Reduced-Order Models for Thermal Radiative Transfer Based on POD-Galerkin Method and Low-Order Quasidiffusion Equations

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Radiation Transport

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- We consider problems of high-energy density physics, where radiative transfer is the main mechanism of energy redistribution
  - Described by complex systems of multiphyiscal differential equations
- Numerical simulations of these complex multiphysical problems are faced with several challenges
  - Strong nonlinearity
  - Multi-scale characterization
  - High-dimensionality
- The Boltzmann transport equation (BTE) drives the dimensionality
  - The solution is 7-dimensional
  - Independent variables include: time (t), spatial position ($\boldsymbol{r}$), direction of motion ($\boldsymbol{\Omega}$), frequency (ν) describing photons
  - Simple discretization - 100 nodes each axis: 10^{12} degrees of freedom
  - The high dimensionality imposes large computational burden and memory footprint
- Reduced order models for the BTE are commonly employed to reduce the problem of dimensionality

Model Order Reduction for the BTE

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- We develop a reduced-order model (ROM) for the BTE to reduce the dimensionality of multiphysical simulations
  - Reducing both computational cost and memory requirements
- Basic idea of the model:
  - Formulate a proper orthogonal decomposition - Galerkin (POD-G) projection for the BTE using known solution data
  - The photon intensities are expanded about the POD basis
  - The projected form of the BTE solves for the coefficients of this expansion for photon intensities
  - Equip the low-dimensional projected BTE with a system of low-order moment equations of the BTE
- The POD-G BTE serves to calculate closures for the moment equations, which are coupled to the specific multiphysics equations of interest

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- The first prototype of this method is formulated on the multigroup thermal radiative transfer (TRT) problem in 1D slab geometry
- The high-order Boltzmann transport equation

$$\frac{1}{c}\frac{\partial I_g}{\partial t}(x,\mu,t) + \mu\frac{\partial I_g}{\partial x}(x,\mu,t) + \varkappa_g(T)I_g(x,\mu,t) = 2\pi\varkappa_g(T)B_g(T) \qquad (1)$$

$$x \in [0,X], \quad \mu \in [-1,1], \quad g = 1,\dots,N_g, \quad t \geq 0,$$

$$I_g|_{\substack{\mu>0\\x=0}} = I_g^{\text{in}+}, \quad I_g|_{\substack{\mu<0\\x=X}} = I_g^{\text{in}-}, \quad I_g|_{t=0} = I_g^0, \qquad (2)$$

- The material energy balance equation

$$\frac{\partial\varepsilon(T)}{\partial t} = \sum_{g=1}^{N_g}\varkappa_g(T)\left(\int_{-1}^{1} I_g(x,\mu,t)d\mu - 4\pi B_g(T)\right), \quad T|_{t=0} = T_0. \qquad (3)$$

- Supersonic radiation flow problem neglecting material motion, photon scattering, heat conduction and external sources

Discretization of the BTE

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

$$\frac{1}{c}\frac{\partial I_g}{\partial t}(x,\mu,t) + \mu\frac{\partial I_g}{\partial x}(x,\mu,t) + \varkappa_g(T)I_g(x,\mu,t) = 2\pi\varkappa_g(T)B_g(T)$$

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

$$\frac{1}{c\Delta t^n}\left(\mathbf{I}^n - \mathbf{I}^{n-1}\right) + \mathcal{L}_h\mathbf{I}^n + \mathcal{K}_h^n(T)\mathbf{I}^n = \mathbf{Q}^n(T)\,, \tag{4}$$

- Discrete operators $\mathcal{L}_h$, $\mathcal{K}_h^n(T)$ determined by scheme
- N_x spatial cells, N_μ discrete directions, N_t time steps,
- $D = 2N_x N_\mu N_g$
- Solution vector: $\mathbf{I}^n = ((\boldsymbol{I}_1^n)^\top \ \ldots \ (\boldsymbol{I}_{N_g}^n)^\top)^\top \in \mathbb{R}^D$
- Construct snapshot matrix

$$\boldsymbol{A} = [\boldsymbol{I}^1, \ldots, \boldsymbol{I}^{N_t}] \tag{5}$$

POD Basis Formulation

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

$$\mathbf{I}_r^u(t^n) = \sum_{\ell=1}^{r} \lambda_\ell^n \boldsymbol{u}_\ell \tag{6}$$

