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A Reduced-Order Model for Thermal Radiative Transfer Based on POD-Petrov-Galerkin Projection of the Normalized Boltzmann Transport Equation

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High Energy Density Physics (Problem Description)

- We consider problems of high-energy density physics (HEDP)
  - Phenomena characterized by extremely high temperatures
  - Significant radiative transfer effects
  - Examples: Supernovae, internal confinement fusion, etc.
- Phenomena in the high energy-density regime are modeled with complex, multi-physical systems of partial differential equations
- Typical challenges faced in the numerical simulation of these systems:
  - Strong nonlinear behavior and coupling between equations
  - Multi-scale characterization in space, time & energy
  - High dimensionality (usually due to the Boltzmann transport equation)

Reduced Order Models for Transport Problems

- The Boltzmann transport equation (BTE) models involved radiation transport physics
  - 7-dimensional solution in 3D geometry
  - 100-point grid in each dimension gives rise to 10^{14} degrees of freedom
- Reduced-order models (ROMs) for the BTE can significantly lower computational costs
  - A ROM uses some low-dimensional equation(s) whose solution approximates the high-dimensional BTE solution
  - Allows for cheaper computation of (typically) the most expensive component of HEDP simulations
- Well-known ROMs for the BTE include:
  - Diffusion-type ROMs (flux-limited diffusion, P_1, ...)
  - Models utilizing maximum-entropy closures (M_n methods)
  - Variable Eddington factor (VEF) ROMs

Data-Based Reduced Order Models

- Data-based ROMs for the BTE offer some advantage to other ROMs
  - The goal: to develop new ROMs which can produce more accurate (or faster) solutions compared to more classical models (e.g. diffusion)
  - The idea: apply methods which create low-dimensional approximations leveraging known data on the solution to a problem
- Data-based ROMs have been successfully developed for:
  - Linear neutral-particle transport problems
  - Reactor physics problems (LWRs & MSRs)
  - Nonlinear radiative transfer problems
- We will introduce a new data-based ROM for the nonlinear thermal radiative transfer (TRT) problem
  - Fundamental model which contains all essential challenges of the broader class of radiation-hydrodynamics problems
  - Useful platform for the development of new models

Thermal Radiative Transfer

- Boltzmann transport equation (BTE):

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I_g + \varkappa_g(T) I_g = \varkappa_g(T) B_g(T) \quad \boldsymbol{r}\in\Gamma\,,\ \forall\boldsymbol{\Omega}\,,\ g\in\mathbb{N}(G)\,,\ t\geq 0\,,$$

$$I_g|_{\boldsymbol{r}\in\partial\Gamma} = I_g^{\text{in}} \ \text{ for }\ \boldsymbol{\Omega}\cdot\boldsymbol{n}_\Gamma < 0, \quad I_g|_{t=0} = I_g^0,$$

- Material energy balance (MEB) equation:

$$\frac{\partial\varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\left(\int_{4\pi} I_g d\Omega - 4\pi B_g(T)\right)\varkappa_g(T), \quad T|_{t=0} = T^0$$

- Material temperature: $T(\boldsymbol{r}, t)$
- Specific radiation intensity: $I_g(\boldsymbol{r}, \boldsymbol{\Omega}, t)$

Multilevel Quasidiffusion Method for TRT

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

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\left(\int_{4\pi} I_g d\Omega - 4\pi B_g(T)\right)\varkappa_g(T)$$

Multilevel Quasidiffusion Method for TRT

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

$$\mathcal{P}^0_\Omega u = \int_{4\pi} u d\Omega,\ \mathcal{P}^1_\Omega u = \int_{4\pi} \mathbf{\Omega} u d\Omega$$

$$\mathcal{P}^0_\Omega\left[\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\nabla I_g + \varkappa_g(T) I_g\right] = \mathcal{P}^0_\Omega\left[\varkappa_g(T) B_g(T)\right]$$

$$\mathcal{P}^1_\Omega\left[\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\nabla I_g + \varkappa_g(T) I_g\right] = \mathcal{P}^1_\Omega\left[\varkappa_g(T) B_g(T)\right]$$

