Multiscale model reduction for neutron diffusion equation

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Abstract. Construction of multiscale method for neutron diffusion equation is provided. The neutron diffusion approximation is mostly used for reactor analysis and applied in most engineering calculation codes. The solution method is based on the use of a generalized multiscale finite element method. The main idea is to create local solutions that can be used to effectively solve on a coarse grid. Numerical results show that multiscale basis functions can well take into account the small-scale characteristics of the medium and provide accurate solutions.

Keywords: multiscale method · parabolic equation · neutron diffusion

1 Introduction

About neutron diffusion equation
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About reduction methods
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About GMsFEM method
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2 Problem statement

Let's consider modelling neutron flux in a one-group diffusion approximation. Neutron flux dynamics is considered within a bounded 2D domain Ω ($\boldsymbol{x} = \{x_1, x_2\} \in \Omega$) with a convex boundary $\partial\Omega$. The neutron diffusion is described by the following set of equations with one group delayed neutron source:

$$\begin{aligned} \frac{1}{v}\frac{\partial \phi}{\partial t} - \nabla \cdot D\nabla\phi + \Sigma_r\phi = \frac{1-\beta}{K_{eff}}\nu\Sigma_f\phi + \lambda c, \\ \frac{\partial c}{\partial t} + \lambda c = \frac{\beta}{K_{eff}}\nu\Sigma_f\phi. \end{aligned} \tag{1}$$

Here $\phi(\boldsymbol{x}, t)$ — neutron flux at point $\boldsymbol{x}$ and time t, v — effective velocity of neutrons, $D(\boldsymbol{x})$ — diffusion coefficient, $\Sigma_r(\boldsymbol{x}, t)$ — removal cross-section, $\Sigma_f(\boldsymbol{x}, t)$ — generation cross-section, β — effective fraction of delayed neutrons, λ — decay constant of sources of delayed neutrons. System of equations (1) is supplement with boundary condition and initial condition.

The albedo-type conditions are set at the boundary of the area $\partial\Omega$:

$$D\frac{\partial \phi}{\partial n} + \gamma\phi = 0, \tag{2}$$

where n — outer normal to the boundary $\partial\Omega$, γ — albedo constant. Let's propose that in the initial time moment (at t = 0) the reactor is in the critical state

$$\phi(\boldsymbol{x}, 0) = \phi^0(\boldsymbol{x}). \tag{3}$$

To solve the problem in computational domain Ω, we approximate the system of equations (1)-(3) using the finite element method. We discretize the time derivatives using finite-difference scheme, and then bring each stationary problem to a variational formulation. For approximation in time, we use a purely implicit scheme with time step τ. To specify the variational formulation, we multiply equations by the test function q and integrate over the domain Ω. Using the integration by parts, we obtain the following variational formulation: find $\phi^{n+1} \in V$ such that

$$\begin{aligned} \int_\Omega \frac{1}{v}\frac{\phi^{n+1}}{\tau}qdx + \int_\Omega D^{n+1}\nabla\phi^{n+1}\cdot\nabla q dx + \int_\Omega \Sigma_r^{n+1}\phi^{n+1}qdx - \\ \int_\Omega \frac{1+\lambda\tau-\beta}{K_{eff}(1+\lambda\tau)}\nu\Sigma_f^{n+1}\phi^{n+1}qdx + \int_{\partial\Omega}\gamma\phi^{n+1}qds = \\ \int_\Omega \frac{1}{v}\frac{\phi^n}{\tau}qdx + \int_\Omega \frac{\lambda c^n}{1+\lambda\tau}qdx, \quad \forall q \in V, \end{aligned} \tag{4}$$

where $V = H^1(\Omega)$ — sobolev space consisting of scalar functions v such that v^2 and $|\nabla v^2|$ have a finite integral in Ω.

Further, it's necessary to pass from the continuous variational problem (4) to the discrete problem. We introduce finite-dimensional space of finite elements

$V_h \subset V$ and formulate a discrete variational problem. We use standard linear basis functions as basis functions to solve the problem on the fine grid and

$$\phi = \sum_{i=1}^{N_f} \phi_i y_i,$$

where N_f is the nunber of vertices on the fine grid.

The problem is solving a system of linear algebraic equations

$$A_f \phi = b_f, \tag{5}$$

where the operator A_f corresponds to the left side of equation (4), and the vector b_f corresponds to the right side of equation (4).

