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COMPARISON OF TWO-DIMENSIONAL DUAL-PHASE-LAG AND FOURIER-KIRCHHOFF MODEL ORDER REDUCTION USING KRYLOV SUBSPACE METHOD

Summary

This paper presents the comparison of the temperature distribution in two-dimensional nanometric structure received using two different heat transfer models. The first one is the classical approach based on Fourier-Kirchhoff model, while the second one uses the modern methodology related to Dual-Phase-Lag equation. In both cases the reduced order models have been also prepared. The reduction process was based on the Krylov subspace method. All results have been carefully analysed and discussed in this paper.

Keywords and phrases: Fourier-Kirchhoff model, Dual-Phase-Lag equation, nanoscale heat transfer, temperature distribution model order reduction, Krylov subspace method, Arnoldi algorithm

1. Introduction

Modelling of the temperature distribution in modern electronic structures is one of the most significant area related to the designing of innovative systems and devices. Proper estimation of the temperature observed inside the electronic appliances prevents the devices malfunctions. Due to this fact the choice of the accurate thermal model is crucial issue.

The most popular model, which is used to temperature distribution modelling, is thermal model based on Fourier-Kirchhoff approach [1],[2]. The mentioned model describes properly the temperature distribution in relatively big structures, however it may not be appropriate for determination of the temperature in very small structures [2]. The research presented in [3] has shown that in the case of the one-dimensional structure, being a simple model of some nanometric transistor, the Fourier-Kirchhoff

model may produce overestimated results, especially in the heat source. It means that investigated model should not be used for such small structures.

The better description of the temperature distribution can be obtained using Dual-Phase-Lag thermal model [4]. According to the research demonstrated in [3],[5], [6], the Dual-Phase-Lag model generates outputs which are more convenient and approximates temperature values more accurate than the Fourier-Kirchhoff model.

However, in the case of more complex nanoelectronic structures, the computation time consuming during the process of the temperature distribution determination can be relatively long [5]. Thus, the model order reduction is needed to be used in order to reduce the complexity of the problem, power consumption and time saving. There exist different order reduction methodologies. One of them, used in this paper, is based on the Krylov subspace method [7].

Obtained results are carefully compared and analysed in detail. Moreover, differences between outputs produced by both investigated thermal model have been also demonstrated. Finally, the conclusions have been included.

2. Heat Transfer Methodology

As it was mentioned previously, for one-dimensional nanometric structures, the Dual-Phase-Lag model produces more adequate results than the Fourier-Kirchhoff model. However, investigation presented in this paper is related to two-dimensional structures. Thus, results obtained using both described thermal models will be compared.

In this section expressions describing mentioned thermal models are demonstrated. All parameters, which are used in these formulas and in figures are shown in Table 1.

The basic form of the Dual-Phase-Lag model can be presented using the following formula:

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

In the case when the value of the temperature time lag is equal to 0, the expression (1) has the form shown below:

$$q\left(x,y,t\right)+\tau_q\frac{\partial q\left(x,y,t\right)}{\partial t}=-k\nabla T\left(x,y,t\right) \tag{2}$$

The foregoing expression is commonly known as Cattaneo-Vernote relation being the hyperbolic-type equation. The other case, when the temperature time lag as well as the heat flux time lag are equal to 0 leads to the following equation:

$$-q\left(x,y,t\right)=k\nabla T\left(x,y,t\right) \tag{3}$$

Table 1. *Parameters' description.*

Parameter symbol	**Parameter interpretation**
q	Heat flux density function
x	Coordinate related to X axis
y	Coordinate related to Y axis
t	Time variable
τ_q	Heat flux time lag
k	Material thermal conductivity
T	Temperature function
τ_T	Temperature time lag
c_v	Volume-specific heat capacity
q_{gen}	Internal generated heat function
L_x	Structure length
L_y	Structure width
n_x	Number of nodes in X axis
n_y	Number of nodes in Y axis

This formula reflects classic Fourier law. On the other hand, the Dual-Phase-Lag model can be represented by the second order differential equation in the following form:

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

This formula is used when the internal heat generation in not observed and the thermal conductivity parameter is independent form the temperature values. However, when both time lags are equal to 0, the equation (4) is transformed to the form demonstrated below:

$$c_v\frac{\partial T\left(x,y,t\right)}{\partial t}=-\nabla\cdot q\left(x,y,t\right)+q_{gen}\left(x,y,t\right) \quad (5)$$

The presented dependencies between Fourier-Kirchhoff and Dual-Phase-Lag model will be used to obtain the temperature distribution inside the analysed 2-dimensional structure.

3. Problem Description

The mentioned two-dimensional structure has the form of the square. It is heated from the one of the corners and perfectly cooled in each point of its perimeter. The detailed description of the investigated structure is presented in [8]. The simple visualisation of this structure is shown in Figure 1.

The temperature distribution inside analysed structure has been obtained using the Finite Difference Method. The discretization mesh has been composed of the same number of nodes in both axes. Nodes are numbered along the rows from the left to the right side of the square. The consecutive rows are filled by nodes from the bottom side to the top one.

