Multiscale Model Reduction for Neutron Diffusion Equation

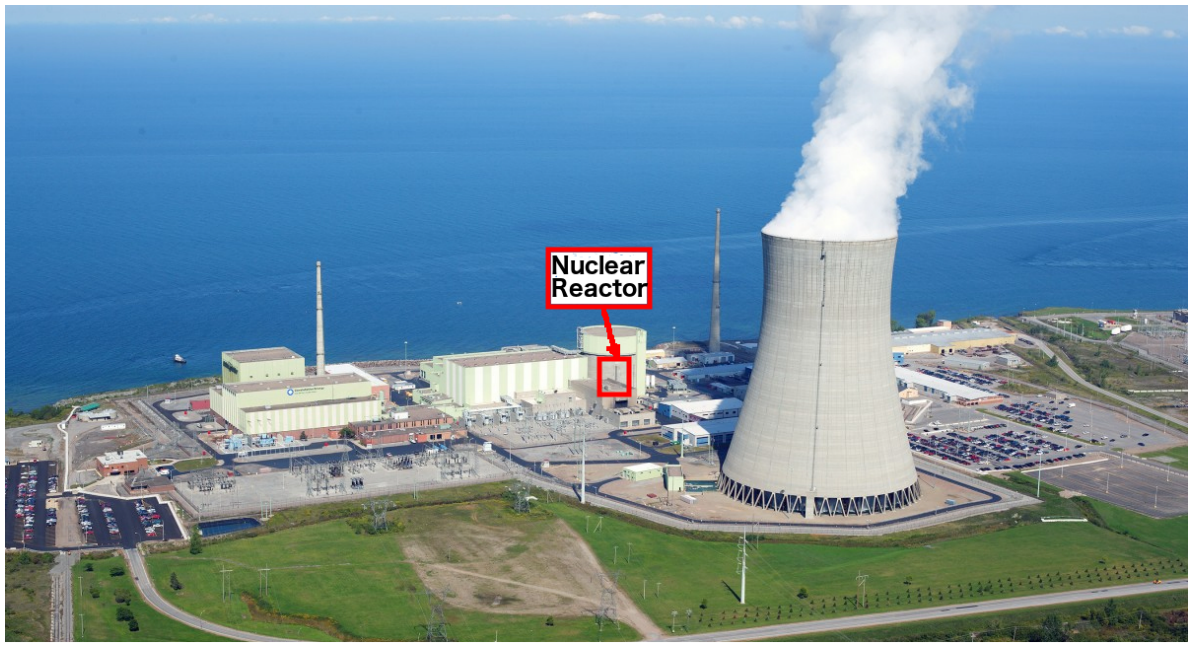
Aleksandr Avvakumov [1] Denis Spiridonov [2]
Aleksandr Vasilev [2]

[1]National Research Center "Kurchatov Institute", Moscow, Russia
[2]North-Eastern Federal University, Yakutsk, Russia

4th MMR& HPC, September 9-12, 2020 Sochi

Introduction

Real dynamic neutronic calculations require the use of large computational grids during large characteristic times. For these reasons, the reactor calculations can be very expensive.

