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Augmented Quadratures for the Discrete Ordinates Method Using Reduced Order Modeling Approaches

John Tencer

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Outline

- Overview of the discrete ordinates method
- Summary of model reduction methodology
- Definitions
- Sample problems / results
- Description of error estimation technique
- Summary
- Q&A

Discrete Ordinates Method

- Radiative Transfer Equation
  - $\vec{\Omega} \cdot \vec{\nabla} I(\vec{\Omega}) + (\sigma_A + \sigma_S) I(\vec{\Omega}) = \sigma_A I_b + \frac{\sigma_S}{4\pi} \int I\left(\vec{\tilde{\Omega}}\right) d\tilde{\Omega}$

1 5-dimensional PDE

- Discrete Ordinates Approximation
  - $\overrightarrow{\Omega_i} \cdot \vec{\nabla} I_i + (\sigma_A + \sigma_S) I_i = \sigma_A I_b + \frac{\sigma_S}{4\pi} \sum w_j I_j$
  - $I_i = \varepsilon I_{bw} + \frac{1-\varepsilon}{\pi} \sum_{\vec{n} \cdot \overrightarrow{\Omega_j} < 0} w_j I_j \left| \vec{n} \cdot \overrightarrow{\Omega_j} \right|$

Up to several hundred coupled 3-dimensional PDEs

- Source Iteration
  - $\overrightarrow{\Omega_i} \cdot \vec{\nabla} I_i^0 + (\sigma_A + \sigma_S) I_i^0 = \sigma_A I_b$
  - $I_i^0 = \varepsilon I_{bw}$

$\overrightarrow{\Omega_i} \cdot \vec{\nabla} I_i^j + (\sigma_A + \sigma_S) I_i^j = \sigma_A I_b + \frac{\sigma_S}{4\pi} \sum w_k I_k^{j-1}$

$I_i^j = \varepsilon I_{bw} + \frac{1-\varepsilon}{\pi} \sum_{\vec{n} \cdot \overrightarrow{\Omega_k} < 0} w_k I_k^{j-1} \left| \vec{n} \cdot \overrightarrow{\Omega_k} \right|$

- Discretized Model
  - $\overline{\overline{K}}(\overrightarrow{\Omega_i}) \vec{I}(\overrightarrow{\Omega_i}) = \vec{S}$

Hundred or thousands of solutions of large linear systems (per time-step or nonlinear iteration)

Why Discrete Ordinates?

- Well established
  - Often the only or one of few options available for treating PMR in commercial applications
  - Lots of literature on solution acceleration
- Equations are intuitive and easy to derive
- Converges to correct answer
- Handles void regions well
- Faster than MC

Reduced Order Modeling

- Reduced order modeling offers to reduce the prohibitive cost of the discrete ordinates method by replacing a significant fraction of the linear system solutions with less expensive solutions to significantly smaller linear systems.
- Take snapshots and construct reduced basis through POD
  - $\overrightarrow{\Omega_1}, \overrightarrow{\Omega_2}, \cdots, \overrightarrow{\Omega_K} \longrightarrow \overrightarrow{I_1}, \overrightarrow{I_2}, \cdots, \overrightarrow{I_K}$
  - $\bar{\bar{M}} = \left[\overrightarrow{I_1}, \overrightarrow{I_2}, \cdots, \overrightarrow{I_K}\right] = \bar{\bar{U}}\bar{\bar{S}}\bar{\bar{V}}^T$
  - $\bar{\bar{\phi}}$ is the primary modes of $\bar{\bar{M}}$ given by the first $k \leq K$ columns of $\bar{\bar{U}}$
- Approximate discretized intensity in low-dimensional space
  - $\vec{I}(\vec{\Omega}) \approx \bar{\bar{\phi}}\vec{x}$
  - $(\bar{\bar{K}}(\vec{\Omega})\bar{\bar{\phi}})\vec{x} = \vec{S}$
- Solve for $\vec{x}$ applying least-squares Petrov-Galerkin projection
  - $(\bar{\bar{K}}(\vec{\Omega})\bar{\bar{\phi}})^T(\bar{\bar{K}}(\vec{\Omega})\bar{\bar{\phi}})\vec{x} = (\bar{\bar{K}}(\vec{\Omega})\bar{\bar{\phi}})^T\vec{S}$

