Data-Driven Grey Reduced-Order Model for Thermal Radiative Transfer Problems Based on Low-Order Quasidiffusion Equations and Proper Orthogonal Decomposition

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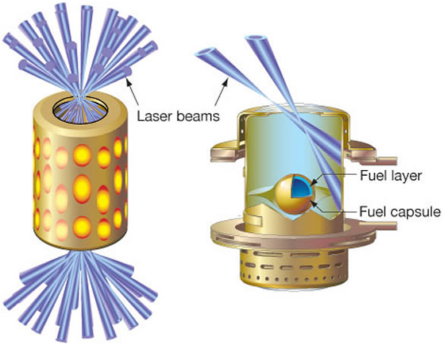
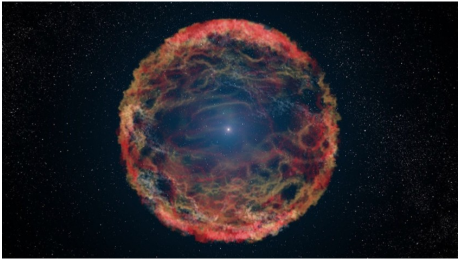
Outline

Introduction

- Thermal radiative transfer (TRT) is an essential piece of many high energy-density multiphysical processes
  - Astrophysics (supernovae)
  - Internal confinement fusion
  - high temperature laser-driven applications





Introduction

- The radiative-hydrodynamics problem models these physical processes, characterized by several fundamental features
  - High dimensionality
  - Multiple scales in time and space
  - Strong nonlinearity and coupling of equations
- There is a need for computational models of various levels of fidelity for
  - Design calculations
  - Parametric studies
  - Modeling experiments
- To lower the computational burden, we formulate a reduced-order model (ROM)
  - Based on a hierarchy of low-order equations for moments of the solution that can reproduce transport effects to an arbitrary degree of accuracy
  - Maintain essential nonlinear future on the original high-fidelity problem
  - Couples low-order radiative transfer model with the material energy balance equation
  - Preserve multiscale nature of the problem

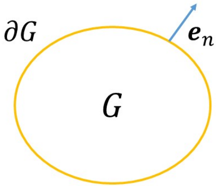
Reduced-Order Modeling

- Classical ROMs that have previously been developed for radiative transfer (P_1, Diffusion) have limitations due to inherent modeling errors
- We propose new data-driven ROMs based on two different techniques
  - The **multilevel nonlinear projective-iterative** (MNPI) methodology
  - The **proper orthogonal decomposition** (POD)
- The MNPI methodology is leveraged to formulate a hierarchy of **effective low-order transport** (ELOT) problems
  - The RT equation is projected into a lower dimensional subspace
  - ELOT equations defined for the angular and energy moments of the specific intensity
  - Exact closures to the ELOT problems allow full recreation of transport physics
- The POD is leveraged to approximate the high-order solution
  - Allows for accurate representation of the high order solution
  - Introduces the limitation of being problem-dependent

Multigroup Thermal Radiative Transfer Problem

- The radiative transfer (RT) equation

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



$$\boldsymbol{r}\in G, \quad \forall\ \boldsymbol{\Omega}, \quad g=1,\dots,N_g, \quad t\geq t_0$$

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

$$I_g|_{t=t_0} = I_g^0, \quad \boldsymbol{r}\in G, \quad \forall\ \boldsymbol{\Omega}$$

$$B_g(T) = \frac{2h}{c^2}\int_{\nu_g}^{\nu_{g+1}} \nu^3 \left(e^{\frac{h\nu}{kT}}-1\right)^{-1} d\nu$$

- The material energy balance (MEB) equation gives a basic model of photon interaction with matter

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

$$T|_{t=t_0} = T^0(\boldsymbol{r}), \quad \boldsymbol{r}\in G, \quad g=1,\dots,N_g$$

Multigroup Low-Order Quasidiffusion Equations

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

- Projection: $\int_{4\pi} \cdot \, d\boldsymbol{\Omega}$ & $\int_{4\pi} \cdot \, \boldsymbol{\Omega} d\boldsymbol{\Omega} \rightarrow \boldsymbol{f}_g = \dfrac{\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} I_g d\boldsymbol{\Omega}}{\int_{4\pi} I_g d\boldsymbol{\Omega}}$
- Functions in the projected space: $E_g = \frac{1}{c}\int_{4\pi} I_g d\boldsymbol{\Omega}$ & $\boldsymbol{F}_g = \int_{4\pi} \boldsymbol{\Omega} I_g d\boldsymbol{\Omega}$

$$\frac{\partial E_g}{\partial t} + \nabla\cdot\boldsymbol{F}_g + c\varkappa_g E_g = 4\pi\varkappa_g B_g$$
$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\nabla\cdot(\boldsymbol{f}_g E_g) + \varkappa_g \boldsymbol{F}_g = 0$$