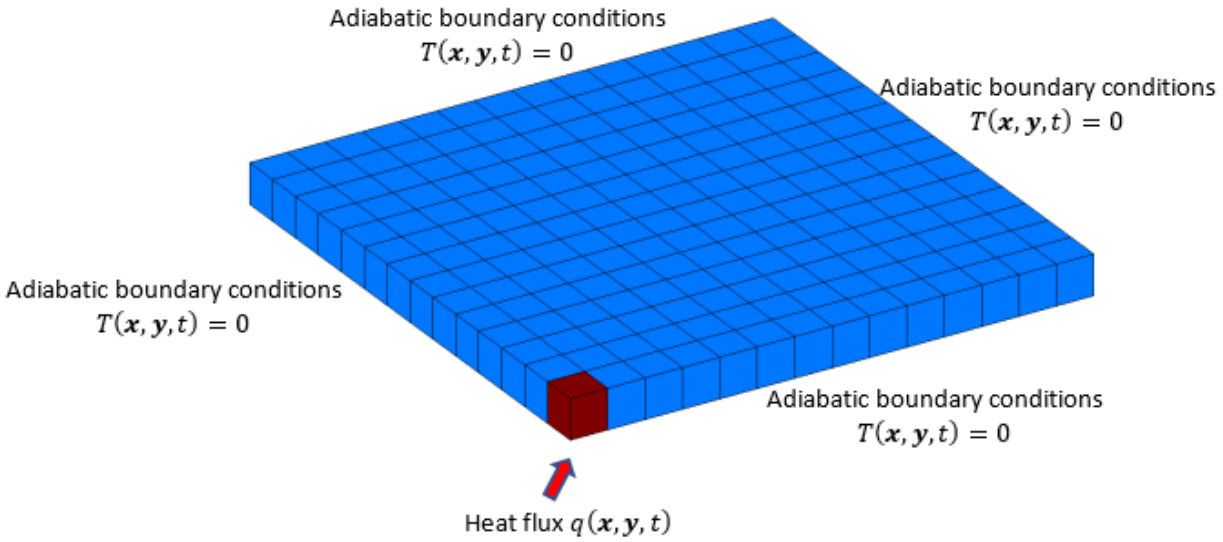

Fig. 1. *The visualization of the investigated structure with marked direction of the heat flux and the adiabatic boundary conditions.*

As it was mentioned earlier, the Krylov subspace methodology [5], [7] has been used due to reduction of the order of the thermal model. Primarily, taking into consideration that the Finite Difference Method is employed, the model (4) has been transformed into the following system of equations [8]:

$$\begin{cases} M\ddot{T}(t) + D\dot{T}(t) + KT(t) = bu(t) \\ \\ y(t) = c^T T(t) \end{cases} \tag{6}$$

Matrices and vectors used in (6) have the forms presented below:

$$M = c_v \cdot \tau_q \cdot \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \tag{7}$$

$$D = \frac{M}{\tau_q} - \frac{k \cdot \tau_T}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -4 & 1 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -4 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & -4 & 1 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 1 & -4 & 1 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 1 & -4 & \cdots & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & -4 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 1 & -4 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 1 & -4 \end{bmatrix} \tag{8}$$

$$K = -\frac{k}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -4 & 1 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -4 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & -4 & 1 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 1 & -4 & 1 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 1 & -4 & \cdots & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & -4 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 1 & -4 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 1 & -4 \end{bmatrix} \tag{9}$$

$$b = \frac{c}{\Delta x} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \tag{10}$$

$$c = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \tag{11}$$

In order to make the analysis easier, the second order model (6) has been equivalently rewritten to the first order system and then, the reduction process based on the moment matching technique has been carried out [5]. Due to numerical problems described in [8] the Krylov subspaces have been used. The final reduced order model matrices have been generated employing one-sided Arnoldi algorithm [9].

The similar analyses have been conducted for Fourier-Kirchhoff thermal model taking the system (5), for which values of the heat flux and temperature time lags are equal to 0. In this case, the system of equations (6) has the following form:

$$\begin{cases} D_{FK}\dot{T}(t) = K_{FK}T(t) + b_{FK}u(t) \\ \\ y(t) = c_{FK}^{T}T(t) \end{cases} \tag{12}$$

where matrices D_{FK}, K_{FK}, b_{FK} and c_{FK} are described as follows:

$$D_{FK} = c_v \cdot \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}, \quad K_{FK} = -K, \quad b_{FK} = b, \quad c_{FK} = c. \tag{13}$$

Finally, four sets of results have been generated during the simulation process:

- two sets related to full thermal models (Fourier-Kirchhoff and Dual-Phase-Lag models),
- two sets related to reduced thermal models (reduced Fourier-Kirchhoff and reduced Dual-Phase-Lag models).

All obtained results have been carefully analysed, compared and presented in the next section.

