A REDUCED-ORDER MODEL FOR THERMAL RADIATIVE TRANSFER PROBLEMS BASED ON MULTILEVEL QUASIDIFFUSION METHOD

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ABSTRACT

Thermal radiative transfer (TRT) is a major piece in various multiphysics phenomena which are driven by interaction between photons and matter. The dimensionality of TRT problems is determined by the radiative transfer (RT) equation. In this paper, we study a new approach for developing physics-based RT reduced-order models. We apply an efficient method for solving coupled multiphysics equations that enables one to reduce the dimensionality of the RT problem and combine it with a decomposition-based approach of reduced order modeling. This paper describes a reduced-order model for TRT problems formulated by means of the multilevel quasidiffusion (QD) method with proper orthogonal decomposition of the QD (Eddington) factors that carry essential information about the RT high-order solution. The numerical results are presented to demonstrate performance of the proposed method.

KEYWORDS: Reduced-order modeling; Radiative transfer; Quasidiffusion method; Proper orthogonal decomposition; Multiphysics problems; Variable Eddington factor

1. INTRODUCTION

We consider the thermal radiation transfer (TRT) problem defined by the time-dependent multigroup radiative transfer (RT) equations

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

coupled with the energy balance (EB) equation

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

where $I_g(\mathbf{r},\mathbf{\Omega},t)=\int_{h\nu_g}^{h\nu_{g+1}} I_\nu(\mathbf{r},\mathbf{\Omega},\nu,t)$ is the group radiation intensity. We use standard notations.

The dimensionality of the TRT problem is driven by the RT equation. In general, the radiation intensity is a 7-dimensional function of the photon spatial position ($\mathbf{r}$), the direction of its flight ($\mathbf{\Omega}$), photon energy group (g) or frequency (ν), and time. In this paper we present analysis of elements of the approach for reduced-order modeling for TRT problems that can be used as the basis for simulation of complex multiphysics radiative transfer problems.

To reduce dimensionality, the proposed approach is based on the multilevel nonlinear projective-iterative (MNPI) methodology [1,2]. The transport problem is recast in a form of a multilevel system of effective low-order transport equations for angular and energy moments of the transport solution. The multilevel system of high-order and low-order equations is closed by means of exact relationships involving factors (functionals) that are weakly dependent on the transport solution. The low-order problem at each level reproduces exactly photon transport physics. This is achieved by averaging with respect to the angular and energy variables without any approximations. The MNPI methodology is combined with the discrete version of the proper orthogonal decomposition (POD) that is capable in generating a low-dimensional description of high-dimensional data and capturing essential pieces of physics [3–5]. This paper describes a reduced-order model (ROM) for TRT problems based on the multilevel quasidiffusion (QD) method [1,6].

2. MULTILVELEL QD METHOD FOR TRT PROBLEMS

The following equations formulate the multilevel QD (MLQD) method for TRT problems in 1D slab geometry for $0 \le x \le H$ and $0 \le t \le t_{end}$ [7–9]:

- The high-order RT equation for the group intensity $(I_g(x,\mu,t))$

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

- The multigroup low-order QD (LOQD) equations for the group radiation energy density $(E_g(x,t))$ and flux $(F_g(x,t))$

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

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

where

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

is the group QD (Eddington) factor.

- The grey LOQD equations for the total radiation energy density $(E(x,t))$ and flux $(F(x,t))$ coupled with the EB equation

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

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

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

where

$$\bar{f} = \frac{\sum_{g=1}^{N_g} f_g E_g}{\sum_{g=1}^{N_g} E_g}, \tag{8}$$

is the grey QD factor,

$$\bar{\varkappa}_E = \frac{\sum_{g=1}^{N_g} \varkappa_g E_g}{\sum_{g=1}^{N_g} E_g}, \quad \bar{\varkappa}_B = \frac{\sum_{g=1}^{N_g} \varkappa_g B_g}{\sum_{g=1}^{N_g} B_g}, \quad \bar{\varkappa}_R = \frac{\sum_{g=1}^{N_g} \varkappa_g |F_g|}{\sum_{g=1}^{G} |F_g|} \tag{9}$$

are different grey opacities averaged with the group low-order solution, and

$$\bar{\eta} = \sum_{g=1}^{N_g} (\varkappa_g - \bar{\varkappa}_R) F_g \Big/ \sum_{g=1}^{N_g} E_g \tag{10}$$

is a compensation term.