3 Multiscale method

For the discretization on the coarse grid we use GMsFEM. We construct two grids: fine grid ($\mathcal{T}_h$) and coarse grid ($\mathcal{T}_H$) (see Figure 1). For multiscale basis construction, we define local domains ω_i, where $i = 1, ..., N_v$ and N_v is the number of coarse grid nodes. We assume that $\mathcal{T}_h$ is a refinement of $\mathcal{T}_H$, where h and H represent the fine and coarse mesh sizes, respectively. We assume that the fine-scale mesh $\mathcal{T}_h$ is sufficiently fine to fully resolve the small-scale information of the domain while $\mathcal{T}_H$ is a coarse mesh containing many fine-scale features. A local domain ω_i is obtained by the combining all the coarse cells around one vertex of the coarse grid.

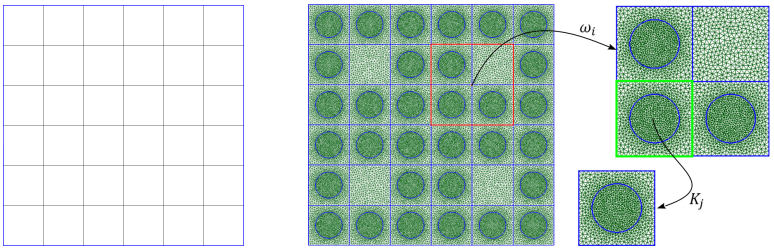

Fig. 1. Coarse grid and local domain ω_i with K_j

GMsFEM involves two basic steps: (a) the construction of multiscale basic functions that take into account small scale heterogeneities in the local domains and (b) the construction of the coarse scale approximation. For the construction of the multiscale basic functions we solve spectral problems in local domains. Spectral problems help to identify the most important characteristics of the solution. In contrast to the available techniques, this method allows to avoid the limitations associated with idealization and limitations on the applicability of

the method. This method also more general technology that takes into account the different scale processes. The construction of basic functions occurs independently for each local domain, doesn't require the exchange of information between processors, and has a high parallelization efficiency. Using constructed multiscale basic functions, we construct a mathematical model on a coarse grid that allows to significant reduce the solution time, the amount of used memory, and can be used to perform calculations for a given configuration of heterogeneous properties.

We construct the mutiscale function space

$$V_{\text{off}} = \text{span}\{y_j\}_{j=1}^{N},$$

where N is the number of coarse basis functions. Each y_j is supported in local domain w_i.

Multiscale space. The firts step is the solution of local spectral problems on the local domains. These spectral problems identify important modes of the problem and used to construct a multiscale space. In order to construct a conforming basis functions, we multiply eigenvectors related to the smallest eigenvalues to the partition of unity functions.

We use following spectral problem in ω_i

$$A\varphi^i = \lambda S\varphi^i, \tag{6}$$

where the elements of the matrices $A = \{a_{ij}\}$ and $S = \{s_{ij}\}$ are defined as follow

$$\begin{aligned} a_{ij} = \int_{\omega_i} D\nabla\phi \cdot \nabla q dx + \int_{\omega_i} \Sigma_r \phi q dx - \int_{\omega_i} \frac{1+\lambda\tau-\beta}{K_{eff}(1+\lambda\tau)} \nu\Sigma_f \phi q dx, \\ s_{ij} = \int_{\omega_i} Duq dx. \end{aligned} \tag{7}$$

We solve this spectral problem on the local domain

$$\tilde{A}\tilde{\varphi}^i = \lambda\tilde{S}\tilde{\varphi}^i, \quad \tilde{A} = PAP^T, \quad \text{and} \quad \tilde{S} = PSP^T. \tag{8}$$

where $P = \{\psi_0, \psi_1, ..., \psi_{J_i}\}$ and $\varphi_k^i = P\tilde{\varphi}_k^i$ for $k = 1, 2, ...$ Then, we choose eigenvectors corresponding to the smallest M_i eigenvalues from (8) and use them for the construction of multiscale basis functions.

Partirion of unity functions. As partition of unity functions, we use linear functions in each domain ω_i. Partitions of unity are calculated in the domain K_j as a linear function from Γ to the vertex A, and 0 is assigned to the entire segment Γ, and at point A is assigned the value 1. Thus, we obtain a linear function from 0 to 1 over the entire domain K_j. Partitions of unity are shown in Figure 2. Domain K_j is one element from a coarse grid.

The multiscale space is defined as the span of $\chi_i\varphi_k^i$, where χ_i is the usual nodal basis function for the node i (linear partition of unity functions). The number of bases can be different, the accuracy of the solution can be improved when we increase the number of bases.