4. Simulation

All simulations have been supported by the computational unit including Intel Core i7 CPU and the Microsoft Windows 10 Operating System. Moreover, parameter values used during the simulation process are listed below:

- $t = 0 \div 1\,\mathrm{s}$,
- $\tau_q = 3\,\mathrm{ps}$ (Dual-Phase-Lag model), $\tau_q = 0\,\mathrm{s}$ (Fourier-Kirchhoff model),
- $k = 0.16\,\frac{\mathrm{kW}}{\mathrm{m\ K}}$,
- $\tau_T = 60\,\mathrm{ps}$ (Dual-Phase-Lag model), $\tau_T = 0\,\mathrm{s}$ (Fourier-Kirchhoff model)
- $c_v = 1780\,\frac{\mathrm{kJ}}{\mathrm{m^3 K}}$,
- $L_x = 5\,\mathrm{nm}$,
- $L_y = 5\,\mathrm{nm}$,
- $n_x = 5 \div 100$ with the step of 5,
- $n_y = 5 \div 100$ with the step of 5,

In order to make analyses more convenient, all temperature values has been transformed into their normalized forms. The normalization has been performed according to the following formula:

$$T_{norm_k}(t) = \frac{T_k(t)}{max\{T_k(t)\}} \quad \text{for} \quad k \in \{1, 2, \ldots, n_x \cdot n_y\}, \quad t \geq 0 \tag{14}$$

The comparisons of normalized steady state temperature rise inside structure obtained using both full and reduced thermal models are presented in Figures 2 - 5.

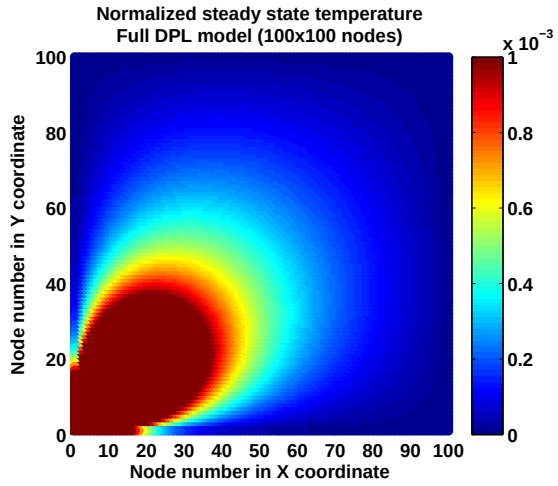

Fig. 2. *Normalized steady state temperature rise inside structure obtained using full Dual-Phase-Lag model for* 10 000 *nodes* [8].

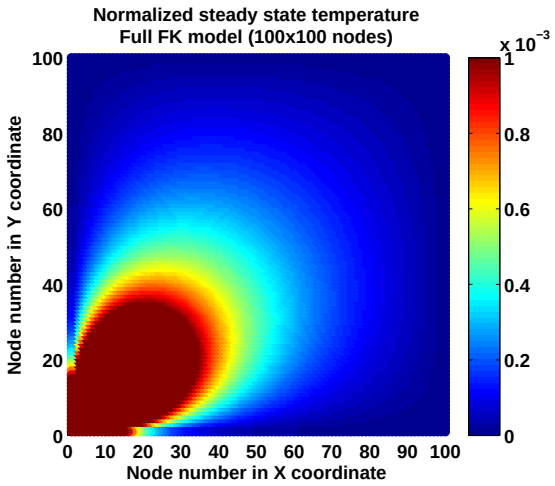

Fig. 3. *Normalized steady state temperature rise inside the structure obtained using full Fourier-Kirchhoff model for* 10 000 *nodes.*

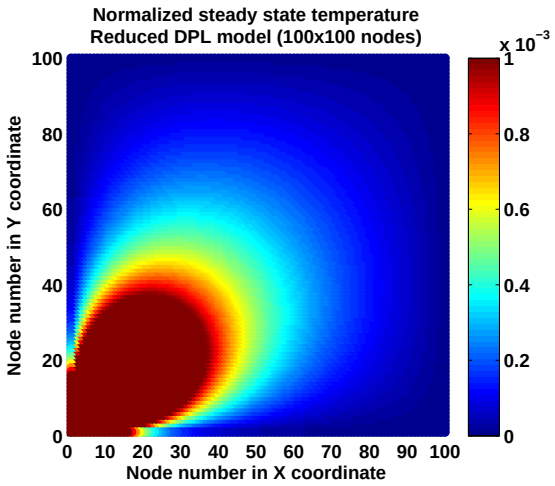

Fig. 4. *Normalized steady state temperature rise inside structure obtained using reduced Dual-Phase-Lag model for* 10 000 *nodes* [8].