The group QD factors are coefficients of the multigroup LOQD equations. They carry all information about the transport solution that the hierarchy of the low-order equations (4) and (6) needs to accurately model photon transport physics. The high-order problem (3) can be viewed as a special one that generates a shape function used to average μ^2 and to compute the group QD factors. The role of the hierarchy of low-order equations is to generate the moments of the transport solution and communicate with the energy balance equation as an element of a multiphysics model. The system of LOQD and EB equations (4)-(7) is the basis for reduced-order modeling in which the group QD factors are components of a compressed data set representing high-order transport solution. To further reduce dimensionality and develop advanced ROMs for TRT problems, we apply POD to the group QD factors. The purpose of this study is to evaluate the potential of developing a parametrized ROM for TRT problems based on MLQD method with POD. We analyze accuracy of the solution obtained by the hierarchy of the LOQD equations with approximate f_g examining POD modes of group QD factors of different scales.

The remainder of this paper is organized as follows. In Sec. 3, the POD approximation of the QD factors is formulated. In Sec. 4, numerical results are presented. We conclude with a brief summary in Sec. 5.

3. POD-BASED REPRESENTATION OF GROUP QD FACTORS

The POD was originally created as a method of solving problems by using previously found data to estimate new results [3–5]. This method involves solving the given problem, creating a database of results for a desired variable. This database is formed as a matrix $\mathbf{A}$ with dimension (X, τ) where X and τ are the number of spatial and temporal discrete nodes respectively. Then the singular value decomposition (SVD) is applied to the data matrix $\mathbf{A}$. The low-rank approximations of $\mathbf{A}$ based on SVD can be used to generate an optimal low-order approximation of the data set and hence reduce dimensionality of the problem. The SVD presents the matrix in the form of $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, where $\mathbf{A} \in \mathbb{R}^{m,n}$, $\mathbf{U} \in \mathbb{R}^{m,k}$ holds the left singular vectors in its columns, $\mathbf{\Sigma} \in \mathbb{R}^{k,k}$ is diagonal and consists of the singular values along its diagonal in decreasing order, $\mathbf{V}^T \in \mathbb{R}^{k,\tau}$ holds the right singular vectors in its rows, where $k = \min(m, n)$ is the rank of $\mathbf{A}$. $\mathbf{A}$ may be approximated as a matrix of rank $r < k$ by reducing the dimension $k \to r$ in its SVD. This effectively removes columns from $\mathbf{U}$, diagonal values from $\mathbf{\Sigma}$ and rows from $\mathbf{V}^T$.

