Dimensionality reduction for thermal radiative transfer problems using a moment-based approach combined with the proper orthogonal decomposition

Joseph M. Coale

Department of Nuclear Engineering
North Carolina State University

Los Alamos National Laboratory

Outline

NC STATE UNIVERSITY

- Fundamental approach and basic ideas
  - Model order reduction for Boltzmann transport problems
  - Thermal radiative transfer (TRT) problems
  - Nonlinear projective approach
- Formulation of data-driven ROMs for nonlinear TRT problems
  - Approximating the Eddington tensor with the POD
  - A POD-Galerkin projection of the Boltzmann transport equation
  - Numerical results for multigroup TRT problems are presented in 2D and 1D Cartesian geometries
- Discussion
- This is a joint work with Dmitriy Anistratov (NCSU)

NC STATE UNIVERSITY

- Radiative transfer is the physical process of energy transfer via the propagation, emission and absorption of photon radiation in the host medium
- Radiative transfer becomes the dominant mode of energy redistribution in materials at extreme temperatures, and is an essential piece of physics for many phenomena spanning several fields
  - high-energy density physics
  - astrophysics
  - plasma physics
  - atmospheric science
- These phenomena are described by complex multiphysical systems of differential equations (radiation hydrodynamics)
- The particle transport physics is modeled by the Boltzmann transport equation (BTE)

Challenges in Simulation of Particle Transport Problems

NC STATE UNIVERSITY

- The numerical simulation of mutiphysical particle transport problems faces several challenges
    - High-dimensionality
    - Strong nonlinearity
    - Strong coupling of equations
    - Multi-scale characterization
    - Distinct characteristic behavior in different energy ranges
    - System of equations of different types
    - Integro-differential BTE
- The BTE is especially challenging to solve
    - Hyperbolic differential operator
    - The solution at any point depends on the solution everywhere in phase space due to the integral operator
    - The solution is high-dimensional
- The BTE largely influences the dimensionality of these problems
- Reduced order models (ROMs) for the BTE are commonly employed to reduce the cost of multiphysics simulations involving radiative transfer

Model Order Reduction for the BTE

- Some ROMs have seen widespread adoption for their usefulness and simplicity
  - Diffusion-based models like flux limited diffusion (FLD)
  - P_1, $P_{1/3}$, P_3
  - Minerbo models
- However, the accuracy of these models is limited
- The development of *advanced* ROMs for the BTE that can achieve both computational efficiency and high accuracy is an active field of research
- Recently substantial research efforts have been made towards developing *data-driven* ROMs for Boltzmann transport
- Many advanced methods for data-driven model order reduction were originally developed in the fluid dynamics community
- The majority of these ROMs focus on linear particle transport problems
- Many questions remain for nonlinear problems of high energy density physics (radiation hydrodynamics problems)
  - How to preserve and reproduce essential features of fundamental physics
  - Dealing with multiscale behavior

Fundamental Approach

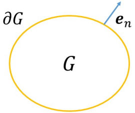
NC STATE UNIVERSITY

- Nonlinear projective approach
  - interpretation
    - nonlinear method of moments
    - multigrid approach
  - Known to give advantage in multiphysical, multiscale applications
- The BTE is coupled with a hierarchy of low-order moment equations
  - Each moment system is exactly closed through nonlinear functionals of the BTE solution (e.g. the Eddington tensor)
  - Moment equations are conservation equations for integral (low-dimensional) quantities
  - Moment equations account for different scales of the problem
  - Multiphysics equations are coupled to moment equations on the same dimensional scale
- Data-driven methods of approximation to estimate closures for low-order equations
  - proper orthogonal decomposition (POD)
  - dynamic mode decomposition (DMD)
  - neural network estimators

Nonlinear Thermal Radiative Transfer Problem

- Prototypes of these ROMs are designed for the fundamental thermal radiative transfer (TRT) problem
  - Supersonic radiation flow problem neglecting material motion, photon scattering, heat conduction and external sources
- The high-order multigroup Boltzmann transport equation (BTE)

$$\frac{1}{c}\frac{\partial I_g(\mathbf{r},\boldsymbol{\Omega},t)}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I_g(\mathbf{r},\boldsymbol{\Omega},t) + \varkappa_g(T) I_g(\mathbf{r},\boldsymbol{\Omega},t) = \varkappa_g(T) B_g(T)$$



$$\mathbf{r}\in G\,,\ \text{for all } \boldsymbol{\Omega}, \quad g=1,\dots,N_g, \quad t\geq t_0,$$

$$I_g|_{\mathbf{r}\in\partial G} = I_g^{in}, \quad \boldsymbol{\Omega}\cdot\boldsymbol{e}_n < 0, \quad t \geq t_0,$$

$$I_g|_{t=t_0} = I_g^0, \quad \mathbf{r}\in G\,,\ \text{for all } \boldsymbol{\Omega},$$