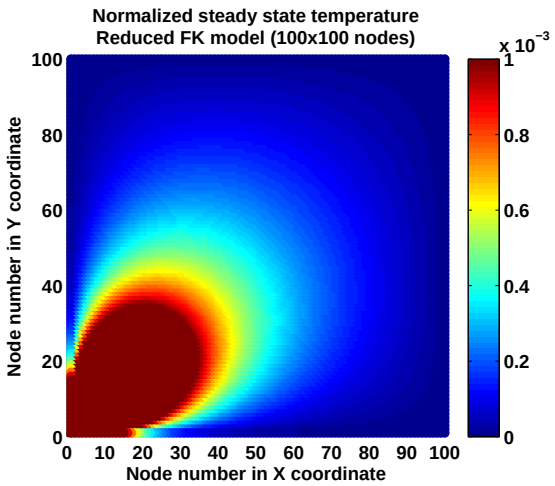

Fig. 5. *Normalized steady state temperature rise inside structure obtained using reduced Fourier-Kirchhoff model for* 10 000 *nodes.*

As it can be seen, the steady state temperature distribution is similar for both full Dual-Phase-Lag and Fourier-Kirchhoff models as well as for both reduced versions of these models. It means that Dual-Phase-Lag and Fourier-Kirchhoff models estimate the final distribution of the temperature in the same way, what is visible in Figures 2 - 3. Moreover, the reduction processes in both cases also produce the similar final steady state temperature distributions, what can be seen in Figures 4 - 5.

However, in the case of Fourier-Kirchhoff model the temperature rises significantly faster than in the case of the Dual-Phase-Lag model, what is confirmed by the transient analysis presented in Figures 6 - 11.

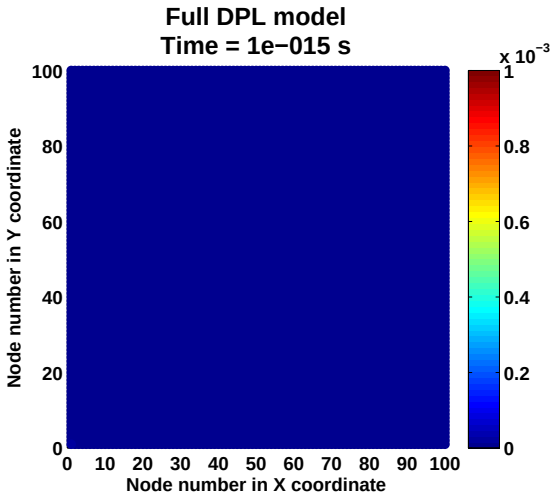

Fig. 6. *Temperature rise inside structure obtained using full Dual-Phase-Lag model for* 10 000 *nodes,* 1 fs *after simulation start.*

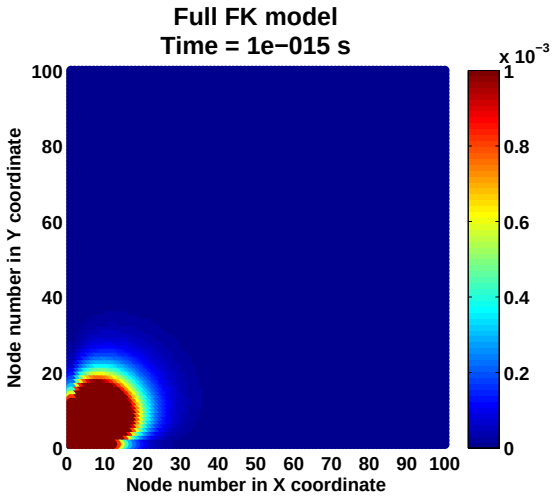

Fig. 7. *Temperature rise inside structure obtained using full Fourier-Kirchhoff model for* 10 000 *nodes,* 1 fs *after simulation start.*

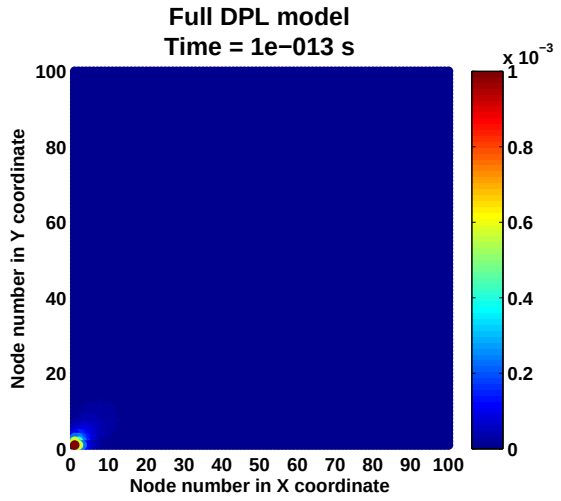

Fig. 8. *Temperature rise inside structure obtained using full Dual-Phase-Lag model for* 10 000 *nodes,* 100 fs *after simulation start.*

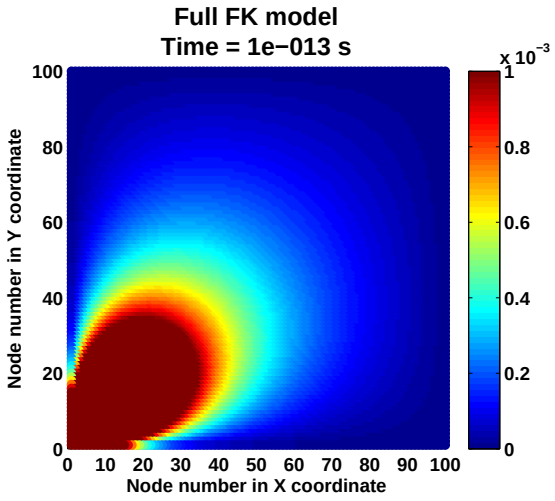

Fig. 9. *Temperature rise inside structure obtained using full Fourier-Kirchhoff model for* 10 000 *nodes,* 100 fs *after simulation start.*