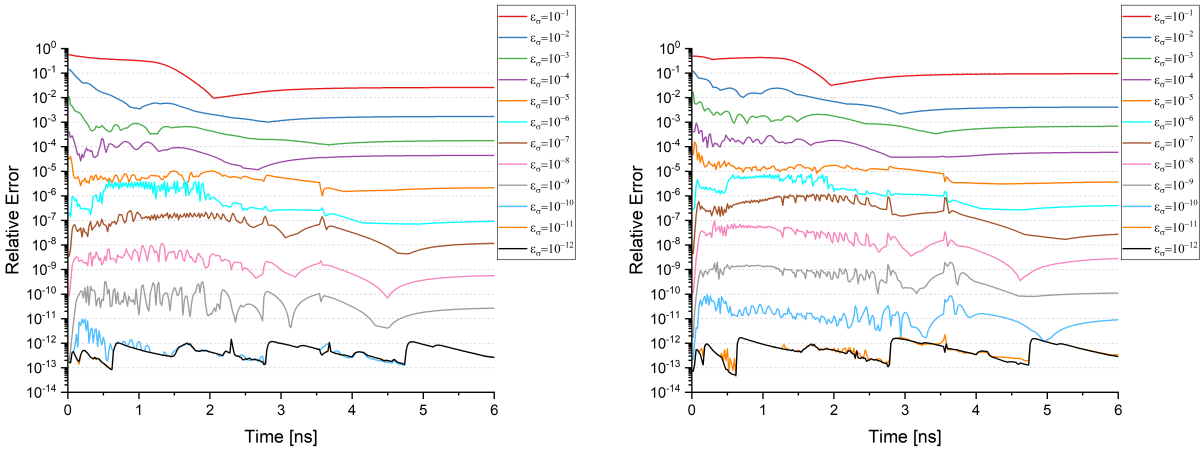
The set of group QD factors $f_g(x,t)$ on grids in energy, space and time is considered as the collection of samples of the physical system behaviour that characterize transport effects. The methodology of the POD is applied to the complete data set of QD factors for the given problem separately in each group. First we solve the TRT problem with the MLQD method to generate the solution for some particular mesh in space and time [9]. Then the QD factors form G group-wise matrices $\mathbf{A}_g^f \in \mathbb{R}^{X,\tau}$ such that each matrix holds one energy group set of QD factors. Each column in $\mathbf{A}_g^f$ contains the spatial vector of QD factors at a separate instant of time (snapshots), ordered chronologically. The SVD is applied to each $\mathbf{A}_g^f$ to cast $\mathbf{A}_g^f = \mathbf{U}_g \mathbf{\Sigma}_g \mathbf{V}_g^T$ where $\mathbf{U}_g \in \mathbb{R}^{X,k}$, $\mathbf{\Sigma}_g \in \mathbb{R}^{k,k}$, $\mathbf{V}_g^T \in \mathbb{R}^{k,\tau}$, and $k = \min(X,\tau)$. We then define a singular value relative cutoff criteria $\varepsilon_\sigma < 1$. For each set of singular values per group, $(\sigma_{1,g}, \ldots, \sigma_{k,g})$, there will be a $r_g \leq k$ such that $\sigma_{n,g}/\sigma_{1,g} \geq \varepsilon_\sigma$ for all $n \leq r_g$. The reduced rank approximations of each group QD factor matrix is computed as $\tilde{\mathbf{A}}_g^f = \tilde{\mathbf{U}}_g \tilde{\mathbf{\Sigma}}_g \tilde{\mathbf{V}}_g^T$ where $\tilde{\mathbf{U}}_g \in \mathbb{R}^{X,r_g}$, $\tilde{\mathbf{\Sigma}}_g \in \mathbb{R}^{r_g,r_g}$, $\tilde{\mathbf{V}}_g^T \in \mathbb{R}^{r_g,\tau}$. The original TRT problem is then solved by means of the hierarchy of the LOQD equations (4) and (6) coupled with the EB equation (7) using the group QD factor approximated by $\tilde{\mathbf{A}}_g^f$. We note that the high-order RT equation is not solved. Hereafter we refer to this ROM as the MLQD-POD model.

4. NUMERICAL RESULTS

In this section we present computational results for a 1-D problem based on the Fleck-Cummings test [10], used to study the accuracy of MLQD-POD models. A 1-D slab of one material is defined as 6 cm thick. The material opacity is given by $\varkappa_\nu = \frac{27}{(h\nu)^3}\left(1 - e^{-\frac{h\nu}{kT}}\right)$. The left boundary has incoming radiation with black-body spectrum at temperature $kT_{in} = 1$ keV and the right boundary is vacuum. The initial temperature of the slab is $kT_0 = 1$ eV and the initial radiation distribution is given by the black-body spectrum at this temperature. We define the material energy as a linear function of temperature $\varepsilon = c_\nu T$ where $c_\nu = 0.5917 a_R T_{in}^3$. The spatial mesh is a uniform 60 cells with length 0.1 cm. We use 17 energy groups and the double S_4 Gauss-Legendre quadrature set. Convergence criteria for temperature and energy density are defined as $\epsilon_T = \epsilon_E = 10^{-12}$.

