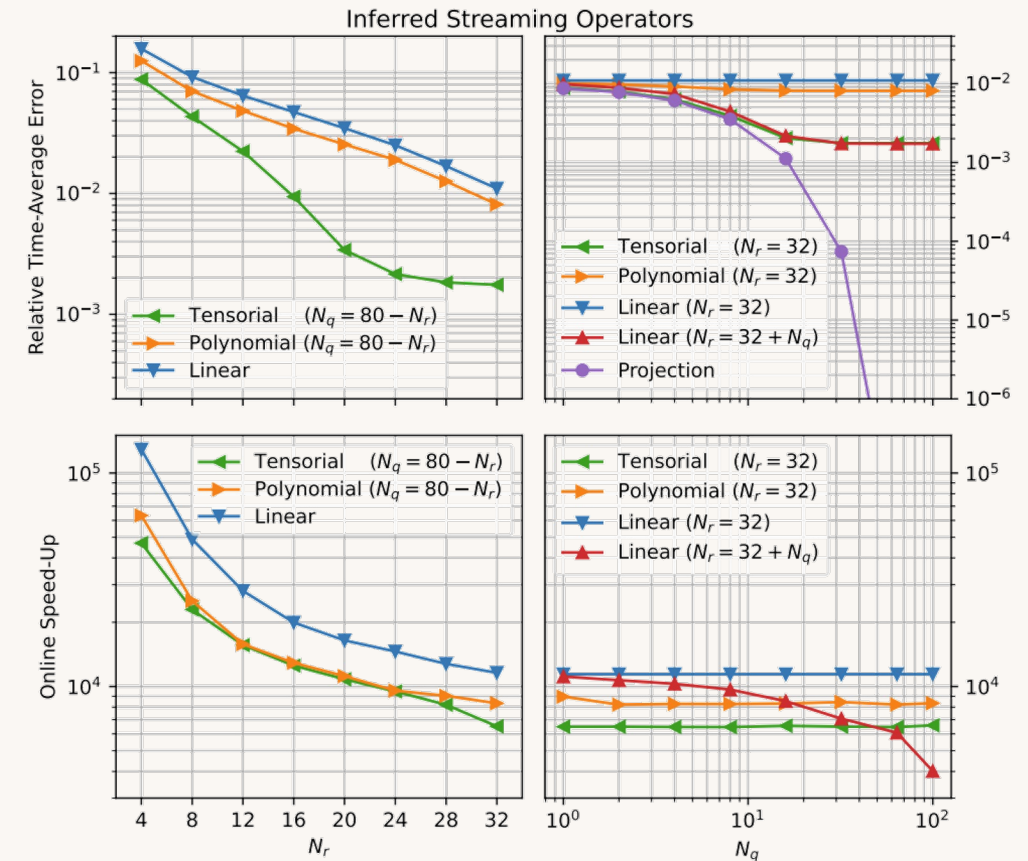


2D Results: Accuracy & Efficiency



2D Results: Accuracy & Speed-Up

- Tensor error up to one order lower than linear
- Convergence vs dimensions: stagnation at $N_r \approx 28 - 32$
- Semi-intrusive avoids global matrix assembly
- Online speed-up: $10^4 - 10^5 \times$ relative to OpenSn FOM
- In absolute terms: 700,000 \rightarrow 80 DOFs and ~ 1 hr $\rightarrow \sim 0.036$ s





Outline

I. Motivation & Problem Setting

- Why ROM for parametric neutron transport?
- The parametric mono-energetic neutron transport problem
- Full order DG- S_N semi-discretization

II. Methodology

- Linear and Nonlinear Manifold ROM
- Proper orthogonal decomposition
- Nonlinear manifolds via quadratic lifting
- Semi-intrusive operator inference

III. Numerical Results

- 1D slab benchmark – projection & inference
- 1D lifting dimension study
- 2D heterogeneous benchmark – scalar flux & convergence

IV. Conclusions & Future Work



Conclusions & Future Work

Summary of Contributions

- Semi-intrusive OpInf avoids global advection FOM matrix, scalable to large \mathcal{N}
- Tensorial nonlinear manifold outperforms linear and element-wise across all tests
- Inferred operators match or surpass projected counterparts
- Hyper-parameter tuning and model stability remain open problems
- 1D: 10^2 – 10^3 × speed-up with $\mathcal{N} \sim 6,000$ DOF
- 2D: 10^4 – 10^5 × speed-up with $\mathcal{N} \sim 700,000$ DOF



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Future Directions

- Parametric ROM for online UQ (varying $\sigma_t(\boldsymbol{\mu})$, $\sigma_s(\boldsymbol{\mu})$, $Q(\boldsymbol{\mu})$)
- Affine decomposition of parametric operators at ROM level
- Multi-group energy: coupled system of transport equations
- 3D geometries with unstructured tetrahedral meshes



Relevant Literature

The following works provide the context for our research:

- [1] J. Barnett, C. Farhat, *Quadratic approximation manifold for mitigating the Kolmogorov barrier in nonlinear projection-based model order reduction*, Journal of Computational Physics 464, 2022
- [2] R. Geelen, L. Balzano, S. Wright, K. Willcox, *Learning physics-based reduced-order models from data using nonlinear manifolds*, Chaos: An Interdisciplinary Journal of Nonlinear Science, 2024
- [3] M. L. Adams, E. W. Larsen, *Fast iterative methods for discrete-ordinates particle transport calculations*, Progress in Nuclear Energy, 2002
- [4] Y. Wang, J. C. Ragusa, *A high-order discontinuous Galerkin method for the SN transport equations on 2D unstructured triangular meshes*, Annals of Nuclear Energy, 2009
- [5] D. Andrs, Z. Hardy, D. Hawkins, J. Morel, D. Q. D. Nguyen, J. C. Ragusa, *OpenSn: A massively parallel, open-source simulation environment for discrete ordinates radiation transport*, Computer Physics Communications, 2025



THANK YOU

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