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\left(\int_{4\pi} I_g d\Omega - 4\pi B_g(T)\right)\varkappa_g(T)$$

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

$$\frac{\partial E_g}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{F}_g + c\varkappa_g(T)E_g = 4\pi\varkappa_g(T)B_g(T)$$

$$\mathfrak{f}_g = \frac{\int_{4\pi}(\boldsymbol{\Omega}\otimes\boldsymbol{\Omega})I_g d\Omega}{\int_{4\pi} I_g d\Omega}$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g = 0$$

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\Big(cE_g - 4\pi B_g(T)\Big)\varkappa_g(T)$$

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$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g = 0$$

$$\mathcal{P}_G u_g = \sum_{g=1}^{G} u_g$$

$$\mathcal{P}_G\left[\frac{\partial E_g}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{F}_g + c\varkappa_g(T)E_g\right] = \mathcal{P}_G\Big[4\pi\varkappa_g(T)B_g(T)\Big]$$

$$\mathcal{P}_G\left[\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g\right] = 0$$

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Multilevel Quasidiffusion Method for TRT

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$$\frac{\partial E_g}{\partial t} + \nabla\cdot\boldsymbol{F}_g + c\varkappa_g(T)E_g = 4\pi\varkappa_g(T)B_g(T)$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\nabla\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g = 0$$

$$\frac{\partial E}{\partial t} + \nabla\cdot\boldsymbol{F} + c\langle\varkappa\rangle_E E = c\langle\varkappa\rangle_B a_R T^4$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}}{\partial t} + c\nabla\cdot(\langle\mathfrak{f}\rangle_E E) + \bar{K}\boldsymbol{F} + \bar{\boldsymbol{\eta}}E = 0$$

$$\frac{\partial \varepsilon(T)}{\partial t} = c\langle\varkappa\rangle_E E - c\langle\varkappa\rangle_B a_R T^4$$

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

$$\mathfrak{f}_g = \frac{\int_{4\pi}(\boldsymbol{\Omega}\otimes\boldsymbol{\Omega})I_g d\Omega}{\int_{4\pi} I_g d\Omega}$$

$$E = \sum_{g=1}^{G} E_g, \quad \boldsymbol{F} = \sum_{g=1}^{G}\boldsymbol{F}_g$$

Effective group-averaged closures:

$$\langle\varkappa\rangle_E, \ \langle\varkappa\rangle_B, \ \langle\mathfrak{f}\rangle_E, \ \bar{K}, \ \bar{\boldsymbol{\eta}},$$

$$\bar{K} = \mathrm{diag}(\langle\varkappa\rangle_{|F_x|}, \langle\varkappa\rangle_{|F_y|})$$

$$\langle u\rangle_W = \frac{\sum_{g=1}^{G} u_g W_g}{\sum_{g=1}^{G} W_g}$$

Idea for the Reduced Order Model

- Fundamental idea: if the Eddington tensor ($\mathfrak{f}_g$) can be approximated, the TRT problem can be solved with only moment equations
- Direct (equation free) data-driven estimation of the Eddington tensor
  - Using proper orthogonal decomposition (POD) & dynamic mode decomposition (DMD)
- Estimation of Eddington tensor using POD-Galerkin projected BTE solution
  - Low-dimensional projected BTE is cheap to solve
  - Resulting closures are coupled to the problem solution
- The ROM introduced here is the next step in this line of work
  - We use a POD-Petrov-Galerkin projection of the *normalized* BTE (NBTE)
  - Allows direct formulation of the Eddington tensor in terms of moments of POD basis
  - The NBTE solution is naturally bounded and easier to project onto few POD modes

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The Normalized Boltzmann Transport Equation

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

$$\Downarrow$$

$$\boxed{\frac{1}{c}\frac{\partial \bar{I}_g}{\partial t} + \mathbf{\Omega}\cdot\nabla \bar{I}_g + \hat{\varkappa}_g(T,\phi_g)\bar{I}_g = \varkappa_g(T)\bar{B}_g(T,\phi_g)}$$

$$\hat{\varkappa}_g = \varkappa_g + \frac{1}{c}\frac{\partial \ln(\phi_g)}{\partial t} + \mathbf{\Omega}\cdot\nabla\ln(\phi_g), \qquad \bar{B}_g = \frac{B_g}{\phi_g}$$