The problem is solved over $0 \leq t \leq 6$ ns using the time step $\Delta t = 2 \times 10^{-2}$ ns. Thus, there are 300 time steps. This is number of snapshots used to build data set of QD factors. We consider approximate MLQD-POD models for this TRT problem defined using different reduced rank representations of the group QD factors computed from our reference solution. We use singular value relative cutoff criteria of $\varepsilon_\sigma = 10^{-1}, 10^{-2}, \ldots 10^{-12}$. Figure 1 presents the relative error of the solution of these MLQD-POD models obtained with $\Delta t = 2 \times 10^{-2}$ ns compared to the reference solution in the ∞-norm at every instant of time that we calculated. These results show how the accuracy of MLQD-POD models improves as ε_σ decreases. Note that both temperature and energy density obtained by means of the MLQD-POQ models eventually reach the solution found using the reference QD factors. Table I displays the number of singular values involved per energy group at different values of ε_σ. The number of singular values used in a particular energy group corresponds to the low-rank approximation of QD factors in the group. Since the test problem has 60 spatial cells the vector of cell-average QD factors in space has 62 values including 2 boundary values. When $\varepsilon_\sigma = 10^{-12}$, all singular values at all groups are used and thus the problem no longer utilizes a reduced rank approximation. We notice that group 2 uses significantly more singular values than any other energy group for large ε_σ. Figure 2 depicts the singular values relative to the largest singular value for 6 sample energy groups $(g = 1, 2, 4, 8, 12, 17)$. Here one can see that the point where the singular values level off to a lower bound is smaller for each successive energy

group excluding group 1. The structure of singular values in group 2 is such that it is required to use most of them to represent the QD factor in this group with a very low value of ε_σ. To show the effective 'worth' of the singular values corresponding to each ε_σ, we use $\gamma_n = \sum_{i=1}^{n} \sigma_i^2 / \sum_{i=1}^{k} \sigma_i^2$ where the numerator can be interpreted as the 'energy' contained in POD modes [11]. Here we set $n = r_g$ as defined in Sec. 3. Table II displays $1 - \gamma_n$ for the energy groups $g = 1, 2, 4, 8, 12, 17$ for the same ε_σ values shown in Table I. $1 - \gamma_n$ is chosen over γ_n for the sake of clarity.



(a) Temperature relative error

(b) Energy density relative error

Figure 1. Relative error in the ∞-norm of MLQD-POD solutions computed for different ε_σ value compared to the reference TRT solution.

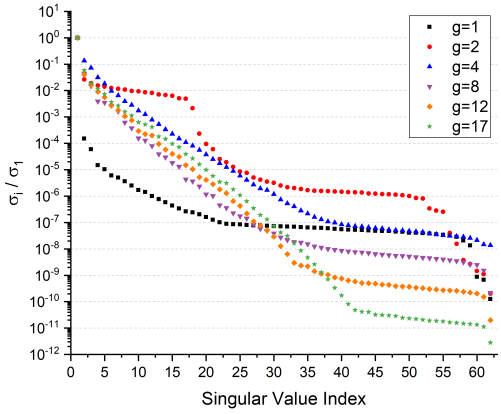


Figure 2. Normalized singular values for energy groups 1, 2, 4, 8, 12, 17.

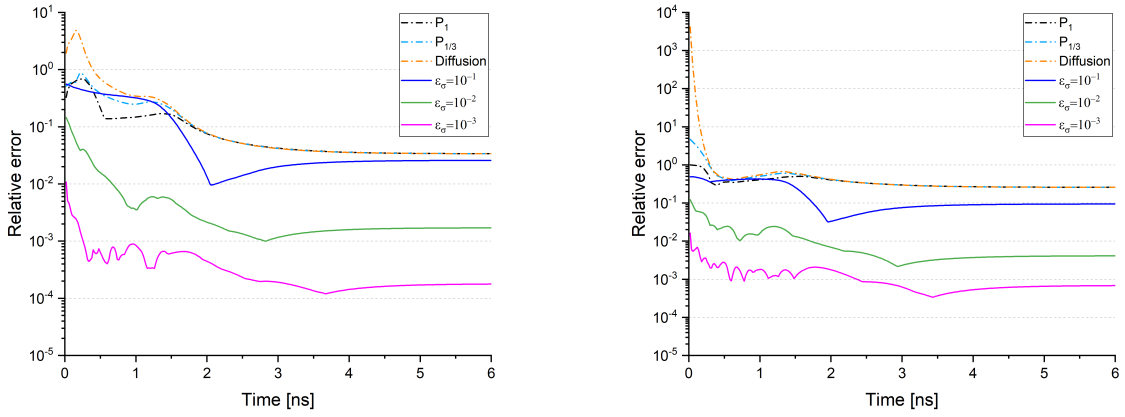
There are well-known classical ROMs for the RT equation, such as the time-dependent diffusion equation, P_1 and $P_{1/3}$ approximations [12]. We solved the above TRT test with $\Delta t = 2 \times 10^{-2}$ ns on the same spatial mesh using these three different RT approximations instead of the high-order RT equation. Figure 3 displays the relative errors in numerical solutions obtained by means of these reduced-order TRT models. The obtained results show that the MLQD-POD models with

