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DUAL-PHASE-LAG MODEL ORDER REDUCTION USING KRYLOV SUBSPACE METHOD FOR 2-DIMENSIONAL STRUCTURES

Summary

In this paper the temperature distribution of nanoscale structure is investigated. Presented analyses focus on two-dimensional rectangular structure. The problem has been solved using the Dual-phase-Lag heat transfer model. In order to reduce the complexity of the problem, the reduction methodology based on Krylov subspace has been used. The reduced-order model matrices generation has been based on the one-sided Arnoldi algorithm. Moreover, comparison of results received using both reduced and full thermal models for different number of discretization mesh nodes and different time instants have been demonstrated. Furthermore, the relative error of generation of reduced thermal model from full model has been considered. Finally, the most important conclusions from the presented research have been also included.

Keywords and phrases: Dual-Phase-Lag model, Fourier-Kirchhoff model, heat transfer, Krylov subspace, order reduction, electronic structures, nanotechnology, temperature distribution

1. Introduction

Nowadays, thermal problems occurring in innovative appliances are one of the most important areas in development of new technology. One of the reasons of this fact is signicifant miniaturization of integrated circuit implemented in almost all latest devices. Another reason is connected with meaningful increase of the operation frequency of mentioned devices. Both these reasons result in rapid growth of the heat density, which is generated inside analyzed structures. Increased internal heat generation causes the dramatic rise of the temperature during the device operation. It is

worth saying that in the case of very small electronic structures the arrangement of productive cooling conditions is often imposible. Thus, the operation of the electronic structure becomes unstabile. Moreover, long-lasting operation in such conditions can cause many device malfunctions and even permanent damages. Described situations cause that the thermal analysis is currently the fundamental development step in modern electronics designing process.

Up to the beginning of twenty first century, the heat transfer problems had been solving using the approach proposed by Fourier [1]. The mentioned approach was based on the Fourier's law and then Fourier-Kirchhoff differential equation presented in formulas (1) and (2), respectively.

$$-q\left(x,y,t\right) = k\nabla T\left(x,y,t\right) \tag{1}$$

$$c_v \frac{\partial T\left(x,y,t\right)}{\partial t} = -\nabla \cdot q\left(x,y,t\right) + q_{gen}\left(x,y,t\right) \tag{2}$$

where c_v is the volumetric heat capacity, while $q\left(x,y,t\right)$, $q_{gen}\left(x,y,t\right)$ and $T\left(x,y,t\right)$ mean the density of the heat flux, the internal heat generation and the temperature function, respectively. All these functions are defined for points (x,y) from two-dimensional space, $x \in \mathbb{R}$, $y \in \mathbb{R}$, and for time $t \geq 0$.

However, the reserach has shown that the Fourier-Kirchhoff model does not reflect the realistic thermal behaviour properly [2], [3] and [4]. For example, in this model the assumptions related to heat propagation with infinite speed and instantaneous changes of temperature gradient and heat flux are postulated, what do not agree with experiments, especially for nanometric electronic structures [5] and [6]. Due to these facts, the Fourier-Kirchhoff model should be replaced by heat transfer model which is appropriate for nano scale. One of such models is Dual-Phase-Lag approach developed by D.Y. Tzou [7].

In this paper the Dual-Phase-Lag model will be considered. Moreover, the model order reduction based on Krylov subspaces methodology will be presented. Apart from that the simulation results obtained using both full- and reduced-order models for 2-dimensional structure will be analyzed and compared. Furthermore, the conclusions will be included.

2. Heat Transfer Model Description

The Dual-Phase-Lag model, considered in this paper, contains some significant modifications of classical Fourier-Kirchhoff model. It includes two relaxation time constants, τ_q and τ_T. The first constant is called the heat flux time lag, while the second one means the temperatuer time lag. Including the existence of these time lags,

the mathematical description of the Dual-Phase-Lag model has the form presented below:

$$\begin{cases} c_v \frac{\partial T(x,y,t)}{\partial t} = -q\left(x,y,t\right) \\ \\ q\left(x,y,t\right) + \tau_q \frac{\partial q(x,y,t)}{\partial t} = -k\nabla T\left(x,y,t\right) - k\tau_T \frac{\partial \nabla T(x,y,t)}{\partial t} \end{cases} \tag{3}$$

where k reflects the value of material thermal conductivity. However, in the case when the thermal conductivity of analyzed material does not depend on the temperature and the internal heat generation is not observed, the Dual-Phase-Lag model can be expressed in the second-order form presented as follows:

$$\begin{cases} c_v \frac{\partial T(x,y,t)}{\partial t} = -q\left(x,y,t\right) \\ \\ c_v \left(\tau_q \frac{\partial^2 T(x,y,t)}{\partial t^2} + \frac{\partial T(x,y,t)}{\partial t}\right) - k\left(\tau_T \frac{\partial \triangle T(x,y,t)}{\partial t} + \triangle T\left(x,y,t\right)\right) = 0 \end{cases} \tag{4}$$