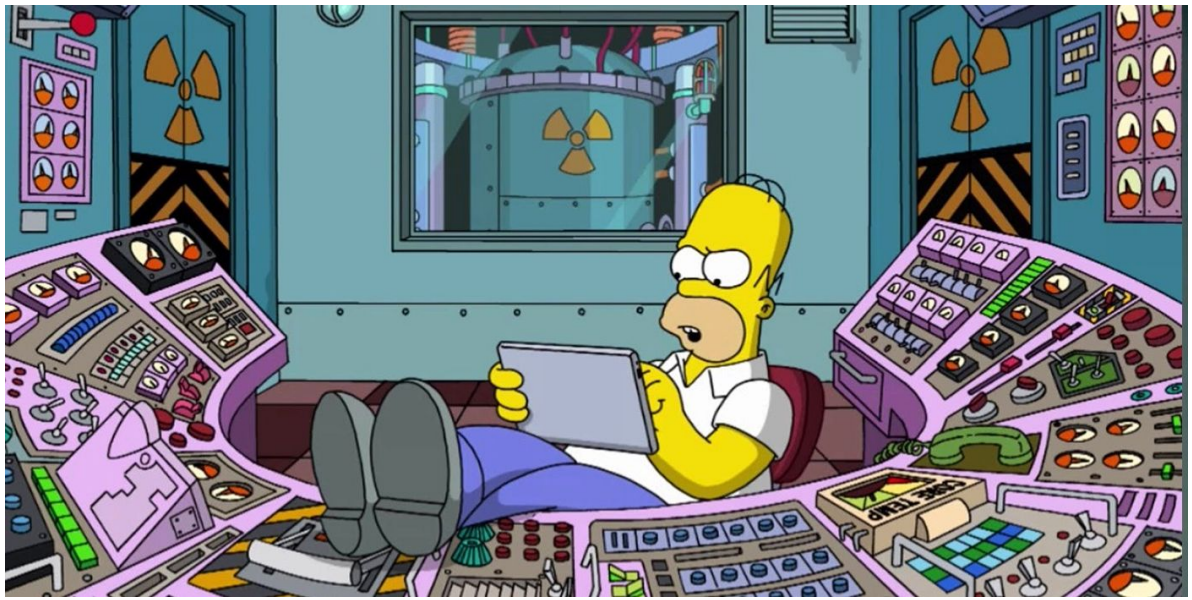


When solving these problems, it is common to use numerical averaging techniques or different multiscale methods that can significantly reduce the number of unknowns, through the construction of coarse-scale model.

Equations

Neutron transport equation: time, energy, spatial and angular variables (7 unknowns)

- Diffusion approximation: one-group, two-group, multi-group
- Spherical Harmonics: P_1, ..., P_N approximations
- Simplified P_N: SP_3, ..., SP_N approximations



Problem statement

We consider a bounded 2D domain Ω ($\boldsymbol{x} = \{x_1, x_2\} \in \Omega$) with a convex boundary $\partial\Omega$. The one-group transport equation in the diffusion approximation with one-group delayed neutron source can be written as follows

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

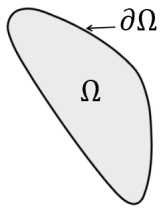
Here $\phi(\boldsymbol{x}, t)$ is the neutron flux at point $\boldsymbol{x}$ and time t, $c(\boldsymbol{x}, t)$ is density of sources of delayed neutrons, v is the effective neutron velocity, D is the diffusion coefficient, Σ_r is the removal cross-section, $\nu\Sigma_f$ is the fission cross-section, β is the effective fraction of delayed neutrons, λ is the decay constant of the delayed neutron source.

Boundary and initial conditons

Let's determine the boundary and initial conditions for Equation (1). The albedo-type conditions are set at the boundary $\partial\Omega$:

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

where n is an outer normal to the boundary $\partial\Omega$, γ is the albedo constant.



Let's propose that at the initial time t $= 0$, the reactor is in steady-state critical condition

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

Time approximation

To solve the problem within the 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 fully implicit scheme with time step τ.

Varitional formulation

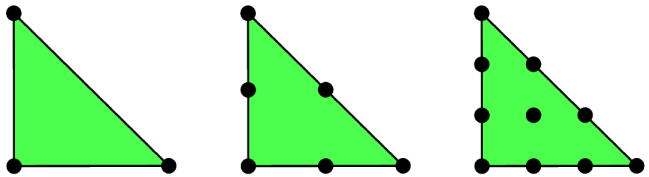
To specify the variational formulation, we multiply equations by the test function q and integrate over the domain Ω. Using the integration by parts, we obtain the following variational formulation: let's find $\phi^{n+1} \in V$ such that

$$\int_\Omega \frac{1}{v}\frac{\phi^{n+1}}{\tau} q d\boldsymbol{x} + \int_\Omega D^{n+1}\nabla\phi^{n+1}\cdot\nabla q d\boldsymbol{x} + \int_\Omega \Sigma_r^{n+1}\phi^{n+1} q d\boldsymbol{x} - \int_\Omega \frac{1+\lambda\tau-\beta}{K_{eff}(1+\lambda\tau)}\nu\Sigma_f^{n+1}\phi^{n+1} q d\boldsymbol{x} + \int_{\partial\Omega}\gamma\phi^{n+1} q d\boldsymbol{s} = \int_\Omega \frac{1}{v}\frac{\phi^{n}}{\tau} q d\boldsymbol{x} + \int_\Omega \frac{\lambda c^n}{1+\lambda\tau} q d\boldsymbol{x}, \quad \forall q \in V, \tag{4}$$

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

Discrete problem

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.



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).

Multiscale method

For the discretization on the coarse grid we use Generalized Multiscale Finite Element Method (GMsFEM).