Table I. Number of singular values used per energy group for decreasing values of ε_σ

$\varepsilon_\sigma \backslash\, g$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
10^{-1}	1	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1
10^{-2}	1	8	6	5	5	4	3	3	3	3	3	3	3	4	4	4	4
10^{-3}	1	18	14	11	10	7	7	7	7	7	7	8	8	8	8	9	9
10^{-4}	2	19	21	17	16	14	12	11	11	12	12	12	13	13	14	14	14
10^{-12}	62	62	62	62	62	62	62	62	62	62	62	62	62	62	62	62	62

Table II. $1 - \gamma_{r_g}$ for select energy groups for decreasing values of ε_σ

$\varepsilon_\sigma \backslash\, g$	1	2	4	8	12	17
10^{-1}	3.9×10^{-9}	1.7×10^{-3}	1.4×10^{-3}	2.5×10^{-4}	3.8×10^{-4}	5.5×10^{-4}
10^{-2}	3.9×10^{-9}	4.2×10^{-4}	6.9×10^{-5}	2.2×10^{-5}	4.4×10^{-5}	2.5×10^{-5}
10^{-3}	3.9×10^{-9}	1.4×10^{-8}	4.8×10^{-7}	1.9×10^{-7}	1.9×10^{-7}	5.1×10^{-7}
10^{-4}	4.1×10^{-10}	5.0×10^{-9}	5.6×10^{-9}	2.9×10^{-9}	6.3×10^{-9}	7.7×10^{-9}
10^{-12}	0	0	0	0	0	0



(a) Temperature relative error

(b) Energy density relative error

Figure 3. Relative error in the ∞-norm of solutions obtained by the diffusion, P_1 and $P_{1/3}$ approximations with $\Delta t = 2 \times 10^{-2}$ ns compared to the one calculated by means of the RT equation.

$\varepsilon_\sigma \leq 10^{-2}$ generate more accurate solutions than these classical ROMs. We also notice that the errors in the solution of the P_1 model is close to one of the MLQD-POD model with $\varepsilon_\sigma = 10^{-1}$.

We now use the POD approximation of the QD factors to solve the test problem with smaller time steps compared to the time step used to generate the QD factors. To perform such calculations we linearly interpolate between values in our database to estimate the QD factors at needed instants of time [13]. Figure 4 shows the relative error in L_1-norm of the MLQD-POD solution computed with $\Delta t = 10^{-2}$ ns using various values of ε_σ. Figure 5 presents the relative error in the solutions computed with $\Delta t = 2 \times 10^{-3}$ ns. The error in the MLQD-POD model saturated at $\varepsilon_\sigma = 10^{-4}$ and smaller values are not shown.

The MLQD-POD models can be used as a basis for developing a parametrized ROM for a class of TRT problems using QD factors estimated from a set of base cases. In this paper we consider ROM with parametrization with respect to temperature T_{in} of incoming radiation at the left boundary. We form a database of the group QD factors for problems with two selected temperatures of incoming radiation $T_{in}^{(1)}$ and $T_{in}^{(2)}$. The MLQD-POD solutions of TRT problems with incoming radiation at some given temperature are calculated using the group QD factors obtained by linear interpolation between values in the database. We present the results for two parametrized ROMs. One model uses $T_{in}^{(1)} = 1$ KeV and $T_{in}^{(2)} = 0.98$ KeV. The second one is formed with $T_{in}^{(1)} = 1$ KeV and $T_{in}^{(2)} = 0.96$ KeV. The data is generated for $\Delta t = 2 \times 10^{-2}$ ns. The spatial and angular mesh is same as above. Figure 6 shows the relative error in L_1-norm in the solution for $T_{in} = 0.99$ KeV computed by means of first parametrized MLQD-POD model with various values of ε_σ. The solution is compared to the reference TRT solution at $T_{in} = 0.99$ KeV. Figure 7 presents the relative error of the MLQD-POD solution for $T_{in} = 0.98$ KeV obtained from the second model that is parametrized with a larger interval of $[T_{in}^{(1)}, T_{in}^{(2)}]$.