- Normalized radiation intensity

$$\bar{I}_g = \frac{I_g}{\phi_g}$$

- Zeroth moment $\phi_g = \int_{4\pi} I_g d\Omega = cE_g$
- The Eddington tensor is a linear function of $\bar{I}_g$

$$\boxed{\mathfrak{f}_g = \int_{4\pi} (\mathbf{\Omega}\otimes\mathbf{\Omega})\bar{I}_g}$$

Discretization of the NBTE

- Rewrite the NBTE (substitute $\bar{I}_g$ into the BTE):

$$\frac{1}{c}\frac{\partial(\phi_g \bar{I}_g)}{\partial t} + \boldsymbol{\Omega}\cdot\nabla(\phi_g \bar{I}_g) + \varkappa_g(T)\phi_g \bar{I}_g = \varkappa_g(T)B_g(T)$$

- We formulate discretization of the NBTE consistent with the simple corner balance (SCB) scheme for the BTE:

$$\mathcal{R}_h^n(\bar{\boldsymbol{I}}^n) = \frac{1}{c\Delta t^n}(\phi^n \odot_\Omega \bar{\boldsymbol{I}}^n - \phi^{n-1} \odot_\Omega \bar{\boldsymbol{I}}^{n-1}) + \mathcal{L}_h(\phi^n)\bar{\boldsymbol{I}}^n - \mathcal{Q}_h^n, \quad \mathcal{R}_h^n(\bar{\boldsymbol{I}}^n) = 0$$

- $\bar{\boldsymbol{I}}^n$ and ϕ^n are discrete vectors over the entire phase space $(\boldsymbol{r}, \boldsymbol{\Omega}, t, g)$
- Goal: project the discrete NBTE over the entire phase space with some inner product onto a low-dimensional space

Generation of data, definition of inner product

- We assume some set of a-priori known solution data to the TRT problem:

$$\mathbf{A}^{\bar{I}} = [\bar{\boldsymbol{I}}^1, \dots, \bar{\boldsymbol{I}}^N], \quad \mathbf{A}^{\phi} = [\phi^1, \dots, \phi^N]$$

- Define the discrete inner product

$$\langle u, v \rangle = \int_0^{\infty} \int_{4\pi} \int_{\Gamma} uv \; d\boldsymbol{r} d\Omega d\nu \;\; \Rightarrow \;\; \langle \boldsymbol{u}, \boldsymbol{v} \rangle = \boldsymbol{u}^{\top} \mathbf{W} \boldsymbol{v}$$

- Using the grid functions of unknowns of the SCB scheme on a 2D square mesh:

$$\mathbf{W} = \bigoplus_{g=1}^{G} \bigoplus_{m=1}^{M} \bigoplus_{j=1}^{J} \frac{w_m a_j}{4} \mathbb{I}_4,$$

  where g, m, j are indices in group, angle, space
- To formulate the weighted SVD induced by the BE time integration scheme we define

$$\mathbf{H} = \mathrm{diag}(\Delta t^1, \; \Delta t^2, \; \dots, \; \Delta t^N),$$

Expansion of the Normalized Intensities

- We seek an expansion basis which optimally captures $\mathbf{A}^{\bar{I}}$ in the norm induced by the derived inner product

$$\bar{\boldsymbol{I}}^n = \sum_{\ell=1}^{k} \lambda_\ell^n \boldsymbol{u}_\ell = \mathbf{U}_k \Lambda^n, \quad k \leq r, \quad r = \text{rank}(\mathbf{A}^{\bar{I}})$$

- Define the weighted singular value decomposition:

$$\hat{\mathbf{A}}^{\bar{I}} = \mathbf{W}^{-1/2} \mathbf{A}^{\bar{I}} \mathbf{H}^{-1/2} = \hat{\mathbf{U}} \hat{\mathbf{S}} \hat{\mathbf{V}}^\top$$

