Data-Driven Grey Reduced-Order Model for Thermal Radiative Transfer Problems Based on Low-Order Quasidiffusion Equations and Proper Orthogonal Decomposition [1]

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1 Introduction

The thermal radiative transfer (TRT) problem is defined by the time-dependent multigroup radiative transfer (RT) equations

$$\frac{1}{c}\frac{\partial I_g(\mathbf{r},\mathbf{\Omega},t)}{\partial t}+\mathbf{\Omega}\cdot\mathbf{\nabla} I_g(\mathbf{r},\mathbf{\Omega},t)+\varkappa_g(T)I_g(\mathbf{r},\mathbf{\Omega},t)=\eta_g(T) \quad g=1,\dots,G \tag{1}$$

coupled with the material energy balance (MEB) equation

$$\frac{\partial\varepsilon(T)}{\partial t}=\sum_{g=1}^{G}\int_{4\pi}\varkappa_g(T)\Big(I_g(\mathbf{r},\mathbf{\Omega},t)-B_g(T)\Big)d\mathbf{\Omega}\,. \tag{2}$$

Here I_g is the group specific radiation intensity; $\eta_g(T)=\varkappa_g(T)B_g(T)$ is the thermal emission term; $B_g(T)$ is the group Planck black-body distribution function; $\mathbf{r}$ is the spatial position; $\mathbf{\Omega}$ is the unit vector in the direction of particle motion; t is time; g is the group index; $\varkappa_g$ is the group opacity; $T(\mathbf{r},t)$ is the material temperature; $\varepsilon(T)$ is the material energy density.

The TRT model (1) and (2) is an essential part of different multiphysics phenomena which are affected by energy redistribution due to photon interaction with matter. It represents well the main features of general radiative hydrodynamic problems, such as high dimensionality, multiple scales, and strong nonlinearity. The dimensionality of TRT problems is determined by the RT equation (1), the solution of which in 3D depends on 7 independent variables. Conversely, the physical quantities that describe the state of matter are functions of just 4 variables in 3D. The high dimensionality of RT equation motivates development of various approximate models. There exist classical reduced-order models (ROMs), for example, P_1, diffusion, and $P_{1/3}$ approximations that are widely used for simulations [1, 2]. The accuracy of these models is well known to have certain limitations.

In this paper, we study a new approach for developing RT reduced-order models. To reduce dimensionality and formulate ROMs for multiphysics problems involving the RT equation, we apply the multilevel nonlinear projective-iterative technique and a hierarchy of low-order quasidiffusion (LOQD) equations (aka Variable Eddington Factor equations) [3, 4, 5, 6]. The LOQD equations are defined for the angular and energy moments of the group specific intensity. The multilevel structure of these equations and the way they are coupled enable us to apply them as a basis for developing a spectrum of ROMs with different degrees of fidelity. It is also possible to formulate flexible ROMs that are capable of resolving accurately physics at different scales of interest. Another component of the proposed ROMs is the proper orthogonal decomposition (POD) of the high-order solution and its moments necessary to generate a database of various parameters of TRT ROMs [7, 8, 9]. Recently this approach was used to develop multigroup ROM based on multilevel LOQD equations with the POD of the group QD (Eddington) factors [10]. This paper presents a grey TRT ROM formulated by means of the grey LOQD equations and POD of group QD factors and group energy densities. We apply this ROM in the case of 1D slab geometry.

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2 Multilevel System of QD Equations for TRT Problems

The general framework for the development of ROMs is the hierarchy of equations of the multilevel QD (MLQD) method [11, 12, 13]. For TRT problems in 1D slab geometry, this multilevel system of equations is given by

- the multigroup high-order RT equations

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \mu\frac{\partial I_g}{\partial x} + \varkappa_g(T)I_g = \varkappa_g(T)B_g(T)\,, \tag{3}$$