- Projection: $\sum_{g=1}^{N_g} \cdot \quad \left(\int_0^\infty \cdot \, d\nu\right)$
- Functions in the projected space: $E = \sum_{g=1}^{N_g} E_g$ & $\boldsymbol{F} = \sum_{g=1}^{N_g} \boldsymbol{F}_g$

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

TRT Model: Multilevel System of QD Equations

- The high-order RT equation

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

$$\Downarrow$$

$$\boxed{\mathbf{f}_g \quad C_{e_n,g}}$$

- The multigroup low-order QD (LOQD) equations

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

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

$$\Downarrow$$

$$\boxed{\bar{\boldsymbol{f}} \quad \bar{C}_{e_n} \quad \bar{\varkappa}_E \quad \bar{\varkappa}_B \quad \bar{\varkappa}_R \quad \boldsymbol{\eta}}$$

- The grey LOQD equations coupled with the MEB equation

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

$$\frac{1}{c}\frac{\partial \boldsymbol{F}}{\partial t} + c\nabla\cdot\left(\bar{\boldsymbol{f}}E\right) + \bar{\varkappa}_R\boldsymbol{F} + \boldsymbol{\eta}E = 0$$

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

Grey ROM: Grey LOQD Eqs. and POD

- Low-rank representation of the high-order solution as POD expanded group QD factors

$$\Downarrow$$

$$\boxed{\tilde{\boldsymbol{f}}_g \quad C_{e_n,g}}$$

- POD expanded multigroup low-order solution $\boxed{E_g}$
- Projection-like POD of the multigroup low-order solution $\boxed{\boldsymbol{F}_g}$

$$\Downarrow$$

$$\boxed{\bar{\boldsymbol{f}} \quad \bar{C}_{e_n} \quad \bar{\varkappa}_E \quad \bar{\varkappa}_B \quad \bar{\varkappa}_R \quad \boldsymbol{\eta}}$$

- The grey LOQD equations coupled with the MEB equation

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

$$\frac{1}{c}\frac{\partial \boldsymbol{F}}{\partial t} + c\nabla \cdot \left(\bar{\boldsymbol{f}} E\right) + \bar{\varkappa}_R \boldsymbol{F} + \boldsymbol{\eta} E = 0$$

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

POD Expansion of E_g and f_g

- Given a database $\mathbf{A} \in \mathbb{R}^{X,\tau}$
- A singular value decomposition (SVD) represents **A** matrix in the form

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$$

  - $\mathbf{U} \in \mathbb{R}^{X,k}$ holds the left singular vectors in its columns
  - $\mathbf{V} \in \mathbb{R}^{\tau,k}$ holds the right singular vectors in its columns
  - $\boldsymbol{\Sigma} \in \mathbb{R}^{k,k}$ holds the k singular values (σ) along its diagonal in descending order

- **A** can be approximated as a matrix of rank $r < k$ by reducing the dimension $k \to r$ in its SVD (using the first r singular values).

$$\boxed{\frac{\sigma_n}{\sigma_1} \geq \varepsilon_\sigma \quad \text{for all } n \leq r}$$

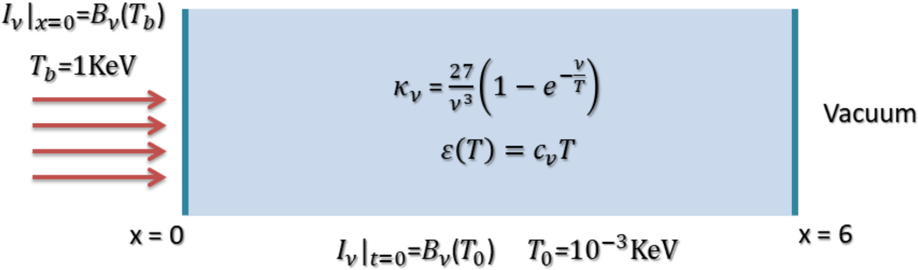
$$\tilde{\mathbf{A}}^r = \mathbf{U}^r\boldsymbol{\Sigma}^r\left(\mathbf{V}^r\right)^T,$$

$$\boldsymbol{\Sigma}^r \in \mathbb{R}^{r,r}, \quad \mathbf{U}^r \in \mathbb{R}^{m,r}, \quad \mathbf{V}^r \in \mathbb{R}^{n,r}.$$