  - $\mathbf{r}$ - spatial position, $\boldsymbol{\Omega}$ - direction of particle motion, g - photon frequency group, t - time, $I_g(\mathbf{r},\boldsymbol{\Omega},t)$ - specific intensity of photons in the group g
- The material energy balance (MEB) equation

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{N_g}\int_{4\pi} \varkappa_g(T)\Big(I_g(\mathbf{r},\boldsymbol{\Omega},t) - B_g(T)\Big) d\boldsymbol{\Omega}\,, \quad T|_{t=t_0} = T^0(\mathbf{r}),\ \text{for } \mathbf{r}\in G.$$

Nonlinear Projective Approach for TRT

NC STATE UNIVERSITY

- Multilevel quasidiffusion (QD) equations:

High order BTE:	$\mathcal{L}I = \mathcal{Q}[T]$
Multigroup QD equations:	$\mathcal{K}[\mathfrak{f}]\zeta = \boldsymbol{q}[T], \quad \zeta = \mathcal{P}I$
Effective grey QD equations:	$\bar{\mathcal{K}}[\varphi]\bar{\zeta} = \bar{\boldsymbol{q}}[T], \quad \bar{\zeta} = \bar{\mathcal{P}}\zeta$
Material Energy Balance:	$\mathcal{R}T = \mathcal{H}[I]$

- Unknowns in projected space:

$$\zeta = (E_g,\ \boldsymbol{F}_g), \quad E_g = \frac{1}{c}\int_{4\pi} I_g d\Omega, \quad \boldsymbol{F}_g = \int_{4\pi} \boldsymbol{\Omega} I_g d\Omega$$

$$\bar{\zeta} = (E,\ \boldsymbol{F}), \quad E = \sum_g E_g, \quad \boldsymbol{F} = \sum_g \boldsymbol{F}_g$$

- Closures of equations:

$$\mathfrak{f}_g[I] = \frac{\int_{4\pi} \boldsymbol{\Omega}\otimes\boldsymbol{\Omega} I_g d\Omega}{\int_{4\pi} I_g d\Omega} = \begin{pmatrix} \mathfrak{f}_{xx,g} & \mathfrak{f}_{xy,g} & \mathfrak{f}_{xz,g} \\ \mathfrak{f}_{xy,g} & \mathfrak{f}_{yy,g} & \mathfrak{f}_{yz,g} \\ \mathfrak{f}_{xz,g} & \mathfrak{f}_{yz,g} & \mathfrak{f}_{zz,g} \end{pmatrix}, \quad \varphi[E_g,\ \boldsymbol{F}_g] = \frac{\sum_g \alpha_g \beta_g}{\sum_g \beta_g}, \ \beta = E_g,\ \boldsymbol{F}_g$$

Nonlinear Projective Approach for TRT

NC STATE UNIVERSITY

- Multilevel quasidiffusion (QD) equations:

High order BTE:	$\mathcal{L}I = \mathcal{Q}[T]$
Multigroup QD equations:	$\mathcal{K}[\mathfrak{f}]\zeta = \boldsymbol{q}[T], \quad \zeta = \mathcal{P}I$
Effective grey QD equations:	$\bar{\mathcal{K}}[\varphi]\bar{\zeta} = \bar{\boldsymbol{q}}[T], \quad \bar{\zeta} = \bar{\mathcal{P}}\zeta$
Material Energy Balance:	$\mathcal{R}T = \tilde{\mathcal{H}}[\zeta]$

- Unknowns in projected space:

$$\zeta = (E_g,\ \boldsymbol{F}_g), \quad E_g = \frac{1}{c}\int_{4\pi} I_g d\Omega, \quad \boldsymbol{F}_g = \int_{4\pi} \boldsymbol{\Omega} I_g d\Omega$$

$$\bar{\zeta} = (E,\ \boldsymbol{F}), \quad E = \sum_g E_g, \quad \boldsymbol{F} = \sum_g \boldsymbol{F}_g$$

- Closures of equations:

$$\mathfrak{f}_g[I] = \frac{\int_{4\pi} \boldsymbol{\Omega} \otimes \boldsymbol{\Omega} I_g d\Omega}{\int_{4\pi} I_g d\Omega} = \begin{pmatrix} \mathfrak{f}_{xx,g} & \mathfrak{f}_{xy,g} & \mathfrak{f}_{xz,g} \\ \mathfrak{f}_{xy,g} & \mathfrak{f}_{yy,g} & \mathfrak{f}_{yz,g} \\ \mathfrak{f}_{xz,g} & \mathfrak{f}_{yz,g} & \mathfrak{f}_{zz,g} \end{pmatrix}, \quad \varphi[E_g,\ \boldsymbol{F}_g] = \frac{\sum_g \alpha_g \beta_g}{\sum_g \beta_g}, \ \beta = E_g,\ \boldsymbol{F}_g$$

