Los Alamos NATIONAL LABORATORY

Transport Corrected Diffusion Reduced Order Model for Thermal Radiative Transfer

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High Energy Density Physics (Problem Description)

- Phenomena which occur in the high-energy density (HED) regime are considered
  - Extremely high temperatures
  - Energy redistribution primarily driven by radiative transfer
  - Found in astrophysics, plasma physics, combustion physics
- Numerical simulation of such phenomena is challenging
  - Multiphysical systems of partial differential equations
  - Strong nonlinear behavior
  - Multiscale characterization in space, time, energy
  - High dimensionality
- 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 for Transport Problems

- In problems involving a particle transport component, it is common practice to use a reduced-order model (ROM) for the BTE
- ROMs are formulated with low-dimensional equations and approximate the BTE solution at lower computational cost
- Common diffusion-type ROMs:
  - Flux-limited diffusion, P_1, $P_{1/3}$...
- Recent literature includes many *data-driven* ROMs for the BTE:
  - Based on methods like the POD, DMD, Neural Networks, etc.
  - Require some databases of known (full-order) solutions
  - Shown effective for linear particle transport, reactor physics, nonlinear radiative transfer
- Idea: Combine diffusion-type models with data-driven methods to improve upon solution accuracy

Thermal Radiative Transfer

- Flux-limited diffusion (FLD) equation:

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

$$\boldsymbol{n}_\Gamma \cdot (-D_g \nabla E_g)|_{r\in\partial\Gamma} = \frac{1}{2}E_g|_{r\in\partial\Gamma} + 2F_g^{\text{in}}, \quad E_g|_{t=0} = E_g^0$$

- Material energy balance (MEB) equation:

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G} \Big(c\varkappa_g(T)E_g - 4\pi\varkappa_g(T)B_g(T) \Big), \quad T|_{t=0} = T^0$$

- FLD coefficient: $D_g(E_g, T) = \left[(3\varkappa_g(T))^2 + \left(\frac{1}{E_g}\nabla E_g \right)^2 \right]^{1/2}$
- Temperature: $T(\boldsymbol{r}, t)$
- Radiation energy density: $E_g(\boldsymbol{r}, t)$

Potential for ROMs Using Data from Diffusion Models

- Diffusion models remain useful for their relatively low computational cost, but suffer from fundamental limitations in solution accuracy
- Improvement for diffusion models can be found in the development of modifications to account for transport effects
- The transport-corrected diffusion (TCD) ROM is developed as a data-driven approach
  - Previous work has shown the Eddington tensor can be well approximated by a BTE solution using a diffusion-evaluated scattering source
- For TRT problems, a diffusion-evaluated temperature distribution can be used in the BTE to find an approximation of the Eddington tensor
- An improved solution (compared to diffusion) can then be found with a variable Eddington factor (VEF) model

Formulation of the TCD ROM

- The Boltzmann transport equation:

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

- MEB equation:

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

Formulation of the TCD ROM

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- Multilevel low-order moment equations:

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

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

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

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

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

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

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

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

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

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

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

Formulation of the TCD ROM

- Let $\hat{T}(\boldsymbol{r}, t)$ be known & calculated from a diffusion-type model:

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

- Multilevel low-order moment equations:

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

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

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

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

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

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

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

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

TCD ROM Algorithm for TRT Problems

Solve TRT problem with Diffusion ROM

$\Downarrow$ $\hat{T}(\boldsymbol{r}, t)$

Solve BTE with fixed opacity, emission source

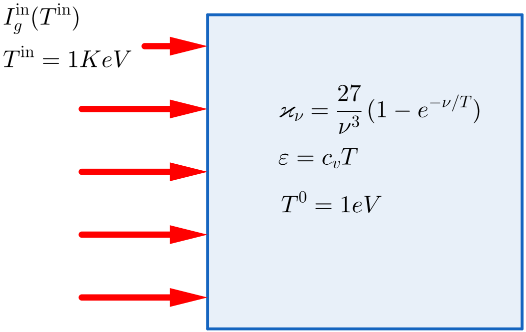
$\Downarrow$ $\hat{\mathfrak{f}}_g(\boldsymbol{r}, t)$