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

$$\min_{\boldsymbol{u}_1,\dots,\boldsymbol{u}_r} \sum_{n=1}^{N_t} \Delta t^n \left\| \mathbf{I}^n - \sum_{\ell=1}^{r} \langle \mathbf{I}^n, \boldsymbol{u}_\ell \rangle_W \boldsymbol{u}_\ell \right\|_W^2, \tag{7}$$

- 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

- 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

$$\int_0^\infty \int_{-1}^1 \int_0^{L_x} u(x,\mu,\nu) dx d\mu d\nu \;\Rightarrow\; \sum_{g=1}^{N_g} \sum_{m=1}^{N_\mu} w_m \sum_{i=1}^{N_x} \frac{\Delta x_i}{2} (\boldsymbol{u}_{g,m,i,L} + \boldsymbol{u}_{g,m,i,R}) \quad (8)$$

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

$$\boldsymbol{W} = \bigoplus_{g=1}^{N_g} \bigoplus_{m=1}^{N_\mu} w_m \hat{\boldsymbol{W}}^x, \quad \hat{\boldsymbol{W}}^x = \bigoplus_{i=1}^{N_x} \begin{pmatrix} \frac{\Delta x_i}{2} & 0 \\ 0 & \frac{\Delta x_i}{2} \end{pmatrix} \quad (9)$$

Calculation of POD Basis

- Construct snapshot matrix

$$\boldsymbol{A} = [\boldsymbol{I}^1, \dots, \boldsymbol{I}^{N_t}] \tag{10}$$

- Calculate weighted snapshot matrix

$$\hat{\boldsymbol{A}} = \boldsymbol{W}^{1/2}\boldsymbol{A}\boldsymbol{D}^{1/2}, \quad \boldsymbol{D} = \text{diag}(\Delta t^1, \dots, \Delta t^{N_t}) \tag{11}$$

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

$$\hat{\boldsymbol{A}} = \hat{\boldsymbol{U}}\hat{\boldsymbol{S}}\hat{\boldsymbol{V}}^\top \tag{12}$$

$$\hat{\boldsymbol{U}} = [\hat{\boldsymbol{u}}_1, \dots, \hat{\boldsymbol{u}}_d], \quad \hat{\boldsymbol{S}} = \text{diag}(\sigma_1, \dots, \sigma_d), \quad \hat{\boldsymbol{V}} = [\hat{\boldsymbol{v}}_1, \dots, \hat{\boldsymbol{v}}_d] \tag{13}$$

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

$$\boldsymbol{U} = \boldsymbol{W}^{-1/2}\hat{\boldsymbol{U}} \tag{14}$$

Truncation Criteria & Rank Determination

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- Full rank system of equations for $\{\lambda_\ell^n\}$ is of size d using all $\boldsymbol{u}_\ell$
- We seek a system of size $r \leq d$ using the first r basis functions in the expansion
- As r decreases, computational efficiency will increase while accuracy decreases
- We seek $r \ll D$ that will give certain level of accuracy
- Truncation criteria (tuning parameter):

$$\xi^2 = \frac{\sum_{\ell=r+1}^{d} \sigma_\ell^2}{\sum_{\ell=1}^{d} \sigma_\ell^2} \tag{15}$$

- Set some ξ and find rank r that satisfies the relation above
- This allows the method to easily trade computational requirements with accuracy at will per simulation

POD Galerkin Projection

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

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

$$\frac{1}{c\Delta t^n}\left(\lambda_\ell^n - \lambda_\ell^{n-1}\right) + \sum_{\ell'=1}^{r} \lambda_{\ell'}^n \left\langle \boldsymbol{u}_\ell, \mathcal{L}_h \boldsymbol{u}_{\ell'} \right\rangle_W + \sum_{\ell'=1}^{r} \lambda_{\ell'}^n \left\langle \boldsymbol{u}_\ell, \mathcal{K}_h^n(T) \boldsymbol{u}_{\ell'} \right\rangle_W = \left\langle \boldsymbol{u}_\ell, \mathbf{Q}^n(T) \right\rangle_W \qquad (16)$$

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

Multilevel Quasidiffusion Method

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- High-order Boltzmann transport equation

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \mu\frac{\partial I_g}{\partial x} + \varkappa_g(T)I_g = 2\pi\varkappa_g(T)B_g(T)$$

- Eddington factor $\mathfrak{f}_g[I] = \int_{-1}^{1}\mu^2 I_g d\mu \Big/ \int_{-1}^{1} I_g d\mu$