GMsFEM involves two basic steps:

1. The construction of multiscale basis functions that take into account small scale heterogeneities in local domains;
2. The construction of the coarse scale approximation.

Coarse and fine grids

We construct two grids: fine grid ($\mathcal{T}_h$) and coarse grid ($\mathcal{T}_H$). We define local domains ω_i, where $i = 1, ..., N_v$ and N_v is the number of coarse grid nodes.

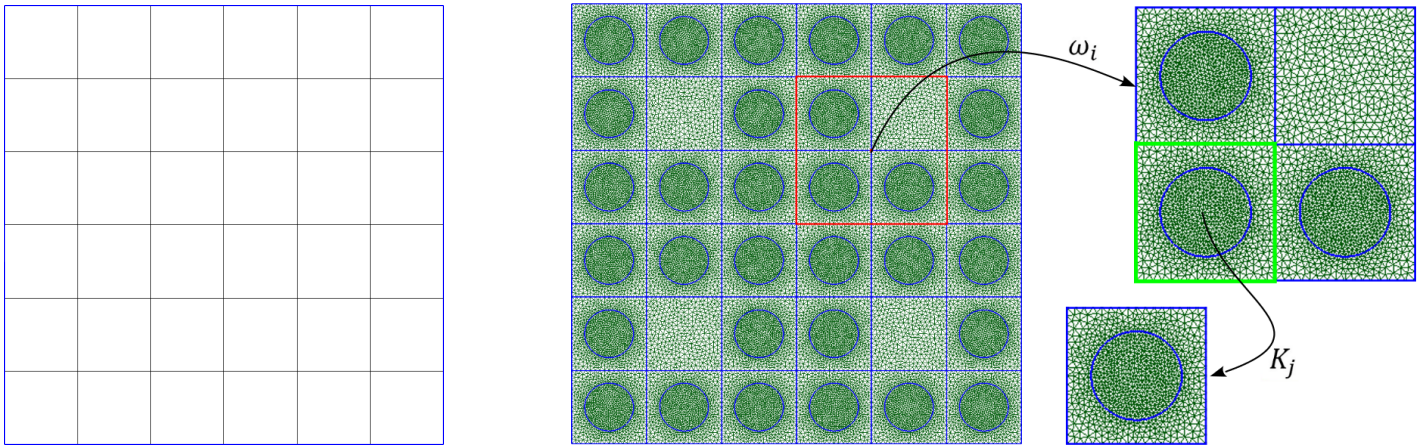


Figure: Coarse grid and local domain ω_i with K_j

A local domain ω_i is obtained by the combining all the coarse cells around one vertex of the coarse grid.

Spectral problems

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. 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

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

Then, we choose eigenvectors corresponding to dominant M_i eigenvalues from (6) and use them to construct the multiscale basis functions.

Partition of unity functions

As partition of unity functions, we use linear functions in each domain ω_i. Thus, we obtain a linear function from 0 to 1 over the entire domain K_j. Domain K_j is one element from a coarse grid.

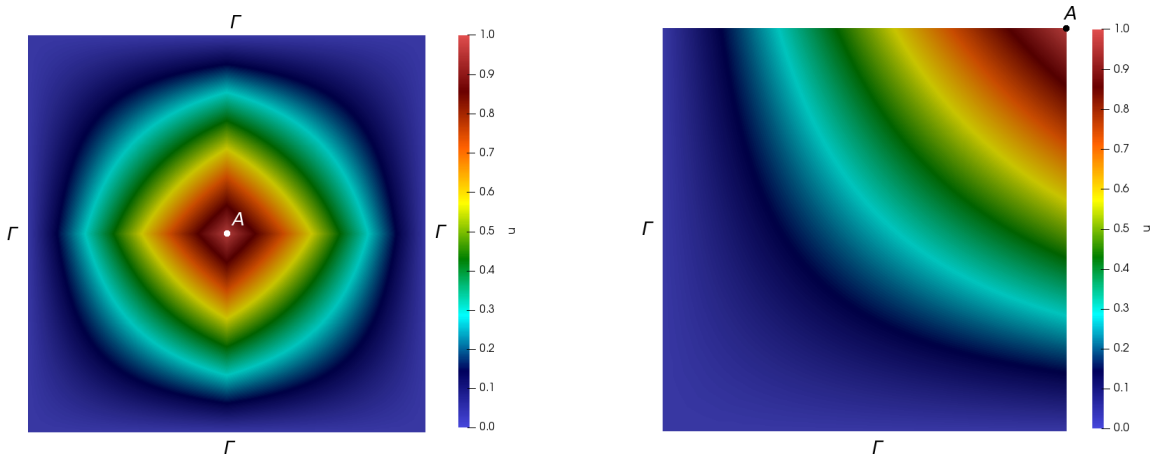


Figure: Partirion of unity functions on the ω_i (right) and K_j (left)

The multiscale space is defined as the span of $y_i = \chi_i \varphi_k^i$, 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.