Solve TRT problem with VEF equations

$\Downarrow$

$T(\boldsymbol{r}, t)$

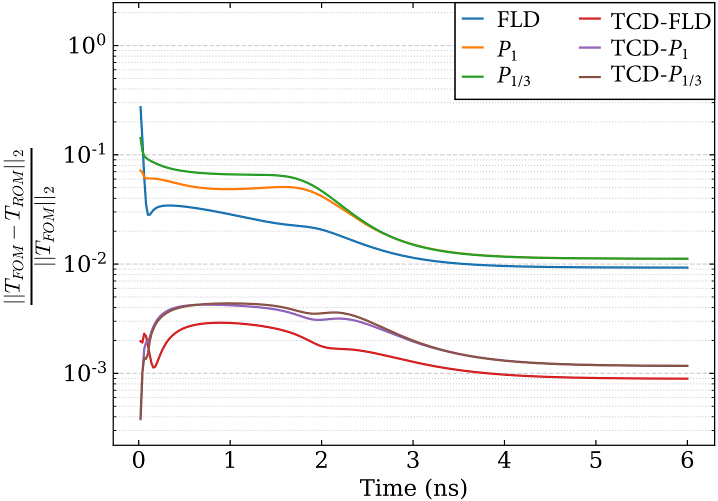
Fleck-Cummings Test Problem Description



- Specification:
  - 2D Cartesian domain 6×6 cm
  - Temporal interval $t \in [0, 6 \text{ ns}]$
- Discretization:
  - 20×20 spatial grid (0.3×0.3 cm cells)
  - 300 time steps of length 0.02 ns
  - 17 frequency groups
  - 144 discrete directions
  - All equations implicitly discretized in time (backward-Euler)
  - BTE discretized in space with method of long characteristics
  - Low-order equations discretized with 2$^{\text{nd}}$ order finite volumes scheme

Error Norms of ROM Solutions

- Relative error in T vs full-order model (FOM)
- FOM defined with the BTE & multilevel moment system
- Calculated in the 2-norm at each time step
- 3 diffusion ROMs and the TCD ROM using them



Error Norms of ROM Solutions

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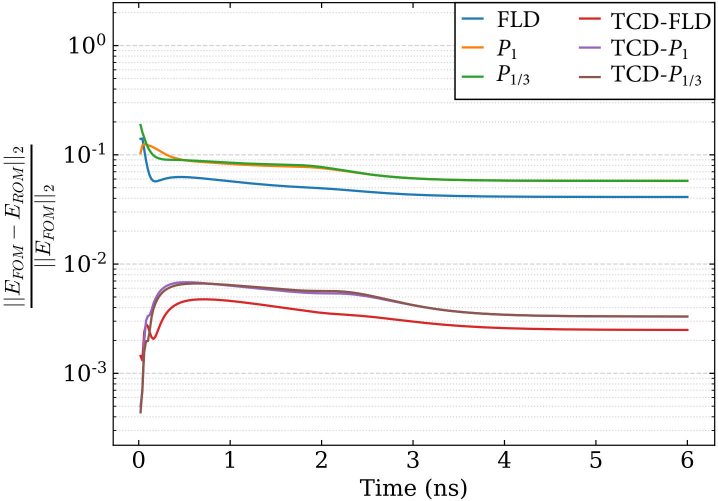

Discussion

- The TCD ROM is developed to use solution data from diffusion-based solutions of TRT problems
  - Can use already-known solutions from databases of large scale simulations
  - Could in the future be extended for parametric applications given parameterized databases
- The TCD ROM is shown to improve upon several diffusion ROMs
  - Accuracy in T, E solution improved by roughly an order of magnitude
  - Frequency spectrum for E_g also shown to improve (several orders of magnitude in high-frequency groups)

Acknowledgments

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Questions?