Center for Hierarchical and Robust Modeling of NonEquilibrium Transport (CHaRMNET)

A Reduced Basis Method for Radiative Transfer Equation

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Building Surrogate for Fusion - Motivation

- In CHaRMNET, we are interested in the fundamental question of optimal design and UQ for fusion.
- Reduced Order Models (ROM) are necessary for outer loop calculations, e.g. UQ, inverse problems and control, see John Jakeman's talk.
- Projection based ROMs are widely accepted as an effective way to construct ROMs for fluid mechanics etc. However, there exists few work for such methods for kinetic equations.

Building Surrogate for RTE

A fundamental model in transport theory: radiative transfer equations

$$\varepsilon\partial_t f + \boldsymbol{v}\cdot\nabla_{\mathbf{x}} f = \frac{\sigma_s}{\varepsilon}(\langle f\rangle - f) - \varepsilon\sigma_a f + \varepsilon G.$$

$t \in \mathcal{R}^+, \mathbf{x} \in \Omega_{\mathbf{x}}, \boldsymbol{v} \in \Omega_v$ Unit sphere

(or its steady state version).

Even with a fixed scattering and absorption coefficient,
this problem is difficult to solve because it is a multiscale problem in high-D.

Connections and overview

Structure-Preserving Machine Learning Moment Closure [with Andrew Christlieb, Juntao Huang et al. – MSU]

$$\partial_x m_{N+1} = \sum_{i=0}^{N} \mathcal{N}_i(m_0, m_1, \cdots, m_N)\partial_x m_i$$

This talk
Projection based ROMs

- Compute surrogate with reduced basis and reduced angular description

Next talk
Data-driven nonlinear manifold ROMs

- By Youngsoo Choi et al.

Outline

The rest of talk will discuss the work on building the ROM when the model parameters are fixed.

- Highlights and challenges.
- Numerical methods.
- Numerical results.

This can be viewed as the inner layer for building ROM for problems with parametric dependence.

Highlights

Background input $FOM(V; U_h^\rho, U_h^g)$

Compress angle

Compress FEM basis

Intermediate $ROM(\mathcal{V}_{\mathrm{rq}}; U_h^\rho, U_h^g)$

Compare to obtain error indicator

$ROM(\mathcal{V}_{\mathrm{train}}; U_{h,r}^\rho, U_{h,r}^g)$

Compress both angle and FEM basis

Output $ROM(\mathcal{V}_{\mathrm{rq}}; U_{h,r}^\rho, U_{h,r}^g)$

Highlights

Never computed

Background input $FOM(V; U_h^\rho, U_h^g)$

Intermediate $ROM(\mathcal{V}_{\mathrm{rq}}; U_h^\rho, U_h^g)$

$ROM(\mathcal{V}_{\mathrm{train}}; U_{h,r}^\rho, U_{h,r}^g)$

Computed in offline stage

Output $ROM(\mathcal{V}_{\mathrm{rq}}; U_{h,r}^\rho, U_{h,r}^g)$

Used in online stage

Challenges addressed

We use the reduced basis method (RBM), which uses a greedy sampling strategy to save offline cost by *avoiding the FOM computation*.

We address several challenges.

1. V is not a parameter, but a true variable. The equations for different angles are coupled.
2. Structure preserving: *positivity* of the weights, equilibrium respecting enhancement (*asymptotic preserving*).

Mathematical justification

Kinetic equations demonstrate multiscale behavior.