Nonlinear Projective Approach for TRT

NC STATE UNIVERSITY

- Multilevel quasidiffusion (QD) equations:

High order BTE:	$\mathcal{L}I = \mathcal{Q}[T]$
Multigroup QD equations:	$\mathcal{K}[\mathfrak{f}]\zeta = \boldsymbol{q}[T], \quad \zeta = \mathcal{P}I$
Effective grey QD equations:	$\bar{\mathcal{K}}[\varphi]\bar{\zeta} = \bar{\boldsymbol{q}}[T], \quad \bar{\zeta} = \bar{\mathcal{P}}\zeta$
Material Energy Balance:	$\mathcal{R}T = \hat{\mathcal{H}}[\bar{\zeta}]$

- Unknowns in projected space:

$$\zeta = (E_g,\ \boldsymbol{F}_g), \quad E_g = \frac{1}{c}\int_{4\pi} I_g d\Omega, \quad \boldsymbol{F}_g = \int_{4\pi} \boldsymbol{\Omega} I_g d\Omega$$

$$\bar{\zeta} = (E,\ \boldsymbol{F}), \quad E = \sum_g E_g, \quad \boldsymbol{F} = \sum_g \boldsymbol{F}_g$$

- Closures of equations:

$$\mathfrak{f}_g[I] = \frac{\int_{4\pi} \boldsymbol{\Omega}\otimes\boldsymbol{\Omega} I_g d\Omega}{\int_{4\pi} I_g d\Omega} = \begin{pmatrix} \mathfrak{f}_{xx,g} & \mathfrak{f}_{xy,g} & \mathfrak{f}_{xz,g} \\ \mathfrak{f}_{xy,g} & \mathfrak{f}_{yy,g} & \mathfrak{f}_{yz,g} \\ \mathfrak{f}_{xz,g} & \mathfrak{f}_{yz,g} & \mathfrak{f}_{zz,g} \end{pmatrix}, \quad \varphi[E_g,\ \boldsymbol{F}_g] = \frac{\sum_g \alpha_g \beta_g}{\sum_g \beta_g}, \ \beta = E_g,\ \boldsymbol{F}_g$$

Model Using Data-Driven Approximation of Closures

NC STATE UNIVERSITY

Approximation of closure:	$\tilde{\mathfrak{f}} = \mathcal{G}[\mathfrak{f}^*], \quad \mathfrak{f}^*$ known
Multigroup QD equations:	$\mathcal{K}[\tilde{\mathfrak{f}}]\zeta = \boldsymbol{q}[T], \quad \zeta = \mathcal{P}I$
Effective grey QD equations:	$\bar{\mathcal{K}}[\varphi]\bar{\zeta} = \bar{\boldsymbol{q}}[T], \quad \bar{\zeta} = \bar{\mathcal{P}}\zeta$
Material Energy Balance:	$\mathcal{R}T = \hat{\mathcal{H}}[\bar{\zeta}]$

- Use data-driven methods to define the operator $\mathcal{G}$
- $\mathcal{G}$ will allow for efficient compression and approximation of data
- Available methods include:
  - Proper orthogonal decomposition
  - Dynamic mode decomposition
  - Neural networks
  - etc.

Approximation of Eddington Tensor

NC STATE UNIVERSITY

- Projection, compression of data
  - Given: full-order solution to some TRT problem for N_t time steps, N_g frequency groups, N_x spatial cells
  - Vectors of each Eddington Tensor component at time t^n

$$\mathbf{f}^n_{\alpha\beta} \in \mathbb{R}^{N_x N_g}, \quad \alpha, \beta = x, y, z$$

  - Construction of snapshot matrices

$$\mathbf{A}^{\mathfrak{f}_{\alpha\beta}} = [\mathbf{f}^1_{\alpha\beta}\ \mathbf{f}^2_{\alpha\beta}\ \dots\ \mathbf{f}^{N_t}_{\alpha\beta}] \in \mathbb{R}^{N_x N_g \times N_t}$$

  - Define projection operator $\mathcal{G}^k$ that will project a given matrix $\mathbf{A}$ onto a rank-k subspace

$$\mathcal{A}^{\mathfrak{f}_{\alpha\beta}}_k = \mathcal{G}^k \mathbf{A}^{\mathfrak{f}_{\alpha\beta}}, \quad k \leq \text{rank}(\mathbf{A}^{\mathfrak{f}_{\alpha\beta}})$$

  - $\mathcal{A}^{\mathfrak{f}_{\alpha\beta}}_k$ is constructed of k sets of various vectors and factors
- Approximation of data from rank k representation
  - A map $\mathcal{M}^n$ is defined by the same method used to define $\mathcal{G}^k$

$$\mathbf{f}^n_{\alpha\beta} \approx \mathcal{M}^n \mathcal{A}^{\mathfrak{f}_{\alpha\beta}}_k$$