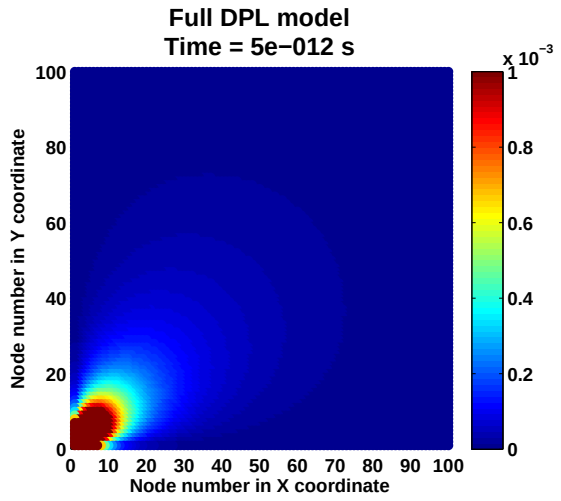

Fig. 10. *Temperature rise inside structure obtained using full Dual-Phase-Lag model for* 10 000 *nodes,* 5 ps *after simulation start* [8].

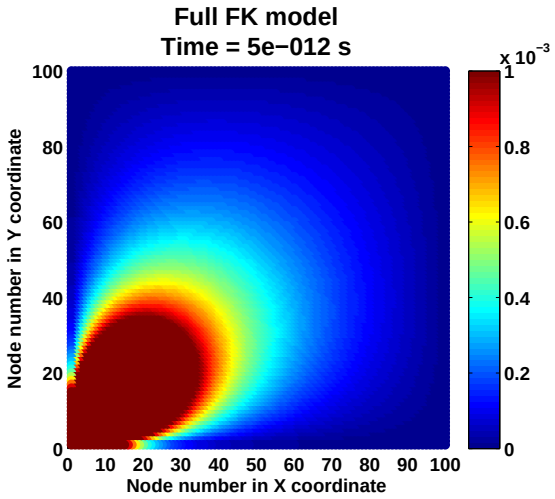

Fig. 11. *Temperature rise inside structure obtained using full Fourier-Kirchhoff model for* 10 000 *nodes,* 5 ps *after simulation start.*

As it can be seen, the steady state temperature distribution, yielded using full Fourier-Kirchhoff model, is achieved meaningfully quicker than in the case of full Dual-Phase-Lag model. The similar results are obtained for reduced-order thermal models, what is shown in Figures 12 - 17.

The analysis of Figures 6 - 17 confirmes that the Fourier-Kirchhoff model overesti-

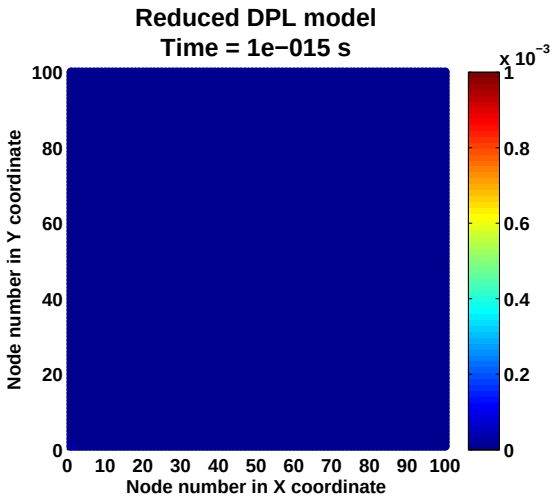

Fig. 12. *Temperature rise inside the analyzed structure obtained using reduced Dual-Phase-Lag model for* 10 000 *nodes,* 1 fs *after simulation start.*

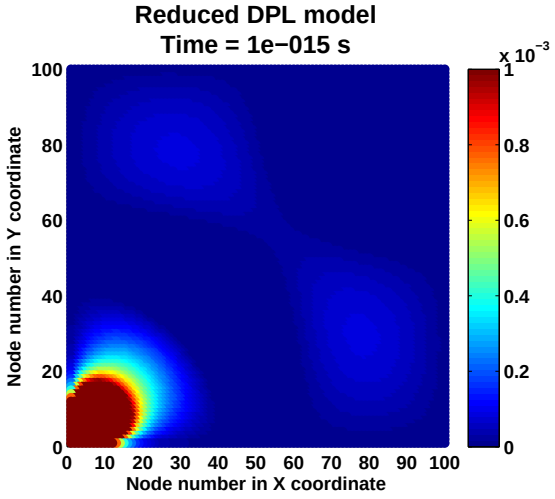

Fig. 13. *Temperature rise inside the analyzed structure obtained using reduced Fourier-Kirchhoff model for* 10 000 *nodes,* 1 fs *after simulation start.*