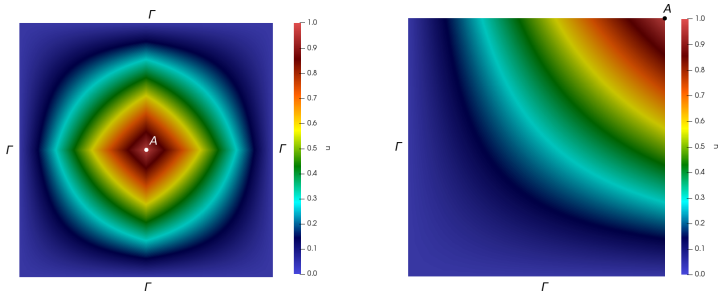

Fig. 2. Partirion of unity functions on the ω_i (right) and K_j (left)

Coarse-scale approximation. Next, we create following matrix for each ω_i

$$R^i = \left[\chi_i\varphi_1^i, \ldots, \chi_i\varphi_{M_i}^i, \chi_i\eta^i\right].$$

and define a transition matrix from a fine grid to a coarse grid to reduce the dimension of the problem

$$R = [R^1, R^2, ..., R^{N_v}],$$

where N_v is the number of local domains ω_i.

Then using transition matrix R and fine grid system (5), we construct coarse grid approximation

$$A_c\phi_c = b_c, \quad A_c = RA_fR^T \quad \text{and} \quad b_c = Rb_f, \tag{9}$$

and using coarse-scale solution ϕ_c, we can reconstruct a fine grid solution $\phi_{ms} = R^T\phi_c$.

4 Numerical results

The test problem for reactor small PWR-2D (Ω — reactor core area) is considered [**?**]. The geometrical model of the small PWR-2D reactor core is presented in Fig.3. The diameter of the fuel rods is 0.82 cm, the cell width is 1.26 cm. Diffusion neutronics constants in the common notations are given in Table 1. There are two types of cassettes, with fuel 1% UO_2 and 2% UO_2. The boundary conditions (2) are used at $\gamma = 0$ (total reflection). The following delayed neutrons parameters are used: $\beta = 6.5 \cdot 10^3$, $\lambda = 0.08$ s^{-1} and $v = 5 \cdot 10^5$ cm/s.

We define the next scenario of the process: The λ-spectral problem is solved [1], the solution is taken as the initial condition; Calculation for the non-stationary model at the time range 0 to 0.4 sec; At a moment of 0.1 sec and 0.3 sec the fuel value Σ_a for the zone 1 changes to +2% and -3% respectively (modeling effect of insertion or withdrawal of control rods). At each time the integrated power is calculated

$$P(t) = a\int_\Omega \Sigma_f\phi d\boldsymbol{x},$$

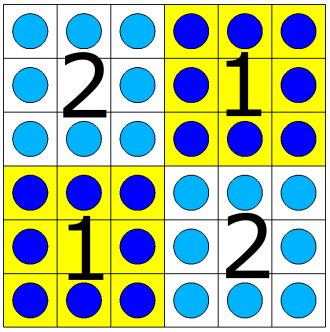

Fig. 3. Geometrcial model of the small PWR-2D reactor core

Table 1. Diffusion neutronics constants for IAEA-2D test problem

Zone	1		2	
	coolant	fuel	coolant	fuel
D	0.34473872445	0.77002585054	0.31679441560	0.80236505122
Σ_a	5.3858400E-03	8.9337900E-02	6.0670900E-03	6.6279500E-02
Σ_f	0.0	5.4731800E-02	0.0	3.3377700E-02
ν	0.0	2.44844861671	0.0	2.45482762443

where a is the normalization coefficient by a given value of the integrated power.

Coarse mesh contains 49 vertices. The fine grid contains 115891 vertices. The time step for both grids is $\tau = 0.001$. As an exact solution, we take the solution by the finite element method on a fine grid. The initial value of K_{eff} was 1.xxxxxxx.

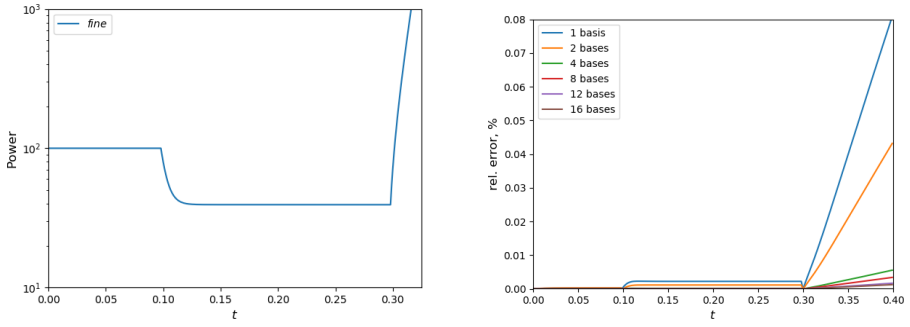

Fig. 4. Interal power on a fine grid and relative errors (%) of the multiscale solution power.