POD of the Eddington Tensor

NC STATE UNIVERSITY

- *Centered* data matrix

$$\hat{\mathbf{A}}^{\mathfrak{f}_{\alpha\beta}} = [\hat{\mathbf{f}}^1_{\alpha\beta}, \dots, \hat{\mathbf{f}}^{N_t}_{\alpha\beta}], \qquad \hat{\mathbf{f}}^n_{\alpha\beta} = \mathbf{f}^n_{\alpha\beta} - \bar{\mathbf{f}}_{\alpha\beta}, \qquad \bar{\mathbf{f}}_{\alpha\beta} = \frac{1}{N_t}\sum_{n=1}^{N_t} \mathbf{f}^n_{\alpha\beta}$$

- A thin singular value decomposition (SVD) represents the matrix in the form

$$\hat{\mathbf{A}}^{\mathfrak{f}_{\alpha\beta}} = \mathbf{U}\mathbf{S}\mathbf{V}^T ,$$

$\mathbf{U} \in \mathbb{R}^{N_x N_g, d}$ holds the left singular vectors $\{\boldsymbol{u}_\ell\}_{\ell=1}^d$ in its columns
$\mathbf{V} \in \mathbb{R}^{N_t, d}$ holds the right singular vectors $\{\boldsymbol{v}_\ell\}_{\ell=1}^d$ in its columns
$\mathbf{S} \in \mathbb{R}^{d,d}$ holds the singular values $\{\sigma_\ell\}_{\ell=1}^d$ along its diagonal in decreasing order,

$$d = \text{rank}(\hat{\mathbf{A}}^{\mathfrak{f}_{\alpha\beta}}) = \min(N_x N_g, N_t)$$

- The rank-k POD representation of $\mathfrak{f}_{\alpha\beta}$

$$\mathcal{A}_k^{\mathfrak{f}_{\alpha\beta}} = \bar{\mathbf{f}}_{\alpha\beta} \cup \{\sigma_\ell, \boldsymbol{u}_\ell, \boldsymbol{v}_\ell\}_{\ell=1}^k$$

$$\boxed{\tilde{\mathbf{f}}^n_{\alpha\beta} \leftarrow \bar{\mathbf{f}}_{\alpha\beta} + \sum_{\ell=1}^{k} \sigma_\ell (\boldsymbol{v}_\ell)_n \boldsymbol{u}_\ell = \mathcal{M}^n \mathcal{A}_k^{\mathfrak{f}_{\alpha\beta}}}$$

Determination of Rank

NC STATE UNIVERSITY

- For each data matrix **A**, the rank k must be calculated to store $\mathcal{A}_k$
- We consider the rank-k truncated SVD

$$\mathbf{A} \approx \mathbf{A}_k = \mathbf{U}_k \mathbf{S}_k \mathbf{V}_k^T$$
$$\mathbf{U}_k = [\mathbf{u}_1 \dots \mathbf{u}_k], \quad \mathbf{S}_k = \mathrm{diag}(\sigma_1, \dots, \sigma_k), \quad \mathbf{V}_k = [\mathbf{v}_1 \dots \mathbf{v}_k]$$

- The error in Frobenius norm

$$\|\mathbf{A} - \mathbf{A}_k\|_F^2 = \sum_{\ell=k+1}^{d} \sigma_\ell^2$$

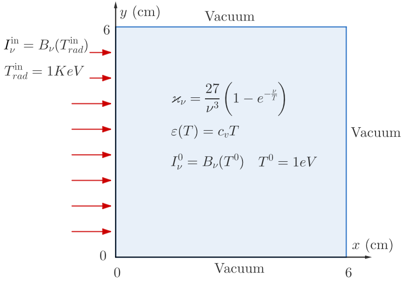
- We calculate k by choosing the relative Frobenius norm error ξ

$$\xi^2 = \frac{\sum_{\ell=k+1}^{d} \sigma_\ell^2}{\sum_{\ell=1}^{d} \sigma_\ell^2} = \frac{\|\mathbf{A} - \mathbf{A}_k\|_F^2}{\|\mathbf{A}\|_F^2}$$

- k increases as ξ decreases
  - Increasing k increases cost in calculating approximate closures
  - Accuracy is also expected to increase with k