The incontestable advantage of Dual Phase-Lag model is fact that it can be applied for parabolit- and hyperbolic-type models. Thus, it is appropriate for many cases and it can replace the classical Fourier-Kirchhoff approach which represents the parabolic type.

However, the Dual-Phase-Lag described by equation (4) is characterized by bigger computational complexity than Fourier-Kirchhoff one. Due to this fact, the determination of temperature distribution using full-order thermal model can take plenty of time, especially when the investigated structure is discretized using relatively big number of nodes. Therefore, the model order reduction of the full thermal model is needed and it will be described in the next sections. Nonetheless, the investigated structure description will be demonstrated at first.

3. Description of the Investigated Structure

The simple two-dimensional rectangular slab is taken into consideration. Without loss of generality, it was assumed that both sides of analyzed rectangle are equal. Moreover, the structure is heated from external heat source. The heat flux is directed towards the one of the corners of the slab. In remaining points of the sturcture edges the adiabatic boundary conditions are imposed. The described situation is presented in Figure 1.

The temperature distribution inside the structure has been modelled using the Finite Difference Method. Due to this fact, the structure had to be primarily discretized. The discretization mesh has been generated using the following dependences:

$$q_k\left(t\right) = q\left(x,y,t\right) \quad \text{for} \quad x = i \cdot \triangle x, \quad y = j \cdot \triangle y \tag{5}$$

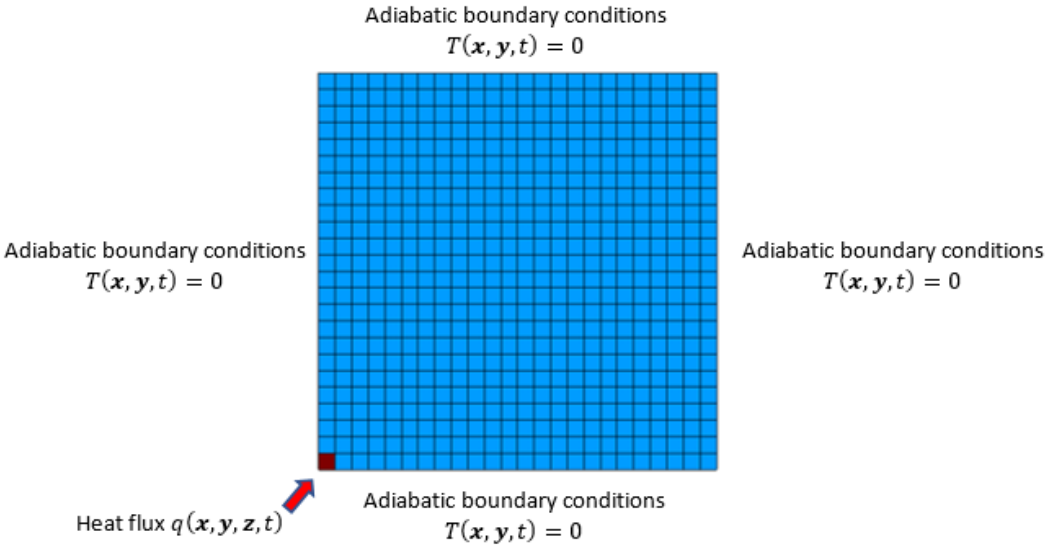

Fig. 1. *The visualization of the investigated two-dimensional rectangular slab with marked adiabatic boundary conditions and direction of the heat flux.*

$$T_k(t) = T(x, y, t) \quad \text{for} \quad x = i \cdot \triangle x, \quad y = j \cdot \triangle y \tag{6}$$