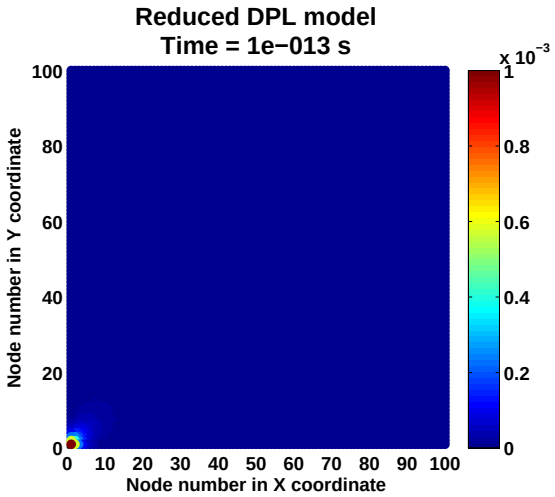

Fig. 14. *Temperature rise inside the analyzed structure obtained using reduced Dual-Phase-Lag model for* 10 000 *nodes,* 100 fs *after simulation start.*

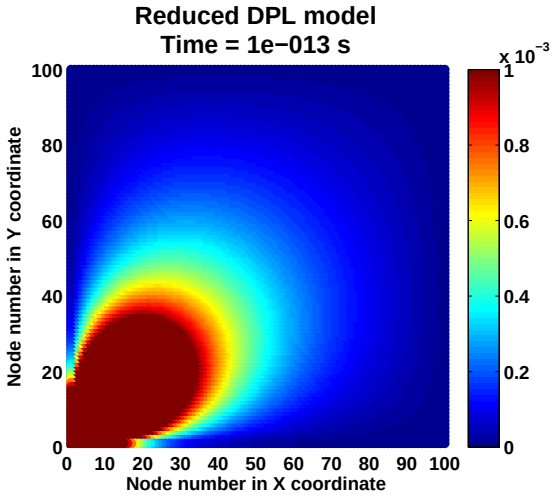

Fig. 15. *Temperature rise inside the analyzed structure obtained using reduced Fourier-Kirchhoff model for* 10 000 *nodes,* 100 fs *after simulation start.*

mated temperatures, especially in areas close to the heat source.

However, the order reduction of the Fourier-Kirchhoff model can give a slightly different outputs than analogous reduction of Dual-Phase-Lag model. It is particularly visible at the beginning of the simulation process. For example, the main difference is observed for time instant equal 1 fs after the simulation start, what is shown in Figures 7 (full Fourier-Kirchhoff model) and 13 (reduced Fourier-Kirchhoff

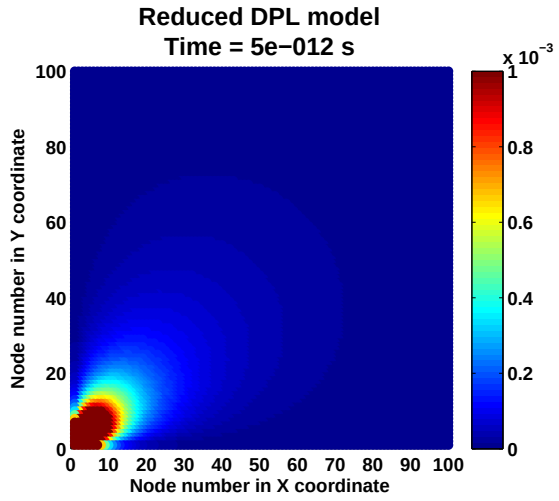

Fig. 16. *Temperature rise inside the analyzed structure obtained using reduced Dual-Phase-Lag model for* 10 000 *nodes,* 5 ps *after simulation start* [8].

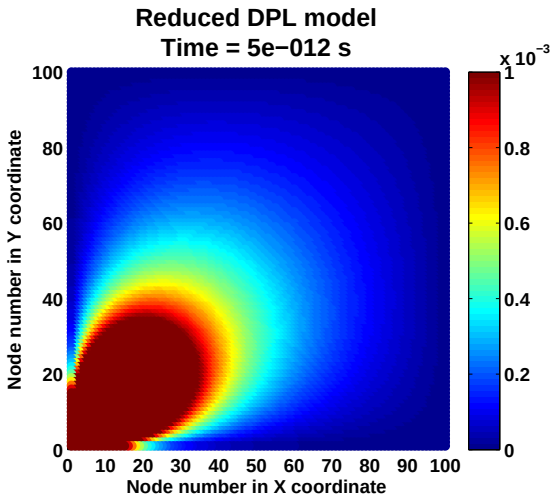

Fig. 17. *Temperature rise inside the analyzed structure obtained using reduced Fourier-Kirchhoff model for* 10 000 *nodes,* 5 ps *after simulation start.*

model). For long times of the analysis, outputs received using full and reduced Fourier-Kirchhoff model are very similar. The described phenomenon is not observed in the case of Dual-Phase-Lag model, for which results yielded using both full and reduced version of this model for all analyzed time instants are comparable. The comparison of fittings of reduced thermal models to their full versions for the steady state are presented in Figures 18 (Dual-Phase-Lag model) and 19 (Fourier-Kirchhoff model). The differences in scale on the vertical axis are caused by very small absolute temperature rises. Small differences between these values can give big differences during the normalization process.