Definitions

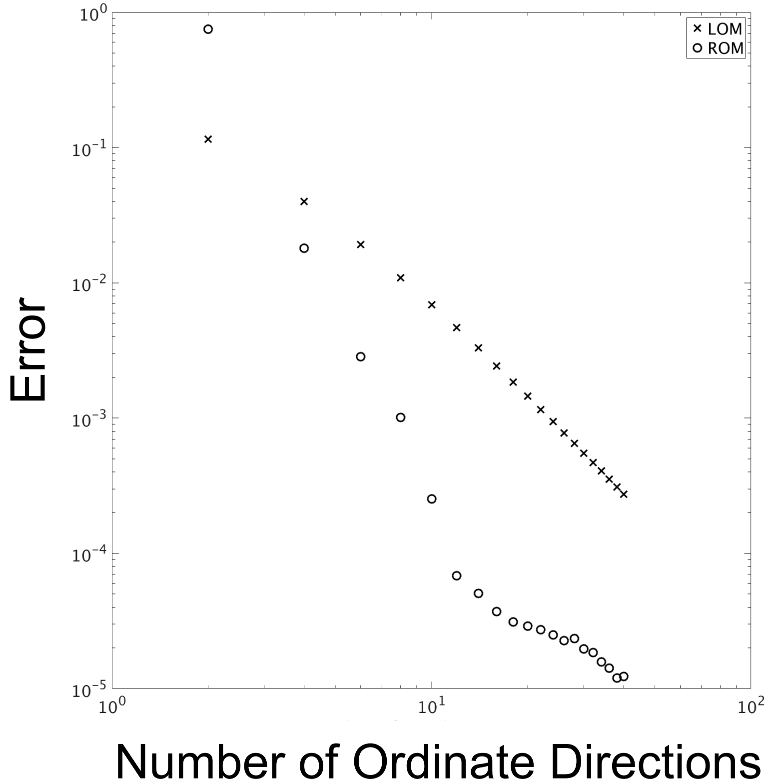
- FOM (Full-Order Model)
  - The discrete ordinates linear system solved in the traditional way
    $\left(\overline{\overline{K}}(\overrightarrow{\Omega})\overline{\overline{\phi}}\right)\vec{x} = \vec{S}$
- ROM (Reduced-Order Model)
  - The approximate linear system
    $\left(\overline{\overline{K}}(\overrightarrow{\Omega})\overline{\overline{\phi}}\right)^T\left(\overline{\overline{K}}(\overrightarrow{\Omega})\overline{\overline{\phi}}\right)\vec{x} = \left(\overline{\overline{K}}(\overrightarrow{\Omega})\overline{\overline{\phi}}\right)^T\vec{S}$
- LOM (Low-Order Model)
  - The set of linear systems corresponding to a low-order quadrature set
  - Reduced accuracy
- HOM (High-Order Model)
  - The set of linear systems corresponding to a high-order quadrature set
  - Typically unattainable using the FOM

Sample Results

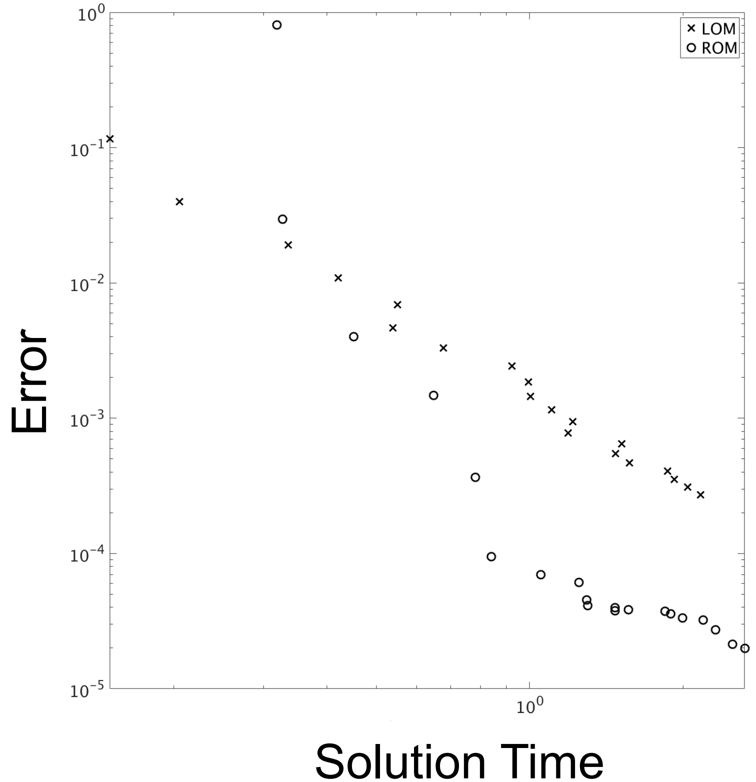
- 1D & 2D
  - Use FOM to evaluate LOM for snapshots to build ROM
  - Use ROM to evaluate HOM
  - Compare accuracy relative to using FOM to evaluate HOM
  - ROM more effective (faster/more accurate) than increasing LOM order
  - Benefits only conferred once minimum LOM order satisfied
- 3D
  - Minimum LOM order to generate accurate ROM too high
    - LOM quadrature is an inefficient way to generate samples
  - Choose subset of HOM points to generate initial snapshots
  - Add additional snapshots adaptively to reduce error
  - Discrete rather than continuous optimization
  - Estimate error at any step (minimum number of FOM evaluations to achieve desired accuracy)