Numerical Test Problem

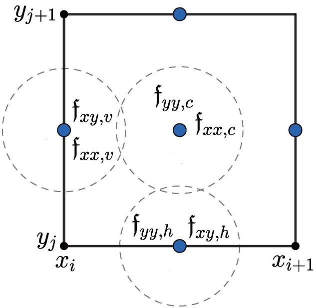
NC STATE UNIVERSITY

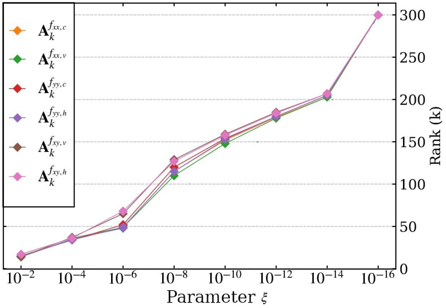


- We test this method on a 2D extension of the Fleck-Cummings (F-C) test
- Fully-implicit time integration
- BTE discretized with simple corner balance scheme
- All low-order equations discretized with 2nd order finite volumes
- Grid:
  - 20x20 spatial cells, 17 groups, 144 discrete directions
  - 300 time steps $\Delta t = .02$ns for $0 \leq t \leq 6$ns
- Degrees of freedom: 1.175×10^9
- ROM degrees of freedom: 1.728×10^7

NC STATE UNIVERSITY

- Databases are formed from the full-order model solution
- Ranks of approximation and memory requirements for the POD with varying ξ

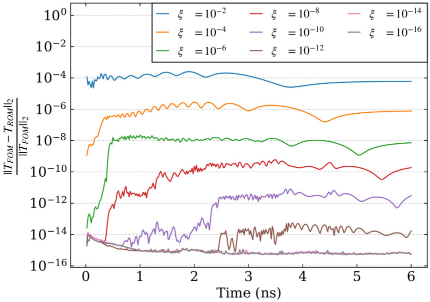




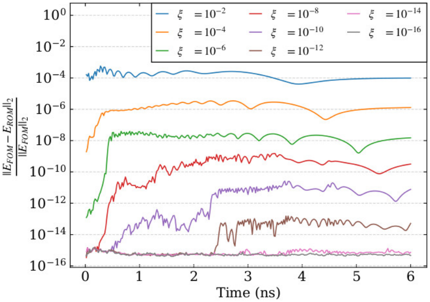
Ranks k vs parameter ξ

NC STATE UNIVERSITY

- Relative errors in the 2-norm using the POD compared to the full-order solution
- Errors plotted vs time, each curve corresponds to a value for ξ



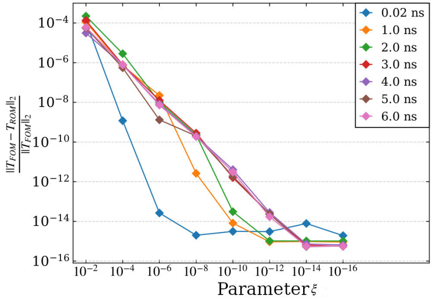
Material Temperature



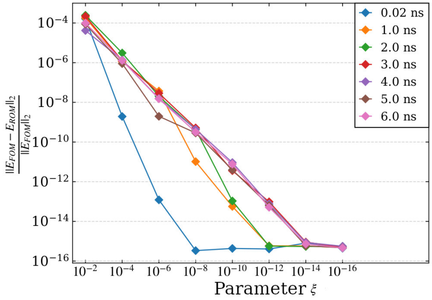
Radiation Energy Density

Convergence of the ROM with Rank (POD)

- Relative errors in the 2-norm using the POD compared to the full-order solution
- Errors plotted vs ξ, each curve corresponds to an instant of time



Material Temperature



Radiation Energy Density

Discussion

NC STATE UNIVERSITY

- The ROM that approximates the Eddington tensor with the POD performs well
- The ROM converges to the full-order solution it was trained on
  - uniform convergence in time
  - linear convergence rate vs ξ
- We have also shown this methodology capable of reproducing fundamental radiative transfer physics
  - Accurate predictions of breakout times of radiation
  - Accurate predictions of radiation spectrum
- Next up: projection of the BTE onto proper orthogonal modes that describe known radiation intensities

Model Using Projection onto Proper Orthogonal Modes

POD-Galerkin Projected BTE:	$\hat{\mathcal{L}}[\boldsymbol{u}]\tilde{\boldsymbol{I}} = \hat{\mathcal{Q}}[\boldsymbol{u}, T]$
Multigroup QD equations:	$\mathcal{K}[\mathfrak{f}[\tilde{\boldsymbol{I}}]]\zeta = \boldsymbol{q}[T], \quad \zeta = \mathcal{P}\boldsymbol{I}$
Effective grey QD equations:	$\bar{\mathcal{K}}[\varphi]\bar{\zeta} = \bar{\boldsymbol{q}}[T], \quad \bar{\zeta} = \bar{\mathcal{P}}\zeta$
Material Energy Balance:	$\mathcal{R}T = \hat{\mathcal{H}}[\bar{\zeta}]$