where $i \in \{1, 2, \ldots, n_x\}$, $j \in \{1, 2, \ldots, n_y\}$, $k \in \{1, 2, \ldots, n_x \cdot n_y\}$, while n_x and n_y reflect the number of discretization mesh nodes along the structure length and width, respectively. The total number of nodes describing the structure is equal to $n_x \cdot n_y$. Nodes are numbered from the heated corner (node no. 1) through nodes located along one side of the rectangular structure to the node in opposite corner (node no. n_x). Then, the numbering process is repeated from the node neighbouring with the heated corner (node no. $n_x + 1$) to the node neighbouring with the opposite corner (node no. $2 \cdot n_x$). The numbering process is finished when the last layer of nodes along the edge of the structure are numbered (nodes no. from $(n_y - 1) \cdot n_x$ to $n_x \cdot n_y$). Additionaly, it was assumed that the distances between nodes located along the structure's lenght and width are equal, i.e. $\triangle x = \triangle y$. The graphical representation of the discretization mesh nodes in the structure and the way of nodes numbering process is demonstrated in Figure 2.

The distribution temperature problem has been solved using the initial conditions described by the following equations:

$$T_k(t) = 0 \quad \text{for} \quad k \in \{1, 2, \ldots, n_x \cdot n_y\}, \quad t = 0 \tag{7}$$

Furthermore, the boundary conditions listed below have been considered:

$$q_k(t) = c \quad \text{for} \quad k = 1, \quad t \geq 0, \quad c \in \mathbb{R}_+ \tag{8}$$

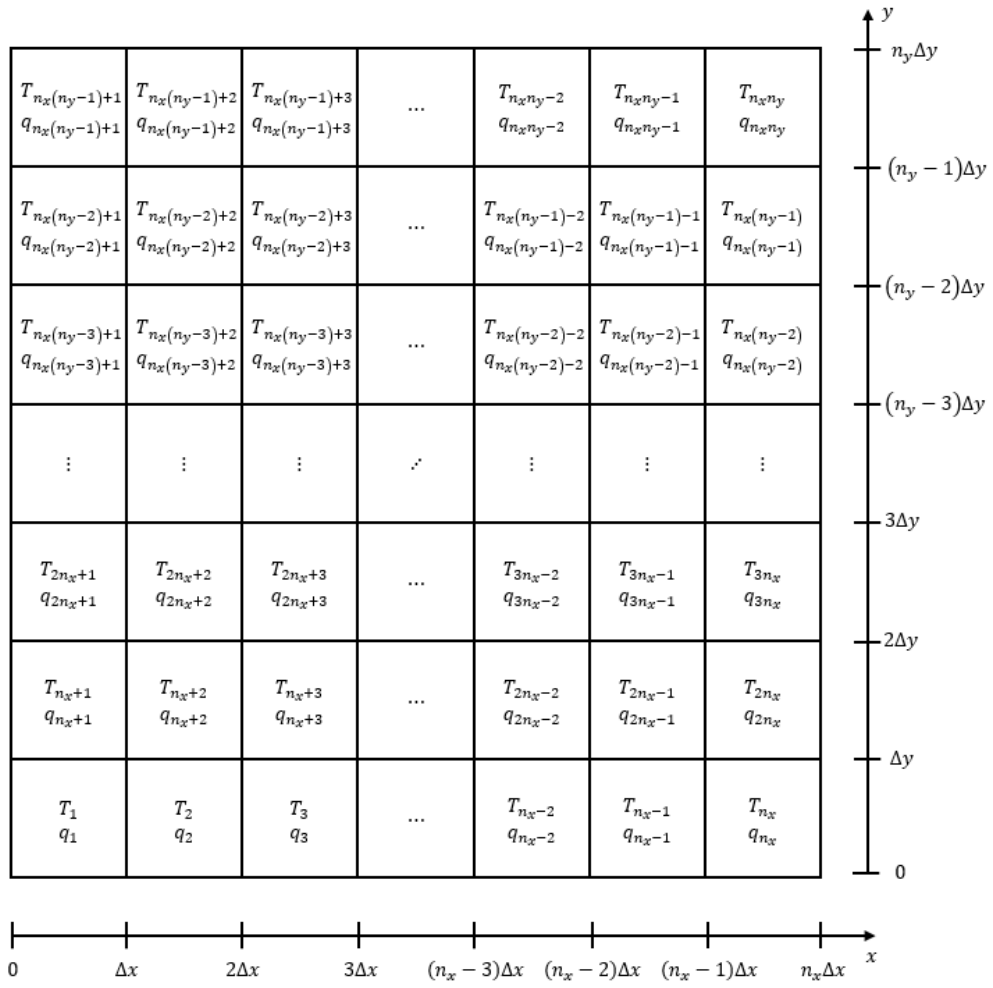

Fig. 2. *The graphical representation of the discretization mesh nodes inside the structure and the way of nodes numbering process.*

$$\begin{gathered} T_k\left(x,y,t\right)=0 \quad \text{for} \quad t\geq 0, \\ (x=0\wedge y>0)\vee(x=n_x\cdot\triangle x\wedge y\geq 0)\vee \\ \vee(y=0\wedge x>0)\vee(y=n_y\cdot\triangle y\wedge x\geq 0) \end{gathered} \tag{9}$$