Additionally, in order to confirm the good agreement of the fittings of reduced models to the full ones, the relative error has been determined according to the following equation [8]:

$$Rel_{error}\left(t\right) = \left| \frac{C^T \overline{T}\left(t\right) - c^T T\left(t\right)}{c^T T\left(t\right)} \right| \qquad t \geq 0 \tag{15}$$

The relative error values, for some chosen time instants and both investigated thermal models, are presented in Figures 20 - 21. The analysis of these figures leads to the conclusion that the biggest relative error values are observed for very small time instants, at the beginning of the simulation, while over the simulation time the relative error becomes inconsiderable. This situation confirmes that the reduction process ensures high quality results. Moreover, the proposed approach is convergent, what is extremely important from the numerical point of view.

Finally, the simulation times have been also compared. Their comparisons are

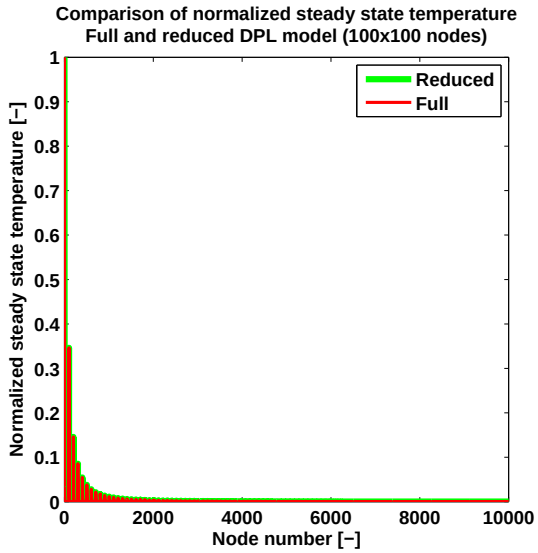

Fig. 18. *Comparison of normalized steady state temperature rise inside structure obtained using full and reduced Dual-Phase-Lag model for* 10 000 *nodes.*

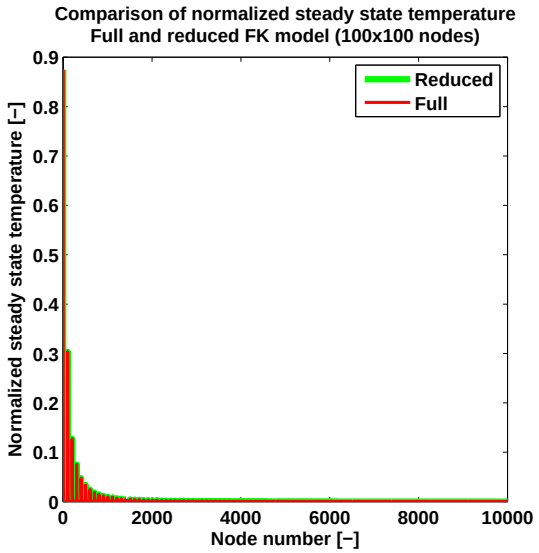

Fig. 19. *Comparison of normalized steady state temperature rise inside structure obtained using full and reduced Fourier-Kirchhoff model for* 10 000 *nodes.*

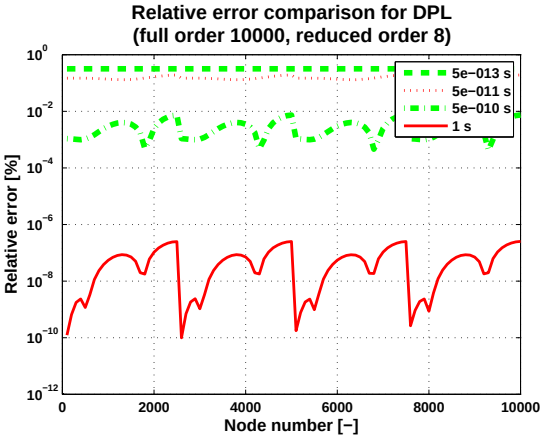

Fig. 20. *Relative error of full thermal model reconstruction from the reduced one in the case of Dual-Phase-Lag model for* 10 000 *nodes.*

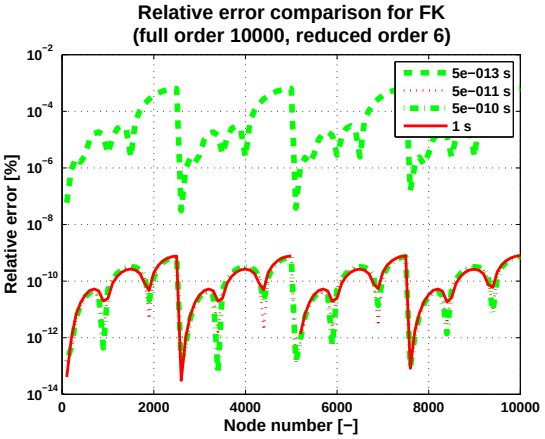

Fig. 21. *Relative error of full thermal model reconstruction from the reduced one in the case of Dual-Phase-Lag model for* 10 000 *nodes.*

shown in Figures 22 - 23.