Formulation of the Grey ROM

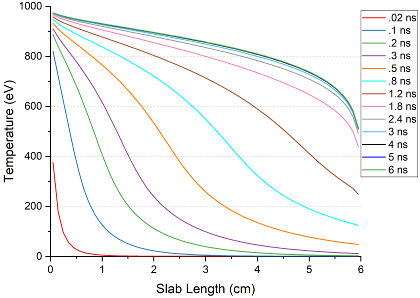
- Given some known TRT problem $\boxed{\mathcal{L}_g I_g = q_g}$
  - The solution is known for $\boxed{I_g,\ E_g}$
- The high-order is used to generate QD factors $\boxed{I_g \rightarrow \boldsymbol{f}_g}$
- For the given set of E_g and $\boldsymbol{f}_g$, the multigroup fluxes F_g are reproduced by means of the multigroup LOQD equations
- A database of QD factors $\boldsymbol{f}_g$ and energy densities E_g is created such that $\boxed{\boldsymbol{f}_g, E_g \in \mathbb{R}^{X,\tau}}$
  - X is the number of discrete spatial nodes
  - τ is the number of discrete temporal nodes
  - The n^{th} column holds the spatial vector of solutions for the n^{th} instant of time
  - $\text{rank}(\boldsymbol{f}_g) = k_g^f = \min(X, \tau)$
  - $\text{rank}(E_g) = k_g^E = \min(X, \tau)$

1D F-C Test Problem

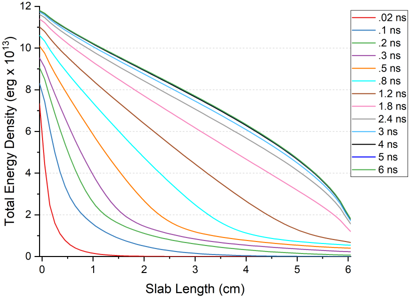


- Fleck & Cummings, 1971
- 17 frequency (energy) groups
- 60 spatial cells, $\Delta x = 0.1$ cm
- $\Delta t = 2 \times 10^{-2}$ ns
- $0 \leq t \leq 6$ ns, 300 time steps
- DS_4 Gaussian quadrature set
- Finite volume in space & fully implicit scheme for LOQD eqs.

Test Problem Solution



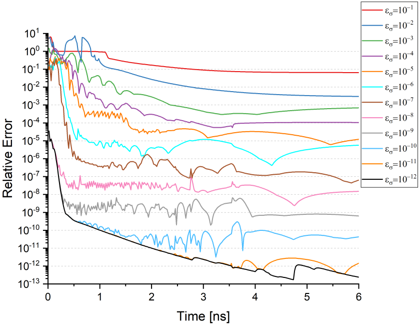
Temperature



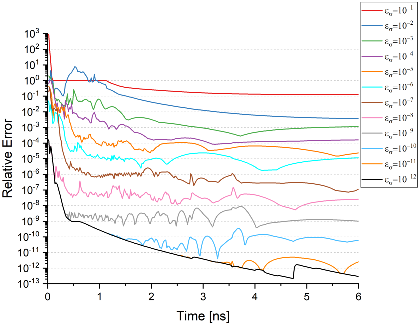
Radiation Energy Density

Solution of the Grey ROM

- The F-C test ($\Delta t = 2 \times 10^{-2}$ ns) is solved to generate the reference solution and form a database of QD factors $\tilde{\boldsymbol{f}}_g$ and energy densities $\tilde{E}_g$
- The same test is solved with the grey LOQD ROM using $\tilde{\boldsymbol{f}}_g$, $\tilde{E}_g$
- Shown is the relative error in the ∞-norm of solutions of the grey LOQD ROM computed for different ε_σ values.



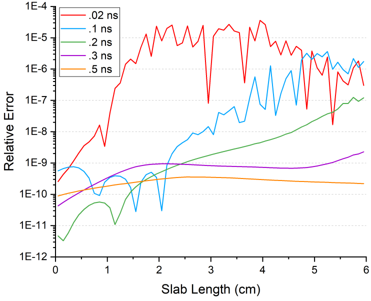
Temperature



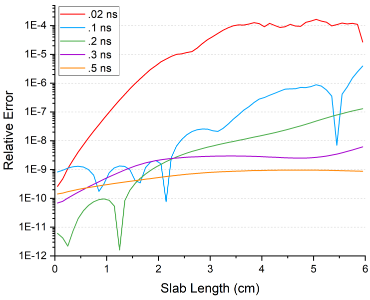
Energy density

Grey ROM High Errors at Early Times

- At early times the grey ROM shows high levels of error, which is produced on the right-hand side of the domain forward of the radiation wave
- Shown are plots of the relative error for early times across the problem domain for the grey ROM using full rank representations of E_g, $\boldsymbol{f}_g$



Temperature



Energy density

Conclusions

- In this study we developed a novel general methodology for developing reduced-order models for TRT problems
  - We apply MNPI methodology based on quasidiffusion low-order equations with POD of radiation energy spectrum and QD factors
- The grey LOQD ROM sufficiently accurately approximates the solution of the considered TRT problem
- Errors are the highest in areas dominated by local radiation
- Future study of the grey LOQD ROM includes
  - Refining how the QD factor and energy density databases are decomposed and compressed
  - Extending the ROM into 2-D
  - Extending the ROM for radiation hydrodynamic problems