4. Second-Order Dual-Phase-Lag Equation Reduction

Taking into consideration the described discretization mesh and the Dual-Phase-Lag model represented by system of equations (4), the distribution of the temperature in investigated structure can be described by the system of equations demonstrated below:

$$\begin{cases} M\ddot{T}(t) + D\dot{T}(t) + KT(t) = bu(t) \\ \\ y(t) = c^T T(t) \end{cases} \tag{10}$$

where $M, D, K, c^T \in \mathbb{R}^{n_x \cdot n_y \times n_x \cdot n_y}$, $b, y \in \mathbb{R}^{n_x \cdot n_y \times 1}$ and $u \in \mathbb{R}$. Moreover, $\ddot{T}$, $\dot{T}$ and $T \in \mathbb{R}^{n_x \cdot n_y \times 1}$ include the second-order time derivatives of the temperature variables, the first-order time derivatives of the temperature variables and the temperature variables, respectively.

However, in order to make analysis easier, this second-order system of Dual-Phase-Lag equations has been equivalently rewritten to the first-order one according to (11):

$$\begin{cases} E\dot{\overline{T}}(t) = A\overline{T}(t) + Bu(t) \\ \\ y(t) = C^T \overline{T}(t) \end{cases} \tag{11}$$

where $E, A, C^T \in \mathbb{R}^{2 \cdot n_x \cdot n_y \times 2 \cdot n_x \cdot n_y}$ and $B \in \mathbb{R}^{2 \cdot n_x \cdot n_y \times 1}$. Moreover, $\dot{\overline{T}}$ and $\overline{T} \in \mathbb{R}^{2 \cdot n_x \cdot n_y \times 1}$ include the first- and the second-order time derivatives of the temperature variables $\left(\dot{\overline{T}}\right)$ and the temperature variables and the first-order time derivatives of the temperature variables $\left(\overline{T}\right)$. Furthermore, forms of matrices E, A, C and B present as follows:

$$E = \begin{bmatrix} I & \Theta \\ \Theta & I \end{bmatrix}, \quad A = \begin{bmatrix} \Theta & I \\ -K & -D \end{bmatrix}, \quad B = \begin{bmatrix} \Theta_1 \\ b \end{bmatrix}, \quad C = \begin{bmatrix} c & \Theta \\ \Theta & c \end{bmatrix} \tag{12}$$

where $I, \Theta \in \mathbb{R}^{n_x \cdot n_y \times n_x \cdot n_y}$ and $\Theta_1 \in \mathbb{R}^{n_x \cdot n_y \times 1}$. The matrix I is the identity matrix, while matrices Θ and Θ_1 are the zero matrices.

Having the second-order system of Dual-Phase-Lag equations equivalently rewritten to the system of the first-order ones, the model order reduction can be carried out in easier way. The description of this process is presented in the next section.

5. Model Order Reduction Methodology

In the case of structures desribed using relatively big number of nodes, the determination of the temperature distribution inside the investigated structure can be time- and power-consuming. Due to this fact, the order of the full thermal model should be reduced. One of the model order reduction methodology is the moment matching technique. The so-called moments m_l can be described as follows [8]:

$$m_l = C^T \left(A^{-1}E\right)^l A^{-1}B \quad \text{for} \quad l \in \mathbb{N} \cup \{0\} \tag{13}$$