- The desired basis $\{\boldsymbol{u}_\ell\}$ is the first k column vectors of $\mathbf{U} = \mathbf{W}^{1/2} \hat{\mathbf{U}}$
- Substitute expansion into the discrete NBTE:

$$\mathcal{R}_h^n(\mathbf{U}_k \Lambda^n) = 0$$

Projection of the NBTE

- Projecting the NBTE onto some test basis $\{\psi_\ell\}$ yields a $k \times k$ dynamical system whose solution is for Λ^n

$$\Psi^\top \mathbf{W}\mathcal{R}_h^n(\mathbf{U}_k\Lambda^n) = 0, \quad \Psi^\top \mathbf{W}\mathbf{U}_k\Lambda^0 = \Psi^\top \mathbf{W}\bar{\boldsymbol{I}}^0$$

- We seek a projection basis which optimally projects the NBTE in the derived inner product (i.e. minimizes its residual)

$$\Lambda^n = \arg\min_{\boldsymbol{\xi}\in\mathbb{R}^{\boldsymbol{k}}} \langle \mathcal{R}_h^n(\mathbf{U}_k\Lambda^n)\rangle$$

- The solution to $\Psi^\top \mathbf{W}\mathcal{R}_h^n(\mathbf{U}_k\Lambda_n)$ satisfies the above with $\{\psi_\ell\}$ defined:

$$\psi_\ell = \frac{d\mathcal{R}_h^n(\lambda_\ell^n \boldsymbol{u}_\ell)}{d\lambda_\ell^n}$$

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Expansion of Eddington Tensor in Moments of POD Modes

- The Eddington tensor:

$$\mathfrak{f}_g = \int_{4\pi} (\boldsymbol{\Omega} \otimes \boldsymbol{\Omega}) \bar{I}_g$$

- In discrete form:
  - M discrete directions with $\{w_m\}$ quadrature weights
  - $\bar{\boldsymbol{I}}_m$ is the portion of $\bar{\boldsymbol{I}}$ corresponding to discrete direction m

$$\boldsymbol{f}^n = \sum_{m=1}^{M} w_m (\boldsymbol{\Omega}_m \otimes \boldsymbol{\Omega}_m) \bar{\boldsymbol{I}}_m^n$$

- Substitute expansion in POD modes:
  - $\boldsymbol{u}_{\ell,m}$ is the portion of $\boldsymbol{u}_\ell$ corresponding to discrete direction m

$$\boldsymbol{f}^n = \sum_{\ell=1}^{k} \lambda_\ell^n \boldsymbol{u}'_\ell, \quad \boldsymbol{u}'_\ell = \sum_{m=1}^{M} w_m (\boldsymbol{\Omega}_m \otimes \boldsymbol{\Omega}_m) \boldsymbol{u}_{\ell,m}$$

Rank of Expansion & Data Collection

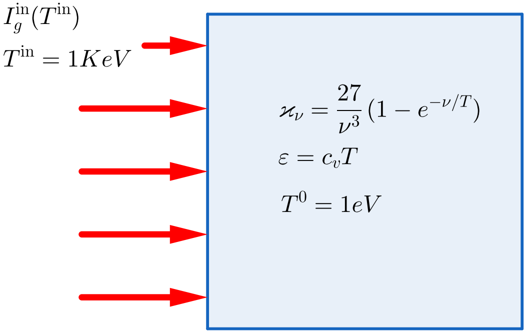
- Rank chosen so that the k-term expansion of $\bar{I}$ has relative error in Frobeinus norm less than some $\xi \in [0, 1]$:

$$k = \min \left\{ p \ : \ \sqrt{\frac{\sum_{\ell=p+1}^{r} \sigma_\ell^2}{\sum_{\ell=1}^{r} \sigma_\ell^2}} \leq \xi \right\}$$

- Data for $\bar{I}$ and ϕ can be generated from the BTE solution given a discretization that is algebraically consistent to the NBTE

$$\mathbf{A}^I = [\boldsymbol{I}^1, \ldots, \boldsymbol{I}^N] \quad \Rightarrow \quad \phi^n = \sum_{m=1}^{M} w_m \boldsymbol{I}_m^n, \quad \bar{\boldsymbol{I}}^n = \frac{\boldsymbol{I}^n}{\phi^n}$$