- the multigroup LOQD equations

$$\frac{\partial E_g}{\partial t} + \frac{\partial F_g}{\partial x} + c\varkappa_g E_g = 2\varkappa_g B_g\,, \tag{4a}$$

$$\frac{1}{c}\frac{\partial F_g}{\partial t} + c\frac{\partial f_g E_g}{\partial x} + \varkappa_g F_g = 0\,, \tag{4b}$$

where the group QD (Eddington) factor is given by

$$f_g = \int_{-1}^{1}\mu^2 I_g d\mu \Big/ \int_{-1}^{1} I_g d\mu\,, \tag{5}$$

- the effective grey LOQD equations coupled with the MEB equation

$$\frac{\partial E}{\partial t} + \frac{\partial F}{\partial x} + c\bar{\varkappa}_E E = c\bar{\varkappa}_B a_R T^4\,, \tag{6a}$$

$$\frac{1}{c}\frac{\partial F}{\partial t} + c\frac{\partial \bar{f}E}{\partial x} + \bar{\varkappa}_R F + \bar{\xi}E = 0\,, \tag{6b}$$

$$\frac{\partial \varepsilon}{\partial t} = c\big(\bar{\varkappa}_E E - \bar{\varkappa}_B a_R T^4\big)\,, \tag{7}$$

where

$$\bar{\varkappa}_E = \frac{\sum_{g=1}^{G}\varkappa_g E_g}{\sum_{g=1}^{G}E_g}\,, \quad \bar{\varkappa}_B = \frac{\sum_{g=1}^{G}\varkappa_g B_g}{\sum_{g=1}^{G}B_g}\,, \tag{8}$$

$$\bar{\varkappa}_R = \frac{\sum_{g=1}^{G}\varkappa_g |F_g|}{\sum_{g=1}^{G}|F_g|} \tag{9}$$

are different grey opacities,

$$\bar{f} = \frac{\sum_{g=1}^{G} f_g E_g}{\sum_{g=1}^{G}E_g}\,, \quad \bar{\xi} = \frac{\sum_{g=1}^{G}(\varkappa_g - \bar{\varkappa}_R)F_g}{\sum_{g=1}^{G}E_g} \tag{10}$$

are the grey QD factor and the compensation term, respectively.

The system of the effective grey LOQD equations (6) is defined for the total energy density and flux. The solution of these moment equations has the same dimensionality as the solution of multiphysics equations that are represented by the MEB equation in the basic TRT problem under consideration. The grey opacities and QD factor in Eqs. (6) and (7) are averaged with the solution of the multigroup LOQD equations. The grey LOQD equations (6) can reproduce radiative transfer effects to an arbitrary degree of accuracy and enable one to model multiphysics phenomena driven by interaction of thermal radiation and matter. We apply them to develop a new class of ROMs for TRT problems.

3 Grey ROM for TRT Problems

The POD is a method of data analysis for obtaining approximate and low-dimensional representations of high-dimensional phenomena. It was developed for creating models of physical phenomena based on a set of experimental data or collection of numerical solutions [7, 8, 9]. This technique involves solving the given problem, generating a database of results for a desired variable. For evolutionary problems, this database is formed as a matrix $\mathbf{A}$ the columns of which are snapshots of the solution at available instants on time. The POD uses a singular value decomposition (SVD) of the database matrix $\mathbf{A}$ that yields its compressed representation. To further significantly reduce dimensionality of the problem a low-rank approximation of $\mathbf{A}$ based on its SVD is applied. This leads to the low-order approximation of $\mathbf{A}$ that is optimal in the 2-norm.

We perform the POD of the discrete set of group energy densities E_g and group QD factors f_g computed on given grids in space and time. The POD is applied to each group data separately to obtain approximations over space and time. We form G group-wise matrices $\mathbf{A}_g^f \in \mathbb{R}^{m_g^f,n}$ and $\mathbf{A}_g^E \in \mathbb{R}^{m_g^E,n}$, where each matrix holds the set of f_g and E_g, respectively. The columns of $\mathbf{A}_g^f$ and $\mathbf{A}_g^E$ are snapshots of the solution at n instants of time, ordered chronologically. m_g^f and m_g^E are dimensions of discrete f_g and E_g in space. The SVD is applied to these matrices to cast them in the form

$$\mathbf{A}_g^\alpha = \mathbf{U}_g^\alpha \mathbf{\Sigma}_g^\alpha \big(\mathbf{V}_g^\alpha\big)^T , \quad \alpha = f, E , \tag{11}$$

where $\mathbf{U}_g^\alpha \in \mathbb{R}^{m_g^\alpha,k_g^\alpha}$, $\mathbf{V}_g^\alpha \in \mathbb{R}^{m_g^\alpha,k_g^\alpha}$ (for $m_g^\alpha < n$) are left and right matrices of singular vectors, $\mathbf{\Sigma}_g^\alpha \in \mathbb{R}^{k_g^\alpha,k_g^\alpha}$ is the matrix of singular values, and $k_g^\alpha = \min(m_g^\alpha, n)$. The low-rank approximation of $\mathbf{A}_g^\alpha$ is given by