Having definition of moments, the transfer function of the model (11) has to be determined according to the following formula:

$$F_{transfer}\left(s\right) = -\sum_{l=0}^{\infty} m_l s^l \tag{14}$$

It is worth saying that transfer functions of full and reduced models are characterized by the same moments up to some degree. However, due to numerical problems, the function $F_{transfer}$ should not be computed directly. The solution of this problem is the use of equivalent techniques which deal with numerical instability of function (14). It turns out that the very useful tool is the Krylov subspace [8] and [9]. Then, using the Arnoldi algorithm [10], the reduced model is generated. It can be described by the following system of equations:

$$\begin{cases} W^T E V \dot{\overline{T}}_r\left(t\right) = W^T A V \overline{T}_r\left(t\right) + W^T B u\left(t\right) \\ \\ y_r\left(t\right) = C^T V \overline{T}_r\left(t\right) \end{cases} \tag{15}$$

where $W, V \in \mathbb{R}^{2 \cdot n_x \cdot n_y \times r}$ are transfer matrices which allow generating the reduced-order models from the full ones. Moreover, $\dot{\overline{T}}_r$ and $\overline{T}_r \in \mathbb{R}^{r \times 1}$. The constant r reflects the order of the reduced thermal model. Furthermore, the output y_r is characterized by the same order like output y. It means that y_r is the reconstruction of the full thermal model from the reduced one.

6. Simulation Results

In this section the simulation results related to 2-dimensional temperature distribution modelling are presented. All simulations have been carried out using the MathWorks Matlab software. The simulation process has been supplied by 4-cores Intel® CORE™ i7 CPU with the maximal operating frequency equal to 3.5 GHz and 32 GB DDR4 RAM Memory under contron the Misrosoft Windows 10 OS. The specially written algorithms include the sparce matrices implementation and support the multi-threading. Moreover, the variable-order solver based on Gear's algorithm has been used. Furthermore, the parameter values demonstrated in Table 1 have been employed.

The research has been conducted for different number of nodes in the structure. The smallest one is equal to 25 nodes (5 per each dimension) while the biggest one equals to 10 000 (100 per each dimension). The temperatures values in each node have been calculated for different time instants up to achieving the maximal possible temperatures (steady state). However, due to the fact that the temperature changes

Table 1. *Algorithm parameter values.*

Parameter name	**Parameter symbol**	**Parameter value**
Volume-specific heat capacity	c_v	$1.78\frac{MJ}{m^3K}$
Material thermal conductivity	k	$160\frac{W}{mK}$
Heat flux time lag	τ_q	$3 \cdot 10^{-12}s$
Temperature time lag	τ_T	$60 \cdot 10^{-12}s$
Structure length	L_x	$5 \cdot 10^{-9}m$
Structure width	L_y	$5 \cdot 10^{-9}m$
Number of nodes in X axis	n_x	$\{5, 10, 15, \ldots, 100\}$
Number of nodes in Y axis	n_y	$\{5, 10, 15, \ldots, 100\}$

are relatively small, the temperature rises have been presented in their normalized forms. Values of normalized temperature rises have been calculated according to the formula presented below:

$$T_{norm_k}(t) = \frac{T_k(t)}{max\{T_k(t)\}} \quad \text{for} \quad k \in \{1, 2, \ldots, n_x \cdot n_y\}, \quad t \geq 0 \tag{16}$$

The normalized temperature rises obtained using both full and reduced thermal models have been compared. Their comparison for 10000 nodes and some chosen time instants are presented in Figures 3 - 5.

It is clearly visible that received results are very similar for all analyzed times. However, in order to determined the rate of fitting of outputs yielded using reduced model to these ones received using full thermal model, the relative error has been calculated according to formula (17):