Coarse-scale approximation

Next, we create the following matrix for each ω_i

$$R^i = [y_1, \ldots, y_{M_i-1}, y_{M_i}].$$

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

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

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

$$A_c\phi_c = b_c, \quad A_c = RA_fR^T \quad \text{and} \quad b_c = Rb_f, \tag{8}$$

and using the coarse-scale solution ϕ_c, we can reconstruct the fine grid solution

$$\phi_{ms} = R^T\phi_c.$$

Small PWR 2D

Let's consider the 2D test problem for small PWR reactor (Ω — reactor core area).

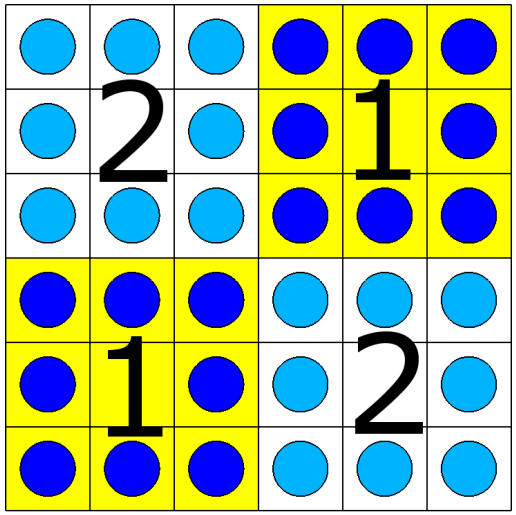


Figure: Geometrcial model of the small PWR-2D reactor core

The diameter of the fuel rods is 0.82 cm, the cell width is 1.26 cm. There are two types of cassettes, with fuel 1% UO_2 and 2% UO_2. The reflective boundary conditions (2) are used ($\gamma = 0$). The following delayed neutrons parameters are used: $\beta = 6.5 \cdot 10^{-3}$, $\lambda = 0.08$ s^{-1} and $\nu = 5 \cdot 10^5$ cm/s.

Scenario

We define the next scenario of the process:

- The λ-spectral problem is solved and the solution is taken as the initial condition;
- Calculation for the non-stationary model at the time range from 0 to 0.4 sec;
- At $t = 0.1$ sec and $t = 0.3$ sec Σ_a for fuel in the zone 1 changes to $+2\%$ and -3%, respectively (simulation of insertion or withdrawal of control rods).

At each time the integrated power is calculated as

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

where a is the normalization coefficient, which corresponds to a given value of the integrated power.

Software

Fine grid solution

The fine grid contains 115891 vertices. The time step for both grids is $\tau = 0.001$. As an exact solution, we take the fine-grid solution. The initial value of K_{eff} is 1.183280.