$$\tilde{\mathbf{A}}_g^\alpha = \tilde{\mathbf{U}}_g^\alpha \tilde{\mathbf{\Sigma}}_g^\alpha \big(\tilde{\mathbf{V}}_g^\alpha\big)^T , \quad \alpha = f, E , \tag{12}$$

where $\tilde{\mathbf{U}}_g^\alpha \in \mathbb{R}^{m_g^\alpha,\ell_g^\alpha}$, $\tilde{\mathbf{V}}_g^\alpha \in \mathbb{R}^{m_g^\alpha,\ell_g^\alpha}$, $\tilde{\mathbf{\Sigma}}_g^\alpha \in \mathbb{R}^{\ell_g^\alpha,\ell_g^\alpha}$. In this study, the reduced rank ℓ_g^α corresponds to

$$\frac{\sigma_{i,g}^\alpha}{\sigma_{1,g}^\alpha} \geq \varepsilon_\sigma \quad \text{for all } i \leq \ell_g^\alpha , \tag{13}$$

where $\sigma_{i,g}^\alpha$ are singular values of $\mathbf{A}_g^\alpha$. There are other ways to choose the reduced rank. For example, the fraction of energy comprised in the first p POD modes

$$\gamma_p^{\alpha,g} = \frac{\sum_{i=1}^{p} \big(\sigma_{i,g}^\alpha\big)^2}{\sum_{i=1}^{k_\alpha} \big(\sigma_{i,g}^\alpha\big)^2} , \tag{14}$$

can be taken into consideration. The denominator in Eq. (14) is the energy of all POD modes [8, 14].

We now formulate a new ROM that is defined by the grey LOQD equations (6) coupled with the MEB equation (7). The coefficients of these grey equations are computed by means of approximate group energy densities $\tilde{E}_g$ and QD factors $\tilde{f}_g$ obtained by the POD of group solutions, namely, by $\tilde{\mathbf{A}}_g^f$ and $\tilde{\mathbf{A}}_g^E$. The database matrices $\mathbf{A}_g^\alpha$ ($\alpha = f, E$) are generated by solving the discretized equations of the MLQD method (3), (4), (6), and (7) on a grid in phase space and time. To compute $\tilde{F}_g$ we apply the discretized group first moment equation (4b) using approximate $\tilde{E}_g$ and $\tilde{f}_g$. Hereafter we refer to this model as the grey ROM for TRT problems. Algorithm 1 shows the iteration scheme for solving TRT problem using this grey ROM. We consider a set of ROMs with a low-rank approximation defined according to the criterion (13) and specified parameter ε_σ.

Algorithm 1: The iteration algorithm for the grey ROM for TRT problems

if $t^n < t^{end}$ **then**
- $n = n + 1$
- compute $\tilde{f}_g^n$ using $\tilde{\mathbf{A}}_g^f$ with the specified rank ℓ_g^f
- compute $\tilde{E}_g^n$ using $\tilde{\mathbf{A}}_g^E$ with the specified rank ℓ_g^E
- $k = 0$, $T^{(0)} = T^{n-1}$
- **if** $||T^{(k)}-T^{(k-1)}||>\tilde{\epsilon}_T||T^{(k)}||+\tilde{\epsilon}_T^*$, $||E^{(k)}-E^{(k-1)}||>\tilde{\epsilon}_E||E^{(k)}||+\tilde{\epsilon}_E^*$ **then**
  - $k = k + 1$
  - update group opacities $\varkappa_g(T^{(k)})$
  - compute $\tilde{F}_g^n$ using $\tilde{f}_g^n$, $\tilde{E}_g^n$ and $\varkappa_g(T^{(k)})$
  - compute grey opacities $\bar{\varkappa}_E^{(k)}$, $\bar{\varkappa}_R^{(k)}$ and factors $\bar{f}^{(k)}$ $\bar{\xi}^{(k)}$ using $\tilde{E}_g^n$, $\tilde{F}_g^n$, $\tilde{f}_g^n$
  - solve the system of grey LOQD and MEB eqs. to compute $T^{(k)}$, $E^{(k)}$, $F^{(k)}$
- $T^n \leftarrow T^{(k+1)}$, $E^n \leftarrow E^{(k+1)}$, $F^n \leftarrow F^{(k+1)}$

4 Numerical Results

To analyze the accuracy of reduced order models, we use the problem based on the Fleck-Cummings (F-C) test [15]. Figure 1 presents its definition.