- Multigroup quasidiffusion equations for $E_g = \frac{1}{c}\int_{-1}^{1} I_g d\mu, \quad \boldsymbol{F}_g = \int_{-1}^{1}\mu I_g d\mu$

$$\frac{\partial E_g}{\partial t} + \frac{\partial F_g}{\partial x} + c\varkappa_g(T)E_g = 4\pi\varkappa_g(T)B_g(T),$$
$$\frac{1}{c}\frac{\partial F_g}{\partial t} + c\frac{\partial}{\partial x}\left(\mathfrak{f}_g[I]E_g\right) + \varkappa_g(T)F_g = 0$$

- Effective grey problem for $E = \sum_{g=1}^{N_g} E_g, \quad \boldsymbol{F} = \sum_{g=1}^{N_g}\boldsymbol{F}_g$

$$\frac{\partial E}{\partial t} + \frac{\partial F}{\partial x} + c\bar{\varkappa}_E E = c\bar{\varkappa}_B a_R T^4$$
$$\frac{1}{c}\frac{\partial F}{\partial t} + c\frac{\partial(\bar{\mathfrak{f}}E)}{\partial x} + \bar{\varkappa}_R F + \bar{\eta}E = 0$$
$$\frac{\partial\varepsilon(T)}{\partial t} = c\left(\bar{\varkappa}_E E - \bar{\varkappa}_B a_R T^4\right)$$

Reduced Order Model

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- POD Galerkin Projected Boltzmann transport equation

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

- Approximate intensities $\mathbf{I}_r^u=\sum_{\ell=1}^{r}\lambda_\ell^n\boldsymbol{u}_\ell \implies \tilde{\mathfrak{f}}_g[\mathbf{I}_r^u]$
- Multigroup quasidiffusion equations

$$\frac{\partial E_g}{\partial t}+\frac{\partial F_g}{\partial x}+c\varkappa_g(T)E_g=4\pi\varkappa_g(T)B_g(T),$$

$$\frac{1}{c}\frac{\partial F_g}{\partial t}+c\frac{\partial}{\partial x}\left(\tilde{\mathfrak{f}}_g[\mathbf{I}_r^u]E_g\right)+\varkappa_g(T)F_g=0$$

- Effective grey problem

$$\frac{\partial E}{\partial t}+\frac{\partial F}{\partial x}+c\bar{\varkappa}_E E=c\bar{\varkappa}_B a_R T^4$$

$$\frac{1}{c}\frac{\partial F}{\partial t}+c\frac{\partial(\bar{\mathfrak{f}}E)}{\partial x}+\bar{\varkappa}_R F+\bar{\eta}E=0$$

$$\frac{\partial\varepsilon(T)}{\partial t}=c\left(\bar{\varkappa}_E E-\bar{\varkappa}_B a_R T^4\right)$$

Numerical Test Problem

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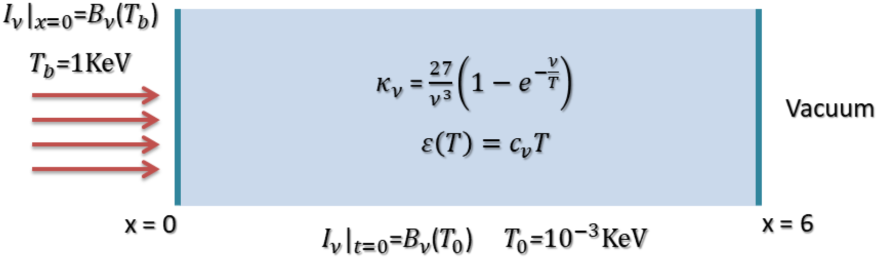

- Fleck & Cummings, 1971
- 17 frequency (energy) groups
- 60 spatial cells, $\Delta x = 0.1$ cm
- $\Delta t = 2 \times 10^{-2}$ ns
- $0 \le t \le 6$ ns, 300 time steps
- DS_4 Gaussian quadrature set
- Finite volume in space & fully implicit scheme for LOQD eqs.