1D Results

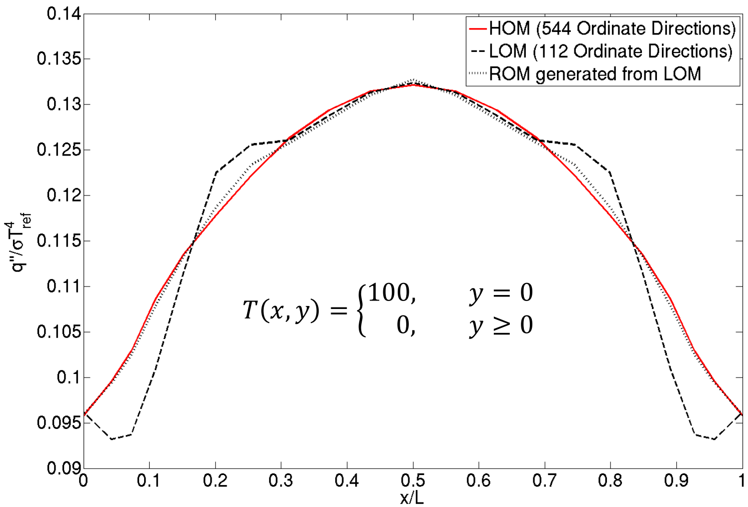
Enriching DOM quadrature with ROM solutions enhances accuracy

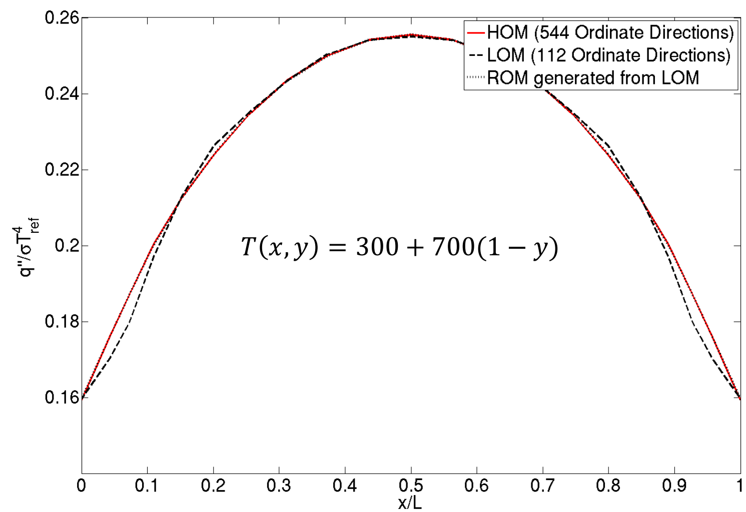


Despite added cost of ROM solutions this is more efficient than increasing quadrature order