Motivation

$$\varepsilon\partial_t f + \boldsymbol{v}\cdot\nabla_{\mathbf{x}} f = \frac{\sigma_s}{\varepsilon}(\langle f\rangle - f) - \varepsilon\sigma_a f + G. \quad \xrightarrow{\varepsilon \to 0} \quad \partial_t\rho - \nabla_{\mathbf{x}}\cdot(\sigma_s^{-1}D\nabla_{\mathbf{x}}\rho) = -\sigma_a\rho + G,$$

$$f(x, v, t) \to \rho(x, t)$$

Therefore, there is an underlying low rank structure. (Low rank is heavily leveraged in Terry Haut et al, previous talk)

Full Order Model (FOM)

We use a FOM discretization by DG method in space, discrete ordinate methods in velocity and the micro-macro decomposition assisted asymptotic preserving method.

$$f = \rho(\mathbf{x}, t) + \varepsilon g(\mathbf{x}, \boldsymbol{v}, t)$$

Macro Micro

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot \langle \boldsymbol{v} g \rangle = -\sigma_a \rho + G,$$
$$\varepsilon^2 \partial_t g + \varepsilon (I - \Pi)(\boldsymbol{v} \cdot \nabla_{\mathbf{x}} g) + \boldsymbol{v} \cdot \nabla_{\mathbf{x}} \rho = -\sigma_s g - \varepsilon^2 \sigma_a g$$

Offline Stage

- **Training set**: define time steps, and velocity sample training set.
- **Initialization**: start with empty RB set, and an initial coarse quadrature rule.
- We then compute ***intermediate ROM with reduced quadrature points*** to generate the snapshots for FEM space.
- We then compute ***intermediate ROM with reduced basis*** *on the full angular spaces*.
- We now use L1 indicator to guide us towards the next important angle and time to sample, and iterate.
- We stop when the difference between the two intermediate ROMs are small.

Offline Stage

- For the construction of quadrature rule on the velocity samples, we use a least square procedure. We use the spherical harmonic function ansatz.
- It is important to maintain positivity of quadrature weights for stability of ROM.
- We adjust the accuracy to satisfy this criteria. We iterate from a Max degree to a Min degree till this criteria can be met.
- We safeguard this procedure by using the quadrature rule in the previous step.
- We add the derivatives of density to the reduced basis of the micro part to enforce self consistency.

Numerical Result

Homogeneous media (2D+sphere): ranks, compression ratio and accuracy. FOM: 80X80 mesh, 590 points in angle.