As it can be seen, full version of the Dual-Phase-Lag model demands significantly more time to obtain the temperature distribution inside the analyzed structure than the Fourier-Kirchhoff model. It is related to bigger computational complexity of the algorithm including the Dual-Phase-Lag system of equations. However, longer simulation time ensures more reliable results. On the other hand, the reduced versions of both investigated thermal models require the similar computational power, what causes that simulation times in both these cases are comparable.

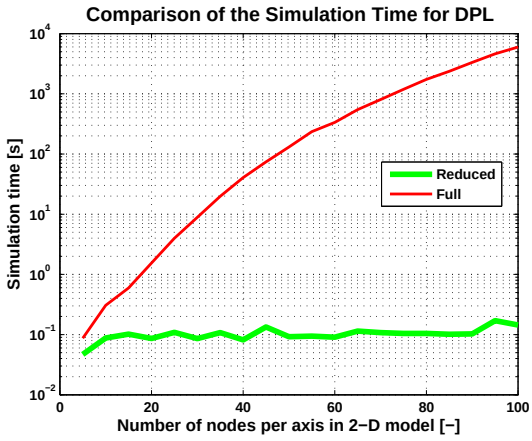

Fig. 22. *Simulation times comparison for full and reduced Dual-Phase-Lag model for* 10 000 *nodes* [8].

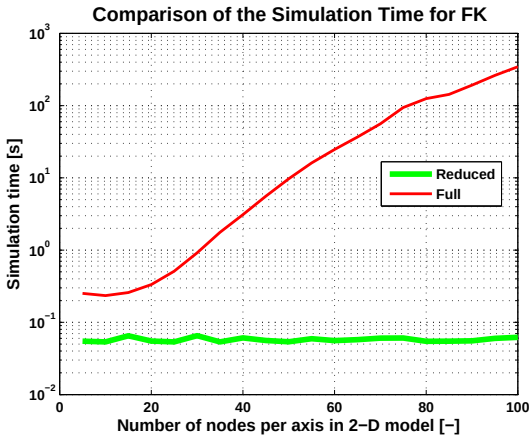

Fig. 23. *Simulation times comparison for full and reduced Fourier-Kirchhoff model for* 10 000 *nodes.*

5. Conclusions

Analyses of obtained results lead to the following conclusions. using the Fourier-Kirchhoff model, the final temperature distribution inside the investigated structure is received in quicker time than that one related to the use of Dual-Phase-Lag model. However, the Fourier-Kirchhoff model overestimates the temperature values, especially near the hear source. Due to this fact the use of Dual-Phase-Lag model is more appropriate for such small nanomertic structures.

In order to reduce the computational complexity of the problem and the simulation time, the model order reduction is needed. The reduction process based on the moment maching using the Krylov subspace method and Arnoldi algorithm ensures obtaining high quality results. The fitting of outputs yeilded using reduced-order models to these ones obtained using full order models is characterized by a very good agreement. This situation is observed in both Fourier-Kirchhoff and Dual-Phase-Lag cases. However, for short times of thermal analyses, the relative error values of full Fourier-Kirchhoff model reconstruction from the reduced one are significantly grather than relative error values of full Dual-Phase-Lag model reconstruction. Neverthless, for longer times of analyses, the relative errors are on a comparatively low level.

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PORÓWNANIE REDUKCJI RZĘDU DWUWYMIAROWYCH MODELI DUAL-PHASE-LAG I FOURIERA-KIRCHHOFFA PRZY UŻYCIU METODY PODPRZESTRZENI KRYLOVA

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

Niniejszy artykuł prezentuje porównanie rozkładów temperatury w dwuwymiarowej strukturze nanometrycznej otrzymanych przy pomocy dwóch różnych modeli przepływu ciepła. Pierwszy z nich wyraża klasyczne podejście bazujące na modelu Fouriera-Kirchhoffa, podczas gdy drugi wykorzystuje nowoczesną metodologię nawiązują do równania Dual-Phase-Lag. W obu przypadkach dokonano również redukcji rzędu modeli termicznych. Proces redukcji oparto na metodzie podprzestrzeni Krylova. Wszystkie wyniki zostały ponadto uważnie przeanalizowane i omówione.

Słowa kluczowe: model Fouriera-Kirchhoff, równanie Dual-Phase-Lag, przepływ ciepła w nanoskali, rozkład temperatury, redukcja rzędu modeli, metoda podprzestrzeni Krylova, algorytm Arnoldiego