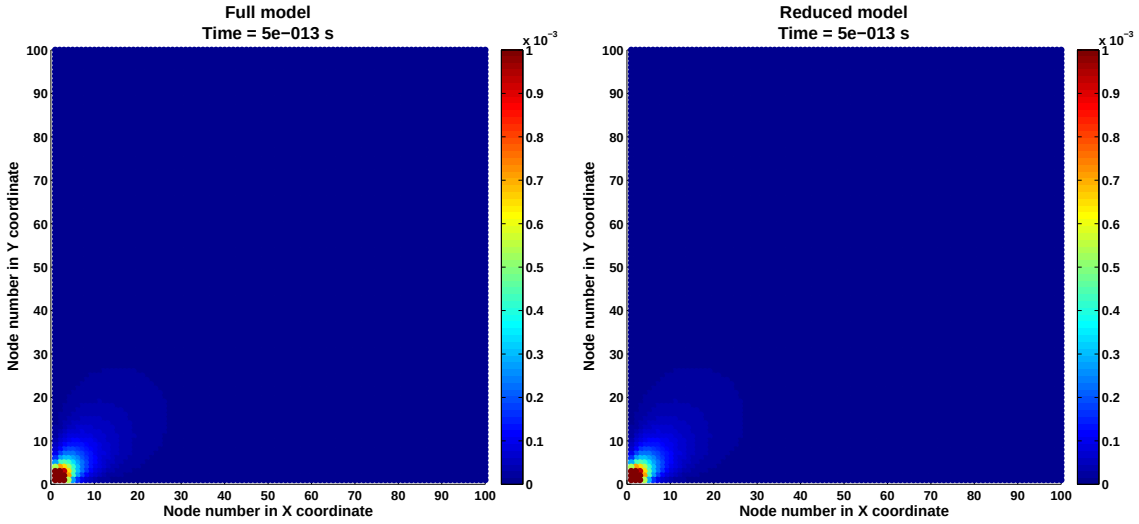

Fig. 3. *The comparison of the temperature distribution inside the investigated structure described by* 10000 *nodes obtained using full and reduced thermal models* $500 \cdot 10^{-15} s$ *after start of the simulation process.*

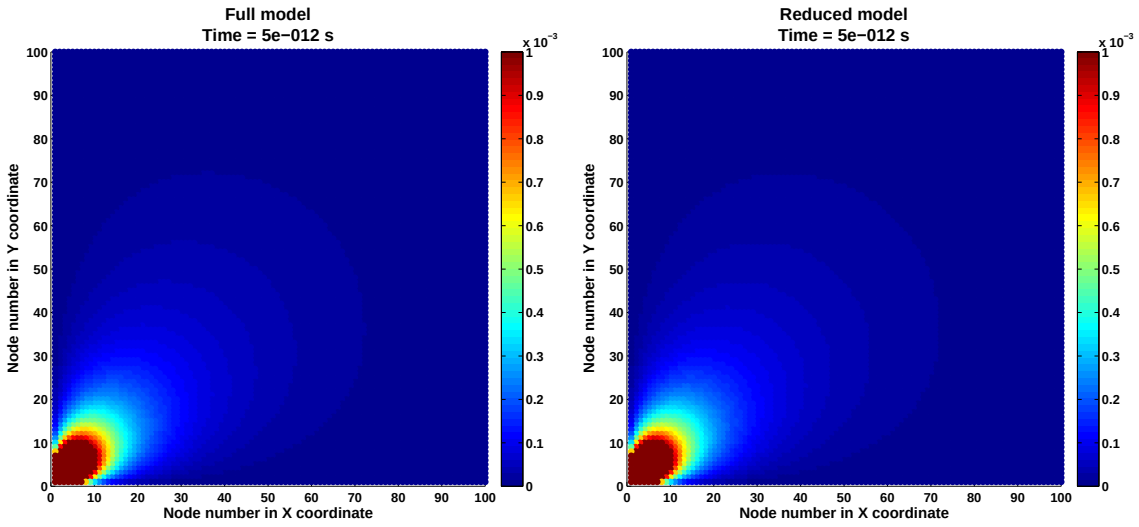

Fig. 4. *The comparison of the temperature distribution inside the investigated structure described by* 10000 *nodes obtained using full and reduced thermal models* $5 \cdot 10^{-12} s$ *after start of the simulation process.*

$$Rel_{error}(t) = \left| \frac{C^T \overline{T}(t) - c^T T(t)}{c^T T(t)} \right| \qquad t \geq 0 \tag{17}$$