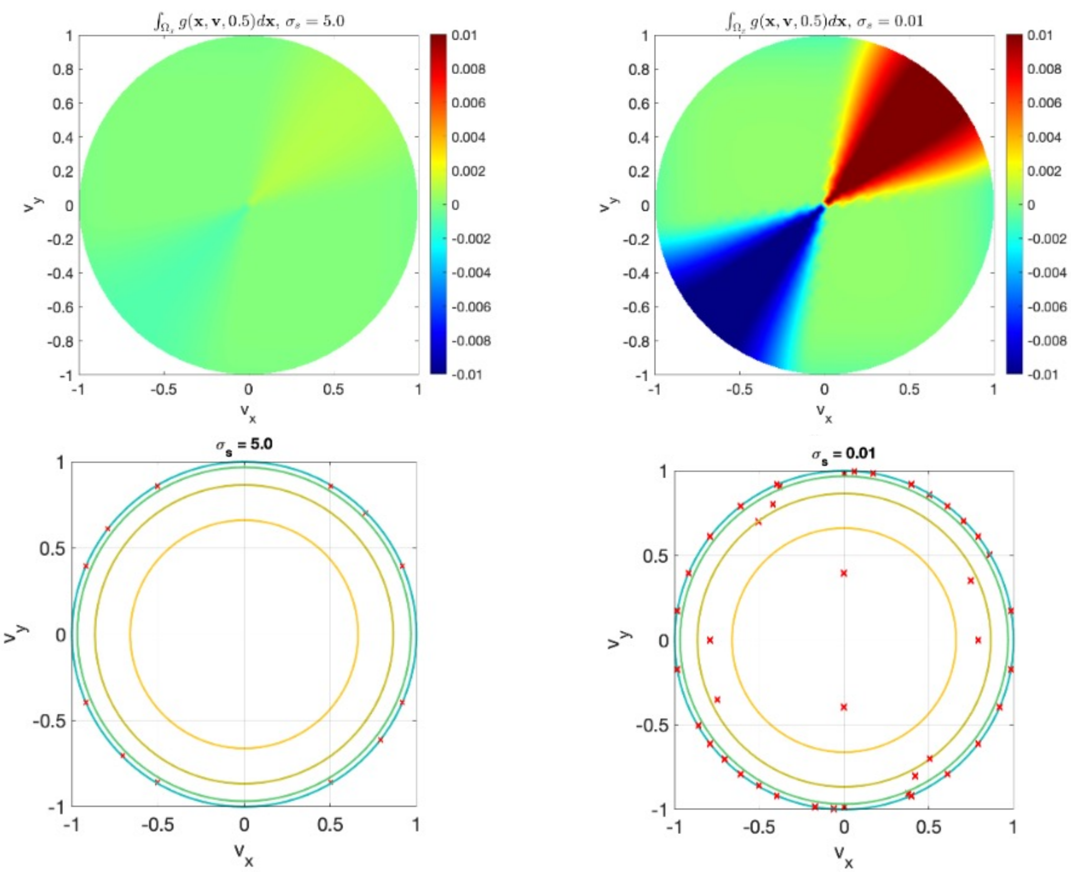
	r_ρ	r_g	N_v^{rq}	C-R	$\mathcal{E}_\rho$	$\mathcal{R}_\rho$	$\mathcal{E}_{\langle \boldsymbol{v} f\rangle}$	$\mathcal{R}_{\langle \boldsymbol{v} f\rangle}$	$\mathcal{E}_f$	$\mathcal{R}_f$
$\varepsilon = 1$	13	52	48	0.07%	1.29e-5	0.22%	1.99e-5	1.29%	1.21e-4	1.74%
$\varepsilon = 0.1$	8	32	40	0.03%	1.44e-5	0.48%	6.48e-6	1.34%	1.05e-4	3.16%
$\varepsilon = 0.005$	3	12	32	0.01%	7.86e-5	0.48%	1.29e-6	1.43%	7.90e-5	0.48%