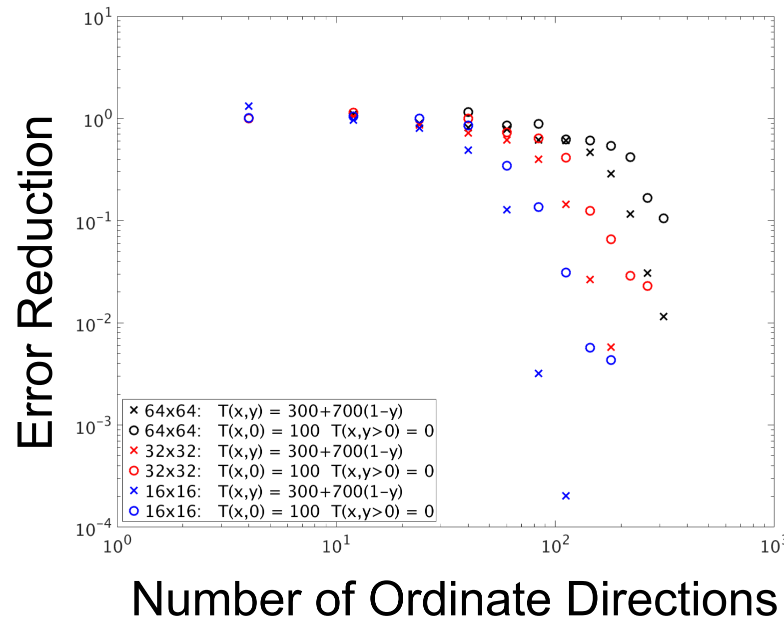


2D Results



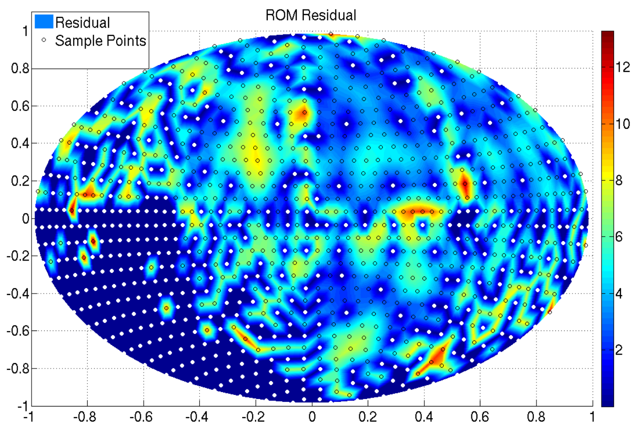


- Significant improvements in accuracy hold true for 2D
- Minimum number of snapshots required prior to rapid accuracy improvements

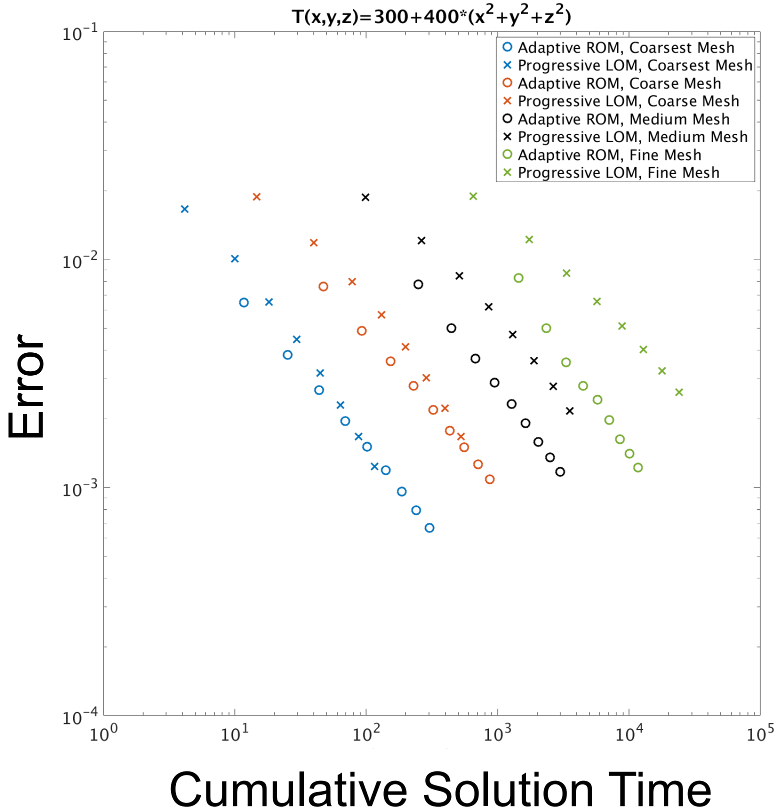


3D Results

- Enrich basis through greedy search to increase ROM solution accuracy
- No need to guess and check appropriate quadrature order
- Adaptive ROM benefits increase with larger meshes