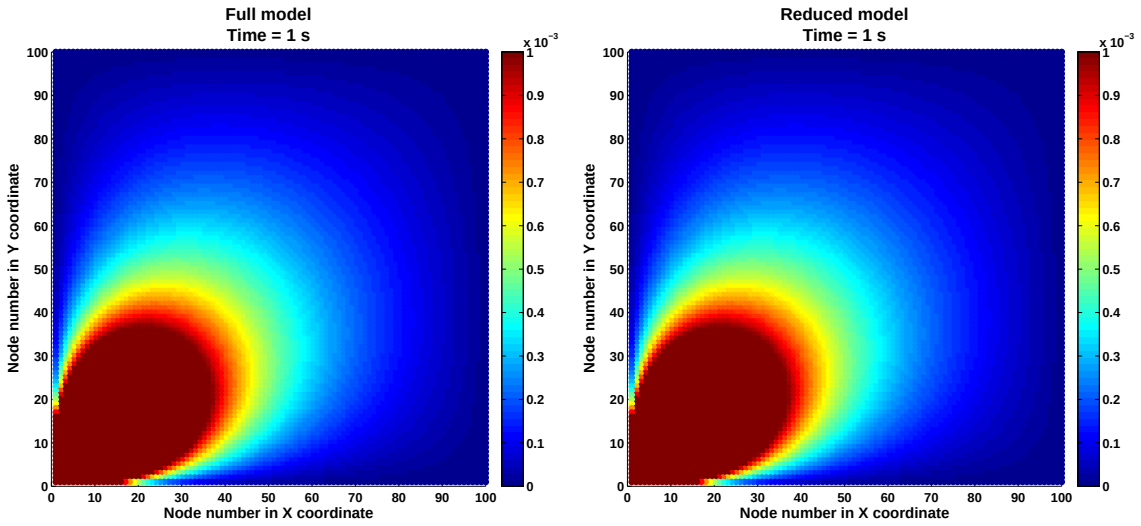

Fig. 5. *The comparison of the temperature distribution inside the investigated structure described by* 10000 *nodes obtained using full and reduced thermal models* 1*s after start of the simulation process.*

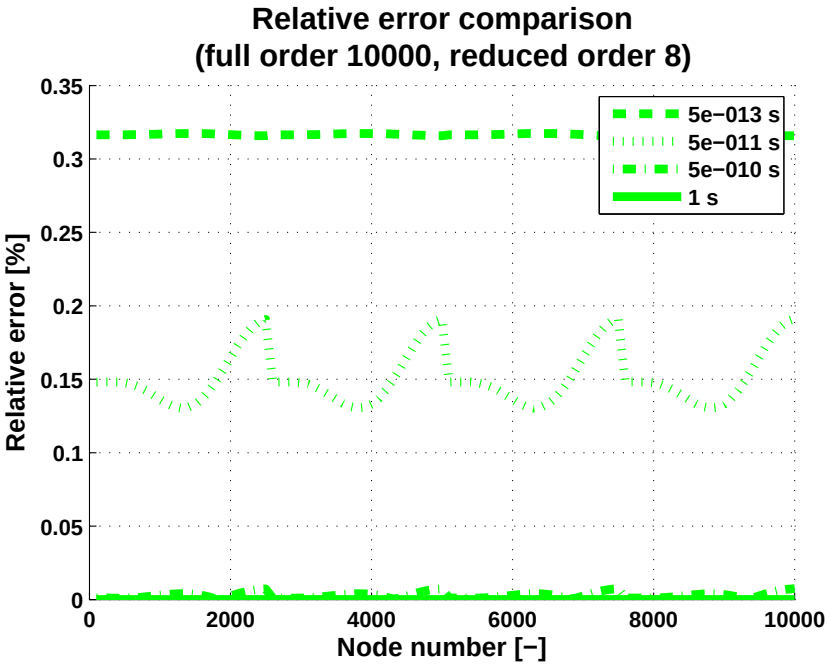

Fig. 6. *The relative error analysis of the reconstruction of the full model consisting of* 10000 *nodes from the reduced thermal model of order 8 for some chosen time instants.*

The sample analysis of the relative error of the reconstruction of the full model

consisting of 10 000 nodes (100 nodes per axis) from the reduced model of order 8 for different time instants is presented in Figure 6. As it can be seen, the maximal value of the relative error does not exceed 0.33%, what means that the results obtained using reduced model are highly reliable. Moreover, the vaue of the relative error becomes smaller over the simulation times, what indicates that proposed approach is convergent.

The times of determination of temperature distribution inside the analyzed structure using full and reduced models have been also compared. Their comparison for different number of nodes is shown in Figure 7.