5. CONCLUSIONS

In this paper we described a new reduced-order method for solving TRT problems. The numerical results demonstrated that the presented MLQD-POD model with a data set generated by means of rather low-rank representation of QD factors in space and time sufficiently accurately approximates the solution of TRT problems. As the rank of the approximation is increased, the accuracy of the model gradually improves. The low-rank version of this QD factor data set can be used as a basis for creating efficient ROMs for multiphysics simulations of evolution of temperature and radiation energy waves. The broad class of TRT problems involves various parameters, for example, material opacities, incoming radiation fluxes, initial distribution of temperature etc. The TRT solution depends differently on these parameters. The obtained results of the MLQD-POD model parametrized with respect to temperature of incoming radiation are promising. They showed that this kind of ROMs has potential in parametric model reduction for TRT problems.

6. ACKNOWLEDGEMENTS

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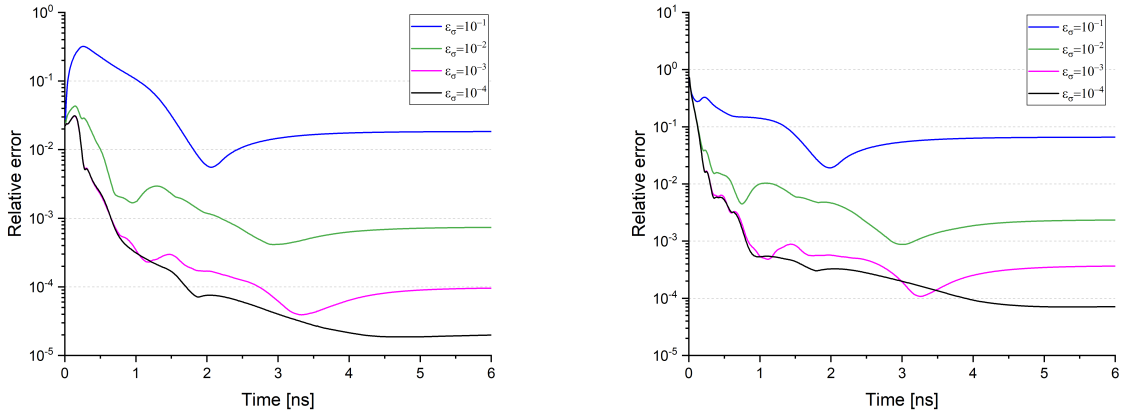
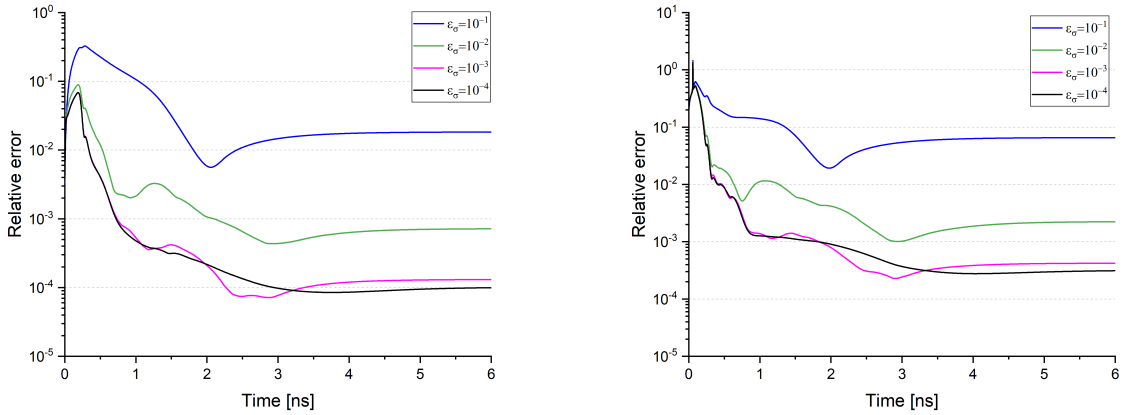