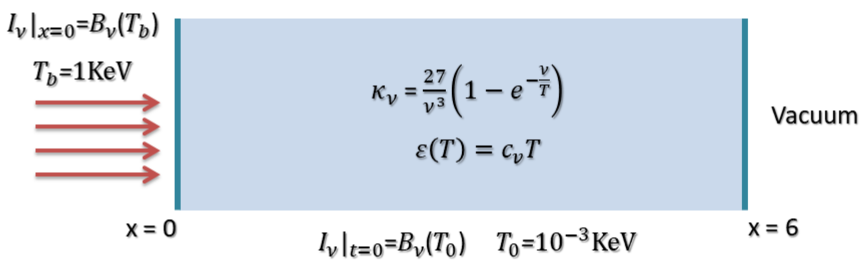

Figure 1: Definition of the test problem.

To form the databases $\mathbf{A}_g^\alpha$ ($\alpha = f, E$) we solve the test with the MLQD method [11, 13]. The multigroup high-order RT equation (3) for the given direction μ_m is approximated with the method of step characteristics. The multigroup LOQD equations (4) are discretized by means of a second-order finite volume method. The spatial discretization of the grey LOQD equations (6) is algebraically consistent with the discretized multigroup LOQD equations [13]. We use 17 frequency groups. The spatial mesh consists of uniform 60 cells with length 0.1 cm. The double S_4 Gauss-Legendre quadrature set is used. The time interval of the problem is $0 \le t \le 6$ ns. The reference numerical solution is computed with constant time step $\Delta t = 2 \times 10^{-2}$ ns and hence n=300. Convergence criteria for temperature and energy density are defined as $\epsilon_T = \epsilon_E = 10^{-12}$.

Figures 2 and 3 show the magnitude of singular values relative to the first one of $\mathbf{A}_g^f$ and $\mathbf{A}_g^E$ for all groups, respectively. Note that there are 60 spatial cells. The vector of group QD factors and energy densities are defined by their cell-average values and two values at the boundaries of the spatial domain. Thus, the original database matrices $\mathbf{A}_g^f \in \mathbb{R}^{62,300}$ and $\mathbf{A}_g^E \in \mathbb{R}^{62,300}$ $\forall g$. The rank of both $\mathbf{A}_g^f$ and $\mathbf{A}_g^E$ equals 62. Figures 4 and 5 present the relative error in the 2-norm of T and E computed with $\Delta t = 2\times 10^{-2}$

ns by means of (i) the grey ROM defined using criterion (13) with different ε_σ and (ii) the multigroup P_1 method. We notice that the grey ROM with low-rank approximation corresponding to $\varepsilon_\sigma = 10^{-3}$ is more accurate then the multigroup P_1 method. These results show that the accuracy of the grey ROM increases gradually as the rank of approximation increases over the most part of the time interval of the problem. The performance of the grey ROM is different during the initial stage the problem ($0 \le t \le 0.5$ ns) when the solution changes very fast and requires higher rank of the POD. The detailed analysis of the grey ROM solutions revealed that the observed effect in the solution at the beginning of the problem is related partially to numerical effects in POD of the solution in the unperturbed part of the spatial domain where there is only local radiation at the background temperature. This feature of the solution requires further analysis and some modifications of the computational method.

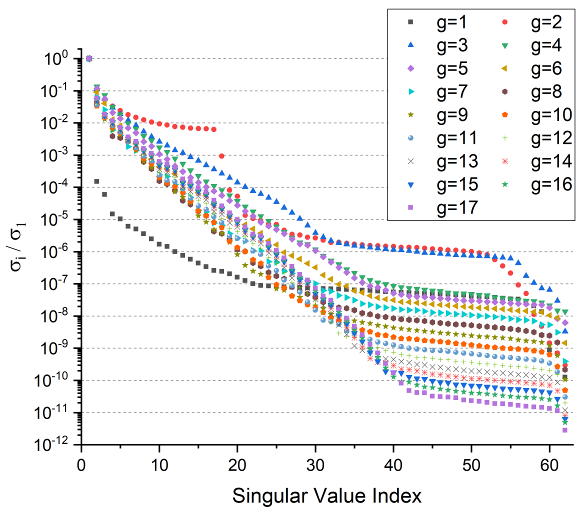

Figure 2: Normalized singular values of $\mathbf{A}_g^f$.