The integral power on a fine grid and relative errors of a integral powers for multiscale soultion shown in Figure 4. When using one basis, the error does not exceed 1%, and for using 4 or more bases it does not exceed 0.01%.

In Figure 5, we present relative L_2 and H_1 errors of multiscale solution vs. time for different number of multiscale basis functions. From the numerical results, we observe a good convergence behavior, when we take sufficient number of multiscale basis functions.

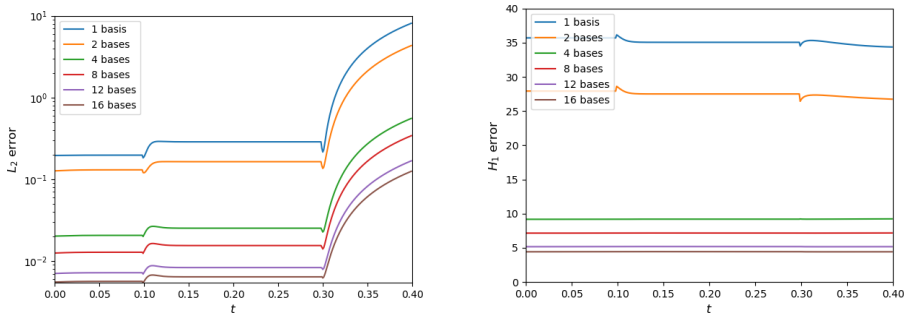

Fig. 5. Relative L_2 and H_1 errors (%) of the multiscale solution.

In Table 2, we present relative L_2 and H_1 errors at final time for different number of multiscale basis functions. For example, when we use 8 spectral basis functions, we obtain 0.34% L_2 error and 7.18% H_1 error. Our comparison showed that it is prefer to use 4 or higher count of bases. The solution of the problem on a fine grid and multiscale solution using 16 basis functions on each local domain ω_i are shown in Figure 6. Relative errors are 0.13% for L_2 and 4.43% for H_1.

Table 2. Relative L_2 and H_1 errors (%) of the solution at final time.

Number of bases	Number of DOF	L_2 error	H_1 error	Calc time
1	xx	8.09	34.36	0.015
2	xx	4.32	26.73	0.018
4	xx	0.56	9.24	0.026
8	xx	0.34	7.18	0.056
12	xx	0.17	5.17	0.102
16	xx	0.13	4.43	0.239
fine	xx	–	–	6.816

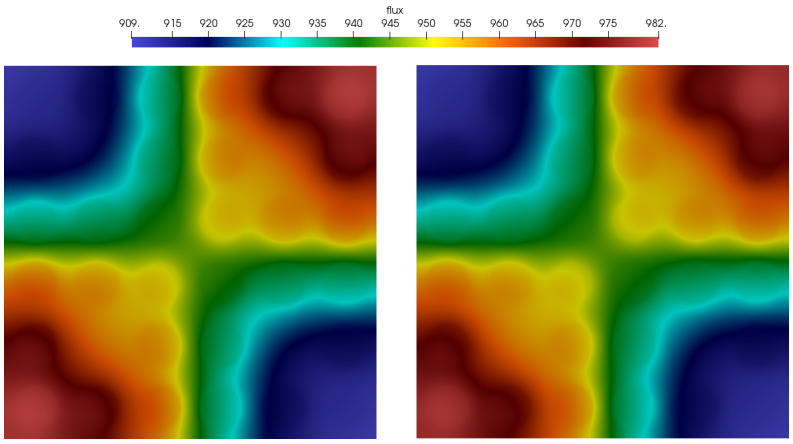

Fig. 6. Fine grid and multiscale solution at final time.

5 Conclusions

A Generalized Multiscale Finite Element method was developed successfully for solving neutron diffusion in one-group approxmimation. We presented an implementation of GMsFEM. We considered each step of GMsFEM algorithm. The results showed that GMsFEM has good accuracy in all cases.

In the current work, we considered the most popular and simplest model of neutron transport equation. Computational expenses are always an issue even for modern computers. In the future, we will consider more complex models of the neutron diffusion and transport equation, such as SP_3 approximation.

Acknowledgements

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