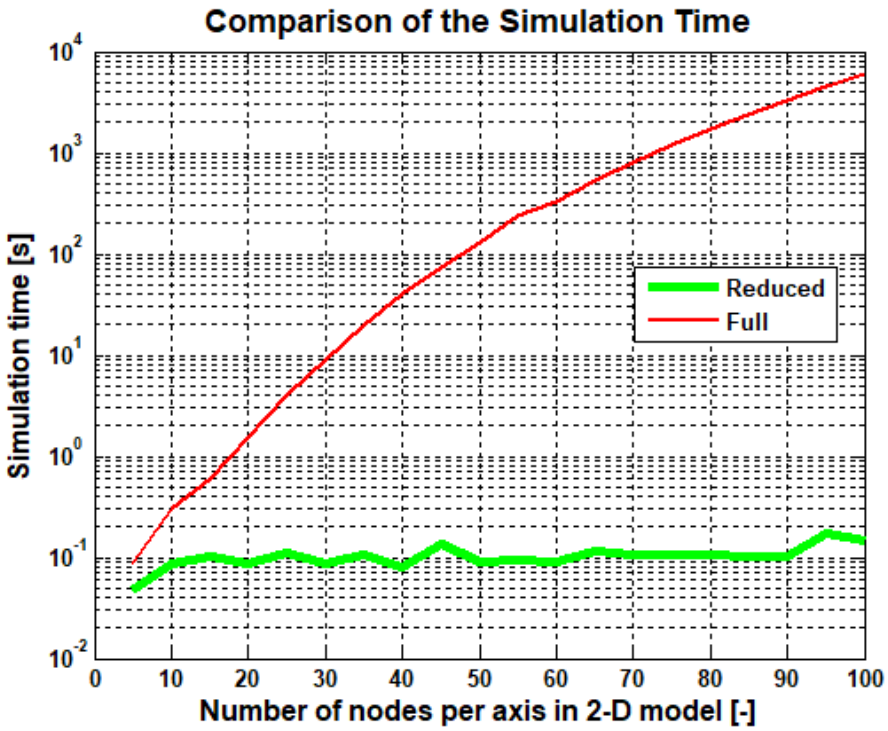

Fig. 7. *The comparison of simulation times of the temperature distribution determination yielded using both full and reduced thermal models for different number of nodes.*

It is easy to see that there exists a huge difference in simulation times depending on employed model. Full thermal model demands even 6 000 s for determination of temperature distribution in the structure described by 10000 nodes while the simulation time needed in the case of reduced model does not exceed 0.1 s. Fluctuations visible along the line reflecting the simulation times demanded by the reduced model are the result of different orders of these models. The smallest number of equations needed for generating the reduced thermal model equals to 8 and is observed in the case $100, 1600, 5625, 6400$ and 10000. On the other hand, the biggest number of equations taken to prepared the reduced order model is equal to 50 and it is recorded for

2025 nodes. Another reason of observed fluctuations is related to memory buffering problems. However, none of them influence significantly on the simulation times.

7. Conclusions

This paper presents the analyses related to order reduction process based on second-order Dual-Phase-Lag model. In order to make the research more convenient, the Dual-Phase-Lag equation has been equivalently rewritten to its first-order form.

The temperature in investigated structure has been modelled using Finite Difference Method. Due to this fact, the structure has been discretized using 2-dimensional rectangular mesh. Without loss of generality, it was assumed that the length and the width of the structure can be described using the same number of nodes. Moreover, distances between neighbouring nodes have been equal.

Presented analysis clearly indicates that application of reduced models produces almost the same temperature distribution like in the case of full models, what has been confirmed by the values of relative error of simulations. Another significant advantage of use of reduced models is fact that all simulations have been obtained in shorter time than using the full models. The reduction was based on Krylov subspace method. Results show that in the case of solving of thausands of differential equations the model order reduction allow solving the same problem but in much easier way, in shorter time and with the acceptable level of the relative error.

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REDUKCJA RZĘDU MODELU DUAL-PHASE-LAG PRZY UŻYCIU METODY PODPRZESTRZENI KRYLOVA DLA STRUKTUR DWUWYMIAROWYCH

S t r e s z c z e n i e

W pracy rozważono rozkład temperatury w strukturach nanometrycznych. Zaprezentowane analizy dotyczą struktury dwuwymiarowej o prostokątnym kształcie. Rezultaty otrzymane zostały przy uyciu modelu termicznego Dual-Phase-Lag. W celu zmniejszenia złożoności problemu, dokonano redukcji rzędu modelu opartą na metodzie podprzestrzeni Krylova. Generacja macierzy redukcyjnych bazuje na wykorzystaniu algorytmu Arnoldiego. Ponadto, porównano także rezultaty otrzymane za pomocą zredukowanego oraz pełnego modelu termicznego dla różnej liczby punktów dyskretyzacyjnych oraz różnych punktów w czasie. Dodatkowo, przedstawiono również analizę błędu względnego wyznaczenia modelu zredukowanego. Finalnie, obszernie opisano najważniejsze wnioski z przedstawionych analiz.

Słowa kluczowe: równanie Dual-Phase-Lag, model Fouriera-Kirchhoff, przepływ ciepła, podprzestrzenie Krylova, redukcja rzędu modelu, struktury elektroniczne, nanotechnologia, rozkład temperatury