- We formulate a POD-Galerkin (POD-G) projection of the BTE
  - A POD basis is calculated based on base-case solutions of the BTE solution
  - Intensities are expanded in the POD basis over the whole phase space
  - The BTE is projected onto the POD basis and solves for coefficients of the expansion
- In this way the POD-G BTE takes the place of the discretized BTE in the multilevel QD hierarchy
  - Large gains in computational efficiency since there are far fewer coefficients than degrees of freedom on the intensities

Discretization of the BTE

- The POD-G projection method is formulated in discrete space
- The high-order Boltzmann transport equation

$$\frac{1}{c}\frac{\partial I_g(\mathbf{r},\boldsymbol{\Omega},t)}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I_g(\mathbf{r},\boldsymbol{\Omega},t) + \varkappa_g(T)I_g(\mathbf{r},\boldsymbol{\Omega},t) = \varkappa_g(T)B_g(T)$$

- Discretize with: Discrete-Ordinates, Backward-Euler, Simple Corner Balance

$$\frac{1}{c\Delta t^n}\left(\mathbf{I}^n - \mathbf{I}^{n-1}\right) + \mathcal{L}_h\mathbf{I}^n + \mathcal{K}_h^n(T)\mathbf{I}^n = \mathbf{Q}^n(T)\,, \tag{1}$$

- Discrete operators $\mathcal{L}_h$, $\mathcal{K}_h^n(T)$ determined by scheme
- N_x spatial degrees of freedom, N_Ω discrete directions, N_t time steps,
- $D = N_x N_\Omega N_g$
- Solution vector: $\mathbf{I}^n = ((\boldsymbol{I}_1^n)^\top \ \dots \ (\boldsymbol{I}_{N_g}^n)^\top)^\top \in \mathbb{R}^D$
- Construct snapshot matrix

$$\boldsymbol{A} = [\boldsymbol{I}^1, \dots, \boldsymbol{I}^{N_t}] \tag{2}$$

- Goal: expand intensities in basis functions $\{\boldsymbol{u}_\ell\}_{\ell=1}^r$

$$\mathbf{I}_r^u(t^n) = \sum_{\ell=1}^{r} \lambda_\ell^n \boldsymbol{u}_\ell \tag{3}$$

- We formulate the POD basis $\{\boldsymbol{u}_\ell\}_{\ell=1}^r$, $r \ll D$ using snapshots in $\boldsymbol{A}$

$$\min_{\boldsymbol{u}_1,\dots,\boldsymbol{u}_r} \sum_{n=1}^{N_t} \Delta t^n \left\| \mathbf{I}^n - \sum_{\ell=1}^{r} \langle \mathbf{I}^n, \boldsymbol{u}_\ell \rangle_W \boldsymbol{u}_\ell \right\|_W^2, \tag{4}$$

- Weighted inner product specific to the discretization: $\langle \boldsymbol{u}, \boldsymbol{v} \rangle_W = \boldsymbol{u}^\top \boldsymbol{W} \boldsymbol{v}$

The Weighted Inner Product

NC STATE UNIVERSITY

- Standard POD uses the identity matrix $\boldsymbol{W} = \mathbb{I}$ so that $\langle \boldsymbol{u}, \boldsymbol{v} \rangle_W = \langle \boldsymbol{u}, \boldsymbol{v} \rangle$
- We seek $\boldsymbol{W}$ to correspond to the discrete integration over space, angle, frequency
- For the considered discretization schemes we have (in 1D geometry)

$$\int_0^\infty \int_{-1}^{1} \int_0^{L_x} u(x,\mu,\nu)\,dx\,d\mu\,d\nu \;\Rightarrow\; \sum_{g=1}^{N_g} \sum_{m=1}^{N_\Omega} w_m \sum_{i=1}^{N_x} \frac{\Delta x_i}{2}\left(\boldsymbol{u}_{g,m,i,L} + \boldsymbol{u}_{g,m,i,R}\right) \quad (5)$$

- We find the matrix $\boldsymbol{W}$ as

$$\boldsymbol{W} = \bigoplus_{g=1}^{N_g} \bigoplus_{m=1}^{N_\Omega} w_m \hat{\boldsymbol{W}}^x, \quad \hat{\boldsymbol{W}}^x = \bigoplus_{i=1}^{N_x} \begin{pmatrix} \frac{\Delta x_i}{2} & 0 \\ 0 & \frac{\Delta x_i}{2} \end{pmatrix} \quad (6)$$

Calculation of POD Basis

NC STATE UNIVERSITY

- Construct snapshot matrix

$$\boldsymbol{A} = [\boldsymbol{I}^1, \ldots, \boldsymbol{I}^{N_t}] \tag{7}$$

- Calculate weighted snapshot matrix

$$\hat{\boldsymbol{A}} = \boldsymbol{W}^{1/2}\boldsymbol{A}\boldsymbol{D}^{1/2}, \quad \boldsymbol{D} = \text{diag}(\Delta t^1, \ldots, \Delta t^{N_t}) \tag{8}$$