(a) Temperature relative error

(b) Energy density relative error

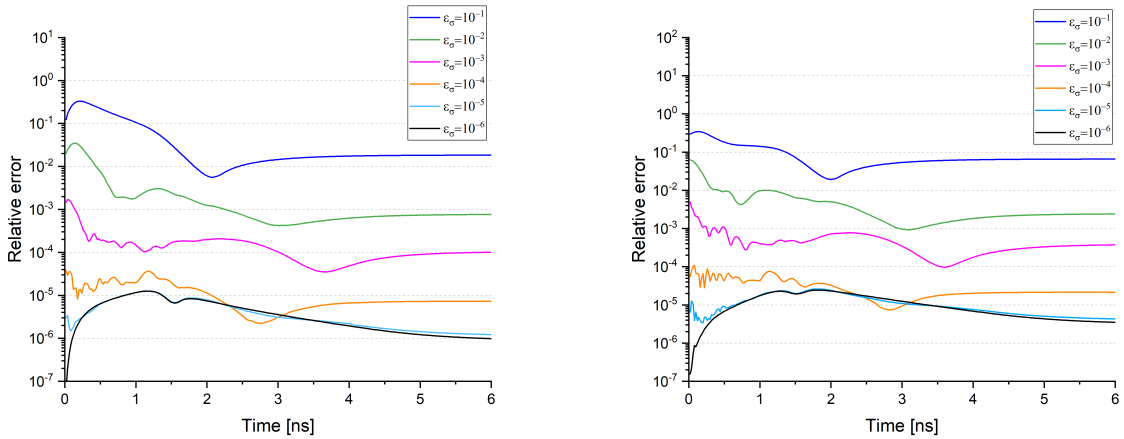
Figure 4. Relative error in the L_1-norm of MLQD-POD solutions computed with $\Delta t = 1\times10^{-2}$ ns versus the reference TRT solution. The MLQD-POD model is generated with $\Delta t = 2\times10^{-2}$ ns.



(a) Temperature relative error

(b) Energy density relative error

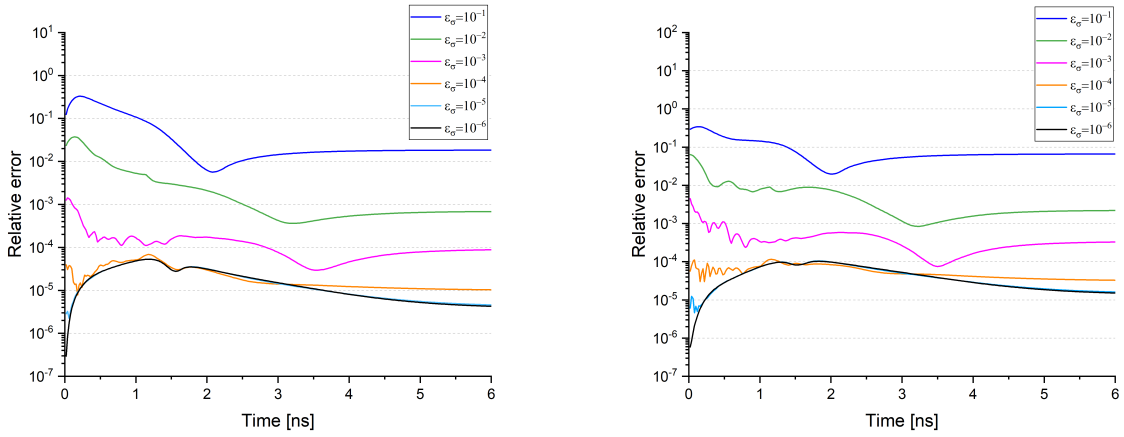
Figure 5. Relative error in the L_1-norm of MLQD-POD solutions computed with $\Delta t = 2\times10^{-3}$ ns versus the reference TRT solution. The MLQD-POD model is generated with $\Delta t = 2\times10^{-2}$ ns.



(a) Temperature relative error

(b) Energy density relative error

Figure 6. Relative error in the L_1-norm of the MLQD-POD solutions computed with $T_{in} = 0.99$ KeV using base cases with $\tilde{T}^1_{in} = 1$ KeV and $\tilde{T}^2_{in} = 0.98$ KeV.



(a) Temperature relative error

(b) Energy density relative error

Figure 7. Relative error in the L_1-norm of the MLQD-POD solutions computed with $T_{in} = 0.98$ KeV using base cases with $\tilde{T}^1_{in} = 1$ KeV and $\tilde{T}^2_{in} = 0.96$ KeV.

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