Compression Ratio

Accuracy

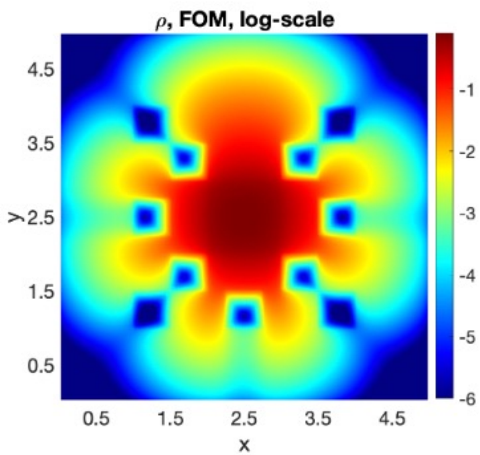
Numerical Result

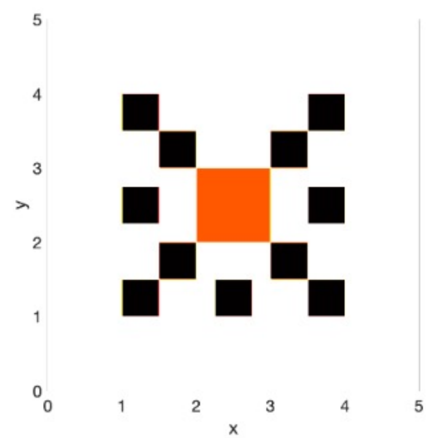
Greedy Angular Samples

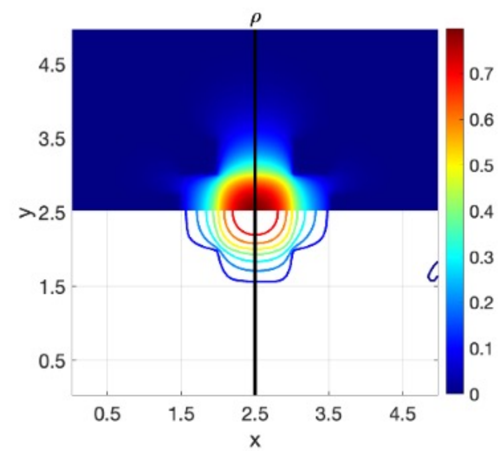


Numerical Result

Two-material lattice problem. The black region is pure absorption $\sigma_a = 100$, while the rest is pure scattering with $\sigma_s = 1$. In the orange region, a constant source is imposed.



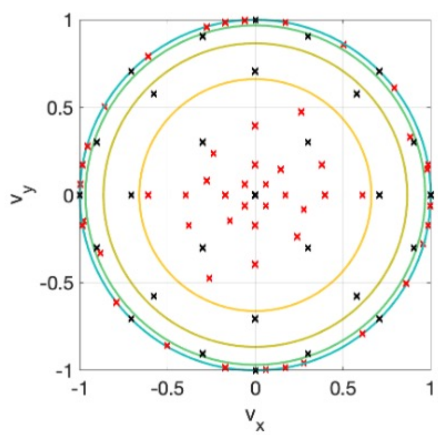




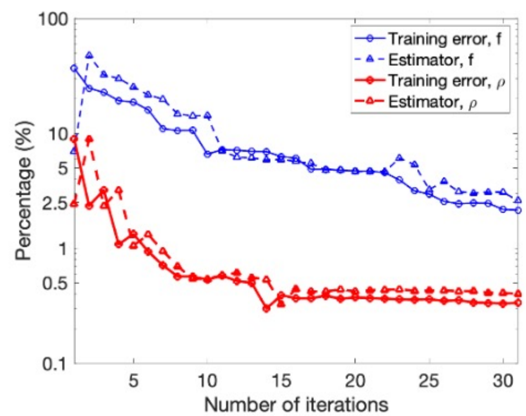
FOM ROM

Numerical Result

r_ρ	r_g	N_v^{rq}	C-R	$\mathcal{E}_\rho$	$\mathcal{R}_\rho$	$\mathcal{E}_{\langle \boldsymbol{v} f\rangle}$	$\mathcal{R}_{\langle \boldsymbol{v} f\rangle}$	$\mathcal{E}_f$	$\mathcal{R}_f$
31	124	102	0.21%	1.85e-3	0.27%	4.45e-3	2.41%	2.38e-2	2.71%