- Find singular value decomposition of $\hat{\boldsymbol{A}}$

$$\hat{\boldsymbol{A}} = \hat{\boldsymbol{U}}\hat{\boldsymbol{S}}\hat{\boldsymbol{V}}^\top \tag{9}$$

$$\hat{\boldsymbol{U}} = [\hat{\boldsymbol{u}}_1, \ldots, \hat{\boldsymbol{u}}_d], \quad \hat{\boldsymbol{S}} = \text{diag}(\sigma_1, \ldots, \sigma_d), \quad \hat{\boldsymbol{V}} = [\hat{\boldsymbol{v}}_1, \ldots, \hat{\boldsymbol{v}}_d] \tag{10}$$

- The POD basis is then found as $\boldsymbol{U} = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_d]$ with $d = \text{rank}(\hat{\boldsymbol{A}})$ using

$$\boldsymbol{U} = \boldsymbol{W}^{-1/2}\hat{\boldsymbol{U}} \tag{11}$$

POD Galerkin Projection

NC STATE UNIVERSITY

$$\frac{1}{c\Delta t^n}\left(\mathbf{I}^n - \mathbf{I}^{n-1}\right) + \mathcal{L}_h \mathbf{I}^n + \mathcal{K}_h^n(T)\mathbf{I}^n = \mathbf{Q}^n(T), \quad \mathbf{I}_r^u(t^n) = \sum_{\ell=1}^{r} \lambda_\ell^n \boldsymbol{u}_\ell$$

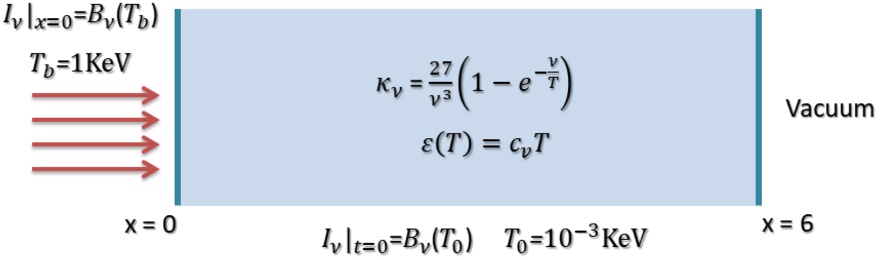
- POD Galerkin-Projected BTE (apply $\langle \boldsymbol{u}_\ell, \cdot \rangle_W$)

$$\frac{1}{c\Delta t^n}\left(\lambda_\ell^n - \lambda_\ell^{n-1}\right) + \sum_{\ell'=1}^{r} \lambda_{\ell'}^n \left\langle \boldsymbol{u}_\ell, \mathcal{L}_h \boldsymbol{u}_{\ell'} \right\rangle_W + \sum_{\ell'=1}^{r} \lambda_{\ell'}^n \left\langle \boldsymbol{u}_\ell, \mathcal{K}_h^n(T) \boldsymbol{u}_{\ell'} \right\rangle_W = \left\langle \boldsymbol{u}_\ell, \mathbf{Q}^n(T) \right\rangle_W \quad (12)$$

- Used orthogonality of basis: $\left\langle \boldsymbol{u}_{\ell'}, \boldsymbol{u}_\ell \right\rangle_W = \delta_{\ell,\ell'}$
- Dense system of equations for $\{\lambda_\ell^n\}$

Numerical Test Problem

NC STATE UNIVERSITY



- Fleck & Cummings, 1971
- 17 frequency (energy) groups
- 60 spatial cells, $\Delta x = 0.1$ cm
- $\Delta t = 2 \times 10^{-2}$ ns
- $0 \leq t \leq 6$ ns, 300 time steps
- DS_4 Gaussian quadrature set
- Finite volume in space & fully implicit scheme for LOQD eqs.

F-C Test Physical Regimes

NC STATE UNIVERSITY

- The F-C test is characterized by three distinct temporal stages
  - Rapid wave formation $t \in [0, 0.3\text{ns}]$
  - Propagation of wave from left to right $t \in (0.3, 1.2\text{ns}]$
  - Slow heating of entire domain towards steady state $t \in (1.2, 6\text{ns}]$
- Finding a POD basis that can represent all three physical regimes is a challenge
- Instead, a separate POD basis can be formulated for each regime