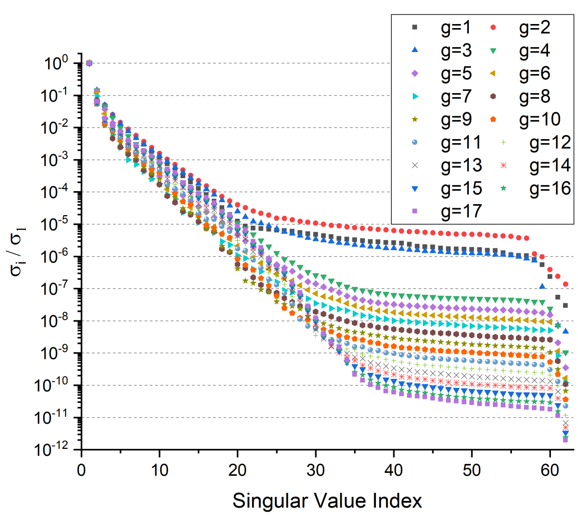

Figure 3: Normalized singular values of $\mathbf{A}_g^E$.

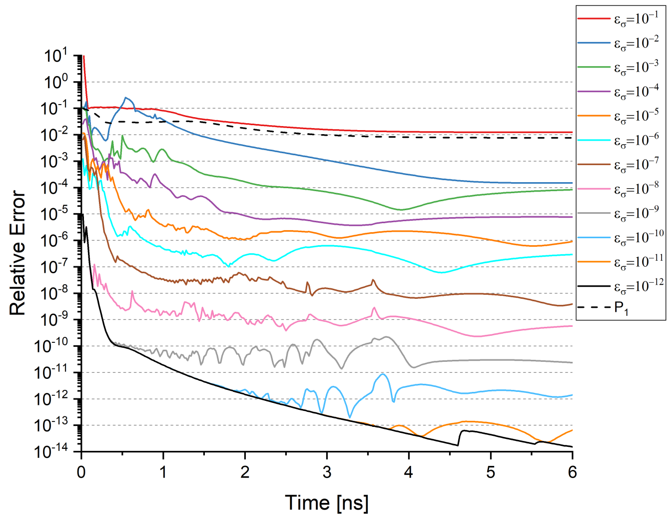

Figure 4: Relative error in temperature in the 2-norm.

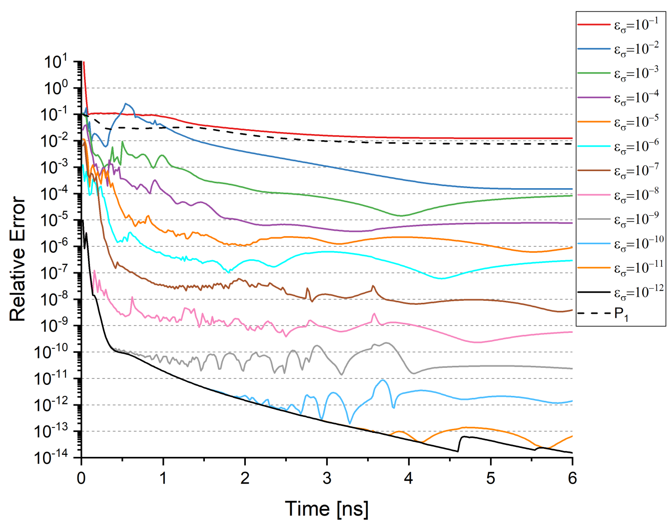

Figure 5: Relative error in total energy density in the 2-norm.

5 Conclusion

We proposed a novel grey reduced-order model for solving TRT problems. The developed grey ROM is based on the grey LOQD equations coupled with the MEB equations and applies the POD of group QD factors and group energy densities in space and time. It does not involve solution of either the high-order RT or multigroup LOQD equations. This is a data-driven model. The RT solution of a given TRT problem is used to generate the database that is approximated with the POD. This grey ROM sufficiently accurately approximates the solution of the considered TRT problem. Further work will include analysis of accuracy of the grey ROM when the time step is different from the one used to generate the database. We will study application of the grey ROM as a basis for developing parametrized ROMs for TRT problems

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