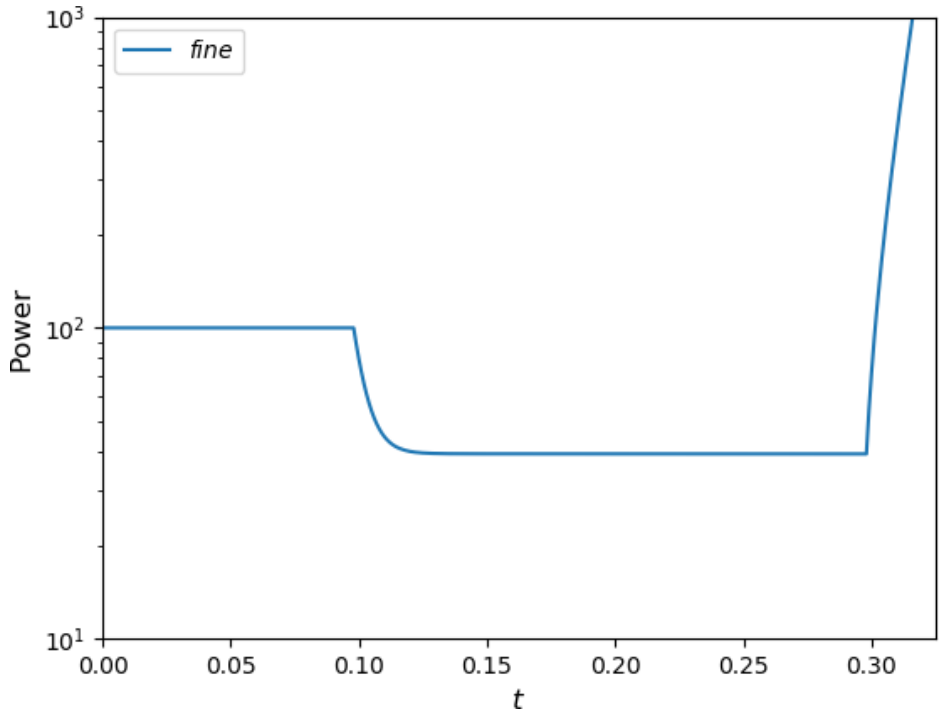


Figure: Integral power on the fine grid.

Coarse grid solution

The coarse grid contains 49 vertices. When using single basis, the error does not exceed 1%, and for using 4 or more bases it does not exceed 0.01%.

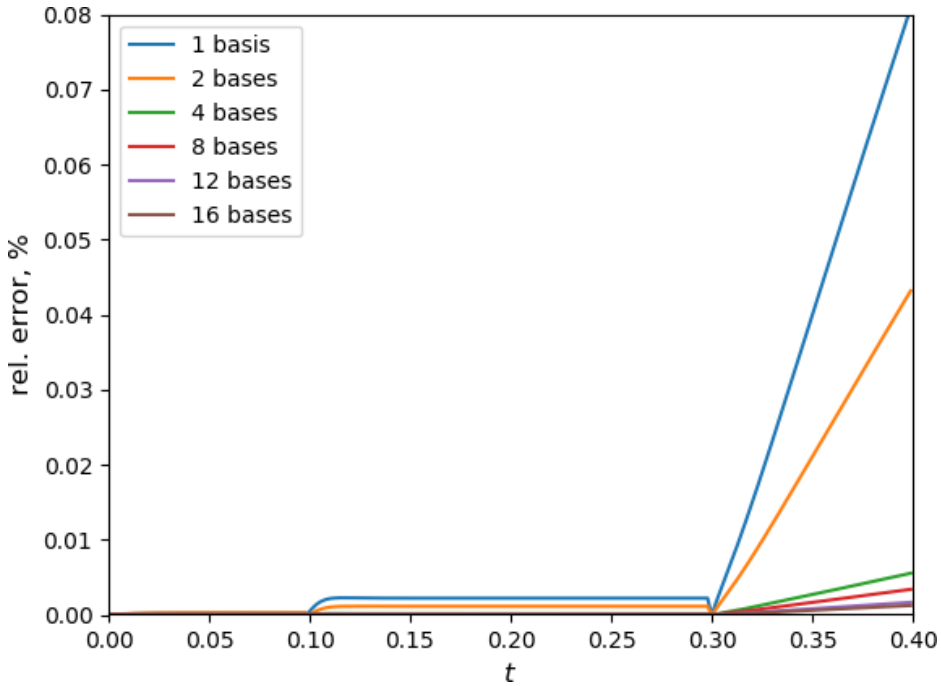


Figure: Relative errors (%) of the multiscale solution power.

L_2 error

We present relative L_2 errors of the multiscale solution vs. time for different number of multiscale basis functions. The numerical results show good convergence behavior, provided that we take sufficient number of the multiscale basis functions.