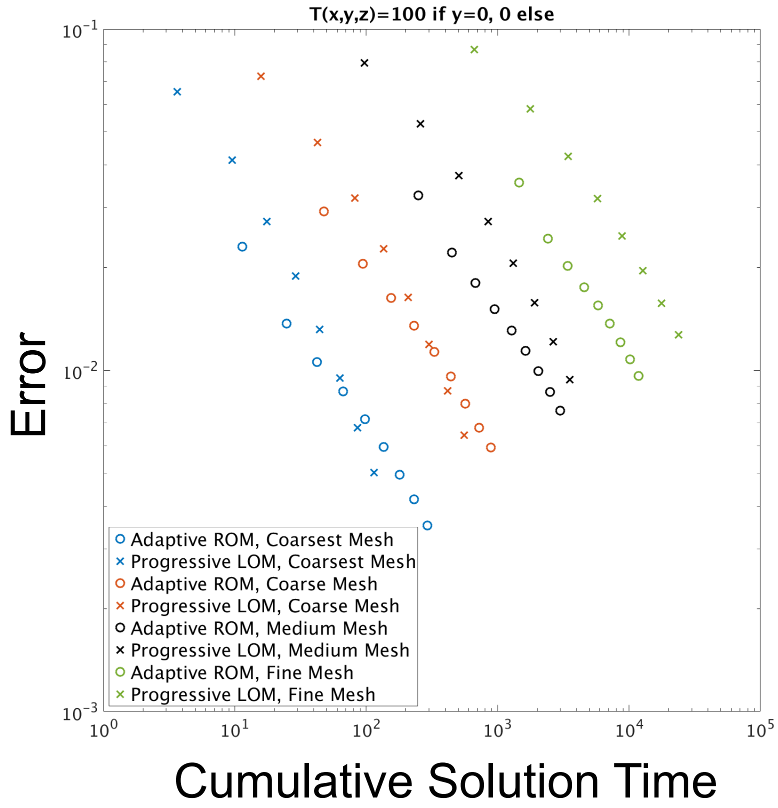
2.4k, 12.2k, 36.5k, 111.8k nodes

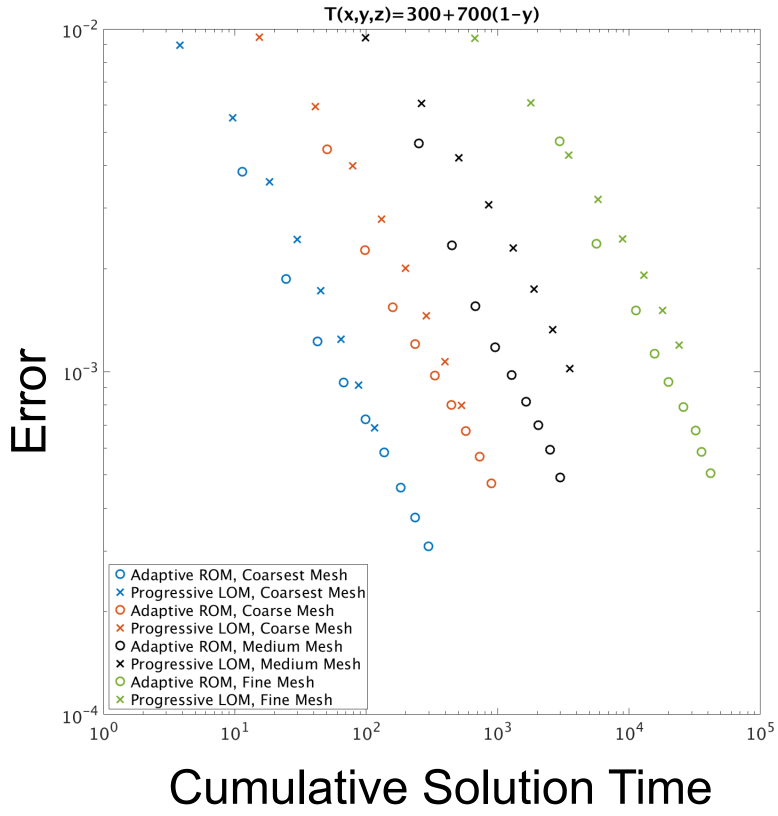


- Smart sample point distribution

3D Results

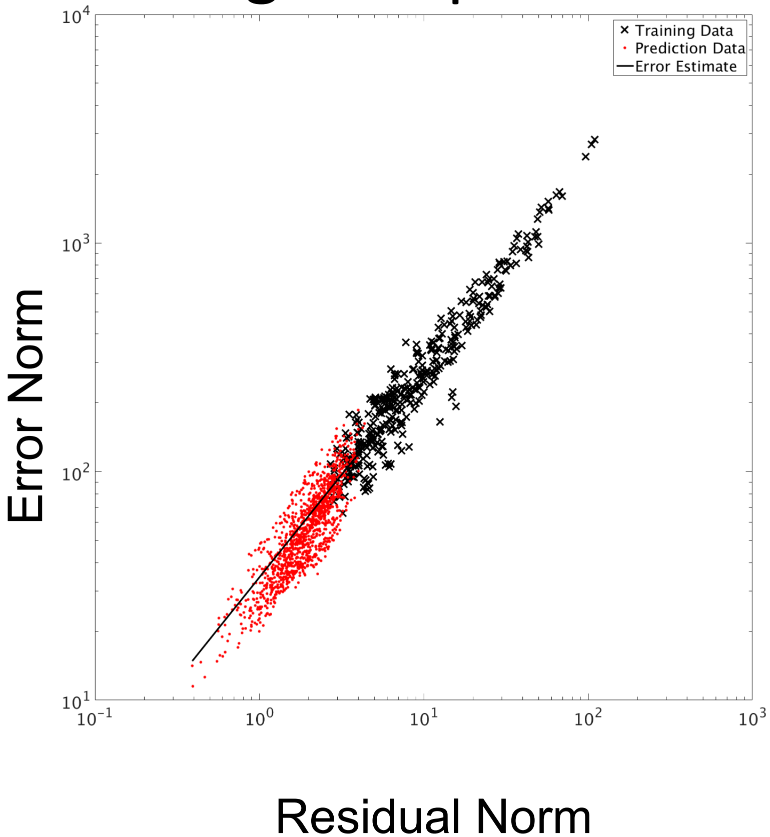
- Performance improvements from adaptive ROM technique are similar for a wide range of possible source distributions.

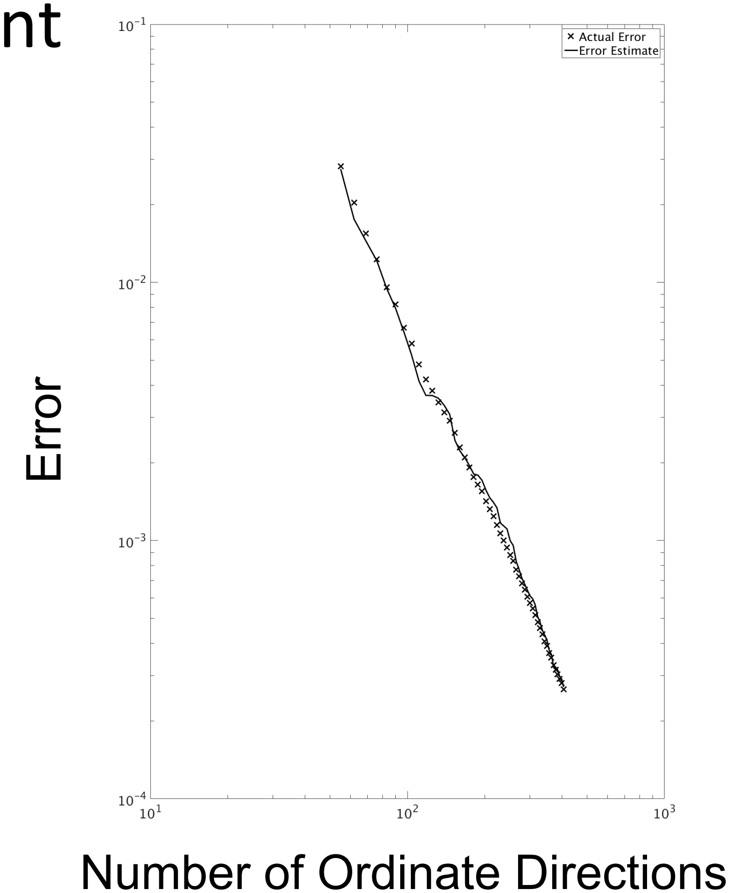




Error Estimation

- Reduced-order model error surrogate (ROMES) model constructed as reduced basis is enriched through adaptive refinement





Summary

- Using the discrete ordinates method to model PMR is computationally expensive
- Reducing the quadrature order to reduce cost results in potentially unacceptable errors of unknown magnitude as well as ray effects
- Reduced order modeling offers an alternative (more efficient) path to reduced computational costs while controlling and quantifying any error introduced
- Cost of ROM evaluations does not scale with mesh size

Questions?