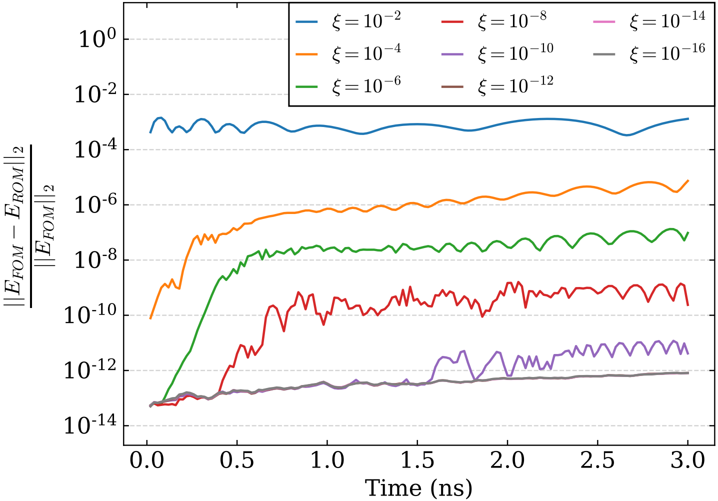
Fleck-Cummings Test Problem Description



- Specification:
  - 2D Cartesian domain 6 $\times$ 6 cm
  - Temporal interval $t \in [0, 3 \text{ ns}]$
- Discretization:
  - 10 $\times$ 10 spatial grid (0.6 $\times$ 0.6 cm cells)
  - 150 time steps of length 0.02 ns
  - 17 frequency groups
  - 144 discrete directions
  - BTE discretized in space with the simple corner balance scheme
  - Low-order QD (LOQD) equations discretized with 2^{nd} order finite volumes scheme
  - The BTE and LOQD equation are discretized in time with the fully implicit (backward-Euler) scheme

Error Norms of ROM Solutions

- Relative error in *E* vs full-order model (FOM)
- FOM defined with the multilevel quasidiffusion system
- Calculated in the 2-norm at each time step



Error Norms of ROM Solutions

- Relative error in T vs full-order model (FOM)
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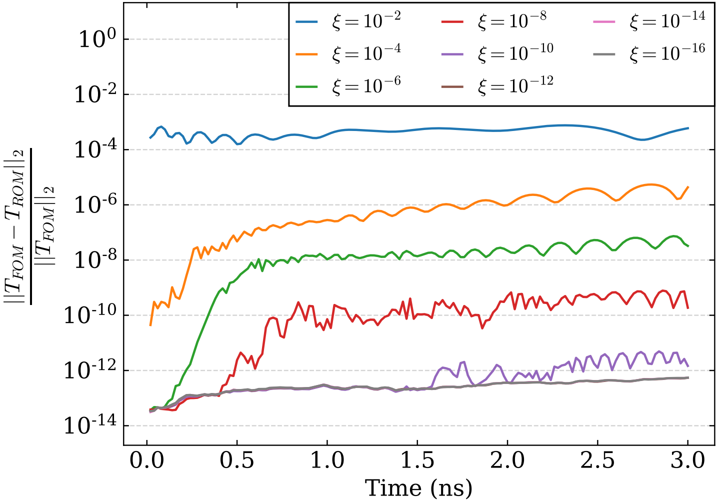

Discussion

- The presented ROM is based on a POD-Petrov-Galerkin projection of the NBTE
  - Solution of projected NBTE yields coefficients of the Eddington tensor expansion in angular moments (integrals) of POD modes of normalized intensity
  - The generated closures are coupled to the multiphysics
- The ROM is demonstrated to effectively reduce the dimensionality of the TRT problem
  - Error levels compared to the FOM are dependent on rank of expansion, and uniformly decrease with increases in rank
  - Iterations at each time step converge rapidly (see paper)
  - The ROM errors are shown to converge approximately linearly with ξ (see paper)

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Questions?