Calculation of Basis

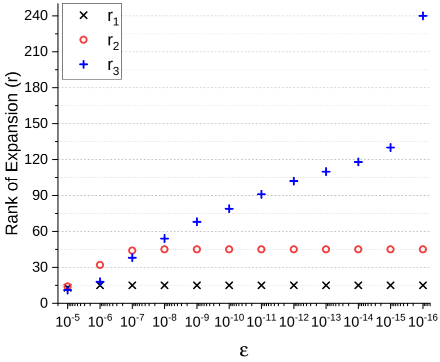
NC STATE UNIVERSITY

- We calculate a unique POD basis for each distinct stage of the F-C test
- $\boldsymbol{A}_1,\ \boldsymbol{A}_2,\ \boldsymbol{A}_3$ with $d_i = \text{rank}(\boldsymbol{A}_i)$

- ranks $r_i \leq d_i$ are calculated based off singular values of $\boldsymbol{A}_i$

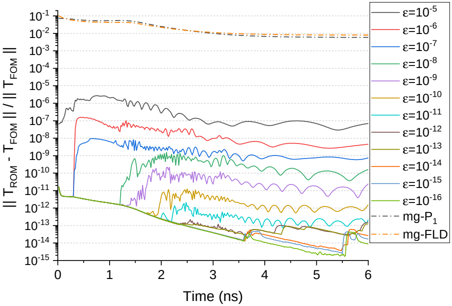
$$\xi^2 = \frac{\sum_{\ell=k+1}^{d} \sigma_\ell^2}{\sum_{\ell=1}^{d} \sigma_\ell^2}$$

- Stage 1 (r_1): full rank $= 15$
- Stage 2 (r_2): full rank $= 45$
- Stage 3 (r_3): full rank $= 240$

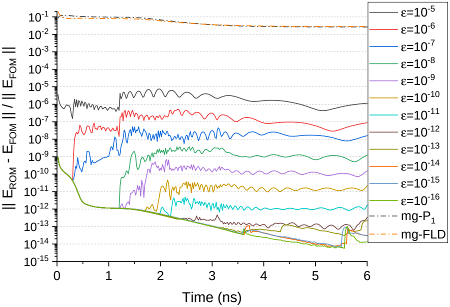


NC STATE UNIVERSITY

- Relative errors in 2-norm at each instant of time



Temperature

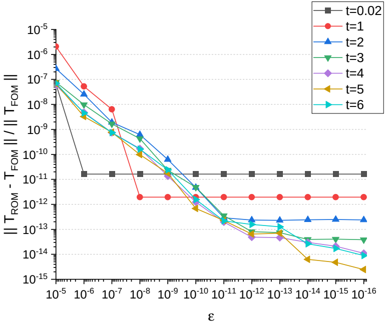


Energy density

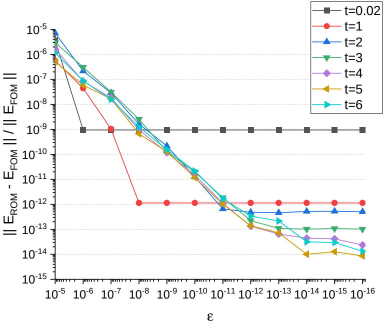
Numerical Results

NC STATE UNIVERSITY

- Relative errors in 2-norm plotted vs ξ for certain times



Temperature



Energy density

Conclusion

NC STATE UNIVERSITY

- Prototype advanced ROMs for TRT have been developed and tested in 1D and 2D geometries
- All models require data on the BTE solution
- Multiphysical equations of interest are coupled moment equations on a low-dimensional scale
- Use of the low-order moment equations enforces conservation of fundamental physics in radiative transfer component
- The proposed methods have been shown to perform well on highly nonlinear thermal radiative transfer problems
- Future research items
  - Optimal sampling techniques for generation of data to inform and train ROMs for TRT
  - Investiagion of more complex data-driven methods for approximation
  - Parametrized ROMs for TRT
- Acknowledgement

  - This research project is funded by the Department of Defense, Defense Threat Reduction Agency, grant number HDTRA1-18-1-0042.

Publications

NC STATE UNIVERSITY

- J. Coale and D. Anistratov, A reduced-order model for thermal radiative transfer problems based on multilevel quasidiffusion method, *Proc. of Int. Conf. on Mathematics and Computational Methods Applied to Nuclear Science and Engineering M&C 2019*, Portland, OR.
- J. Coale and D. Anistratov, Data-driven grey reduced-order model for thermal radiative transfer problems based on low-order quasidiffusion equations and proper orthogonal decomposition, *Transactions of American Nuclear Society*, **121** (2019)
- J. Coale and D. Anistratov, Reduced order models for nonlinear radiative transfer based on moment equations and POD/DMD of Eddington tensor, *arXiv*: 2107.09174 (2021)
- J. Coale and D. Anistratov, Reduced-order models for thermal radiative transfer based on POD-Galerkin method and low-order quasidiffusion equations, *Proc. of Int. Conf. on Mathematics and Computational Methods Applied to Nuclear Science and Engineering M&C 2021*, Raleigh, NC.

Questions?