Sample points. Black: initial point, red:greedy sampled points

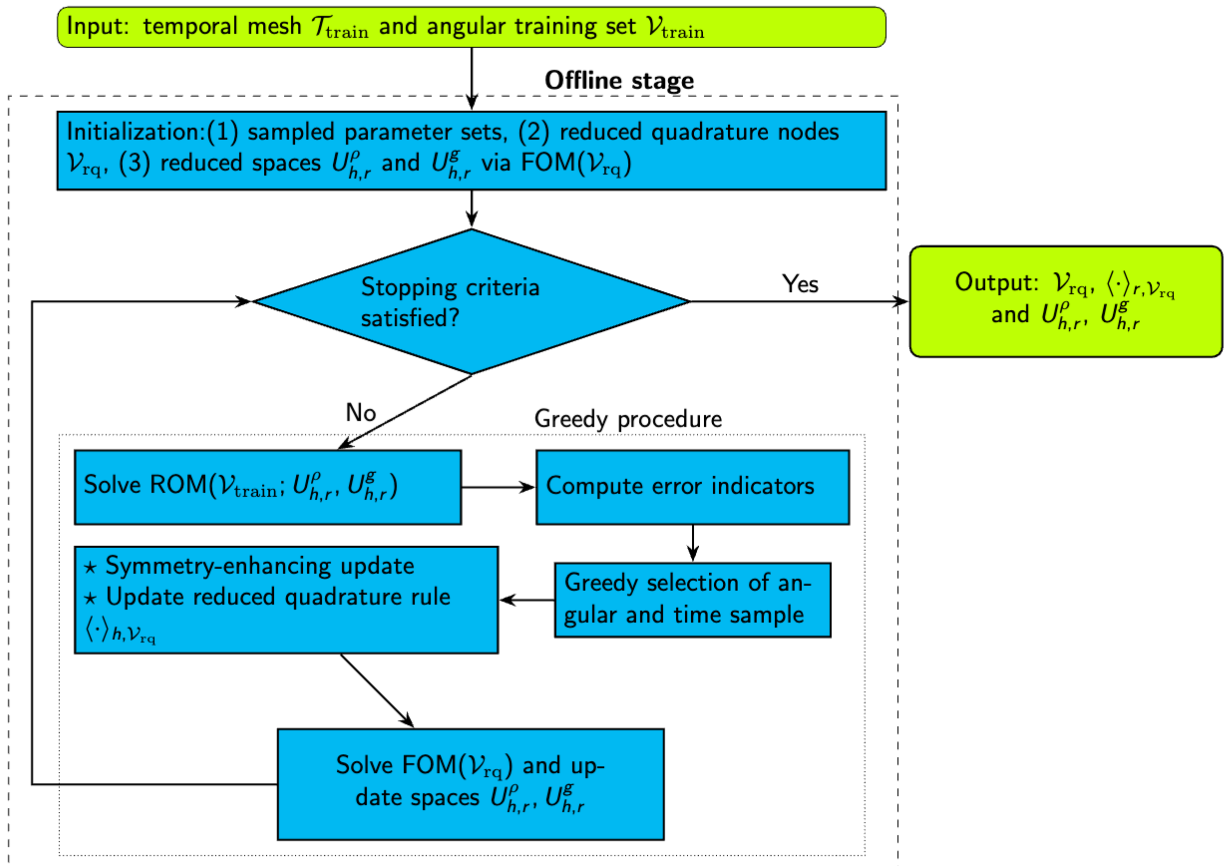


Training history

Conclusions

- We developed a RBM based Surrogate for reducing the velocity variable for RTE.
- There is also a version for ROM for steady state RTE.
- The ROM reduces both basis and angles to achieve max comp ratio.
- We never need to use FOM in the training.
- Next step: Use Sci-ML for transport dominated regime, auto-encoder based ML method with greedy indicators, see next talk by Youngsoo Choi, to work towards Y2 goal.

Algorithm



Input: temporal mesh $\mathcal{T}_{\mathrm{train}}$ and angular training set $\mathcal{V}_{\mathrm{train}}$
Offline stage
Initialization:(1) sampled parameter sets, (2) reduced quadrature nodes $\mathcal{V}_{\mathrm{rq}}$, (3) reduced spaces $U^{\rho}_{h,r}$ and $U^{g}_{h,r}$ via FOM($\mathcal{V}_{\mathrm{rq}}$)
Stopping criteria satisfied?
Yes
Output: $\mathcal{V}_{\mathrm{rq}}$, $\langle\cdot\rangle_{r,\mathcal{V}_{\mathrm{rq}}}$ and $U^{\rho}_{h,r}$, $U^{g}_{h,r}$
No
Greedy procedure
Solve ROM($\mathcal{V}_{\mathrm{train}}$; $U^{\rho}_{h,r}$, $U^{g}_{h,r}$)
Compute error indicators
⋆ Symmetry-enhancing update
⋆ Update reduced quadrature rule $\langle\cdot\rangle_{h,\mathcal{V}_{\mathrm{rq}}}$
Greedy selection of angular and time sample
Solve FOM($\mathcal{V}_{\mathrm{rq}}$) and update spaces $U^{\rho}_{h,r}$, $U^{g}_{h,r}$