Numerical Test Problem

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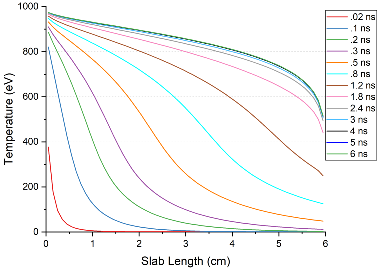
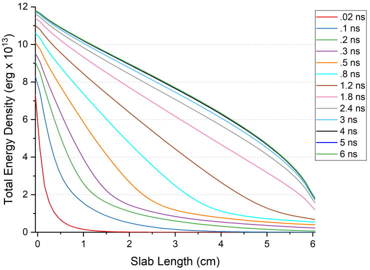
- The F-C test is characterized by three distinct temporal stages
  - Rapid wave formation $t \in [0, 0.3\text{ns}]$
  - Propagation of wave from left to right $t \in (0.3, 1.2\text{ns}]$
  - Slow heating of entire domain towards steady state $t \in (1.2, 6\text{ns}]$



Temperature



Energy density

Calculation of Basis

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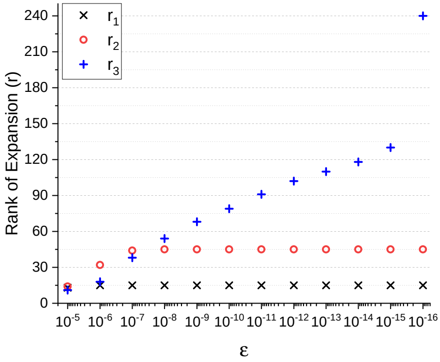
- We calculate a unique POD basis for each distinct stage of the F-C test
- $\boldsymbol{A}_1,\ \boldsymbol{A}_2,\ \boldsymbol{A}_3$ with $d_i = \text{rank}(\boldsymbol{A}_i)$

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

$$\left(\sum_{\ell=r_i+1}^{d_i} \sigma_\ell^2 \Big/ \sum_{\ell=1}^{d_i} \sigma_\ell^2 \right)^{\frac{1}{2}} < \xi$$

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



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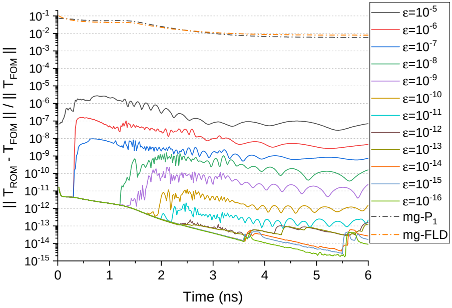
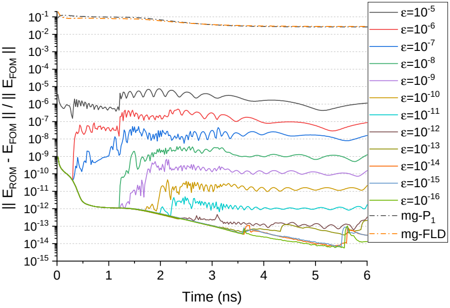
- Relative errors in 2-norm at each instant of time



Temperature



Energy density

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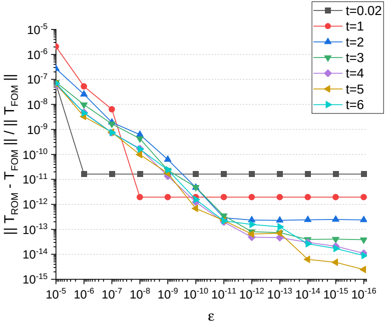
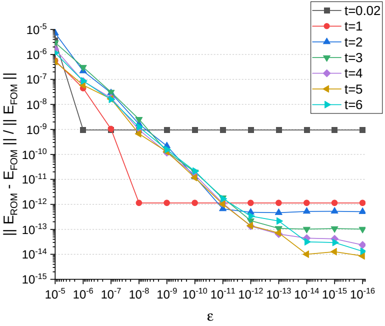
- Relative errors in 2-norm plotted vs ξ for certain times



Temperature



Energy density

Conclusion

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- We developed and tested a prototype advanced ROM for TRT in 1D geometry
- A POD Galerkin-Projected BTE is coupled with the low-order quasidiffusion equations to give approximate closure
- The Projected BTE is dense but contains many less degrees of freedom compared to the original BTE
- The expansion coefficients directly depend on material temperature, making the ROM naturally parametric
- The ROM was shown to produce highly accurate solutions, and converge uniformly to the reference solution as rank is increased
- Results are promising, and future work includes:
    - Extension of the method into 2D geometry
    - Investigation into performance over given parametric spaces