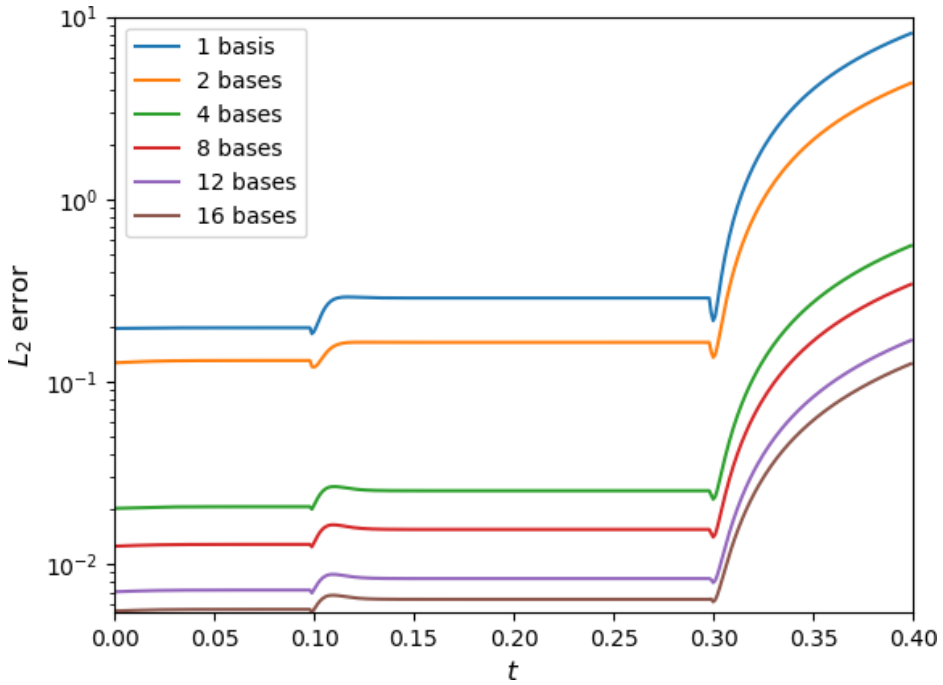


Figure: Relative L_2 errors (%) of the multiscale solution.

H_1 error

We present relative H_1 errors of the multiscale solution vs. time for different number of multiscale basis functions. The numerical results show good convergence behavior, provided that we take sufficient number of the multiscale basis functions.

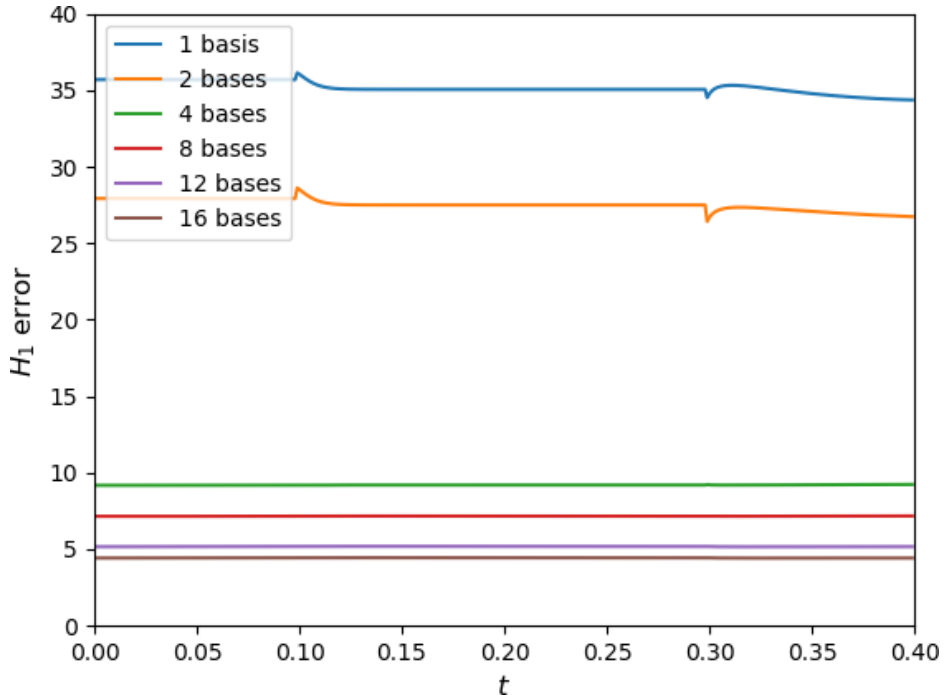


Figure: Relative H_1 errors (%) of the multiscale solution.

Errors at final time

In Table we present relative L_2 and H_1 errors at final time for different number of the multiscale basis functions. For example, when we use 8 spectral basis functions, we obtain 0.34% for L_2 error and 7.18% for H_1 error. Our calculations show that it is necessary to use 4 or more basis functions.

Table: 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	49	8.09	34.36	0.015
2	98	4.32	26.73	0.018
4	196	0.56	9.24	0.026
8	392	0.34	7.18	0.056
12	588	0.17	5.17	0.102
16	784	0.13	4.43	0.239
fine	115891	–	–	6.816

Bases

We present first four (of 16) multiscale basis functions in local domain ω_i.

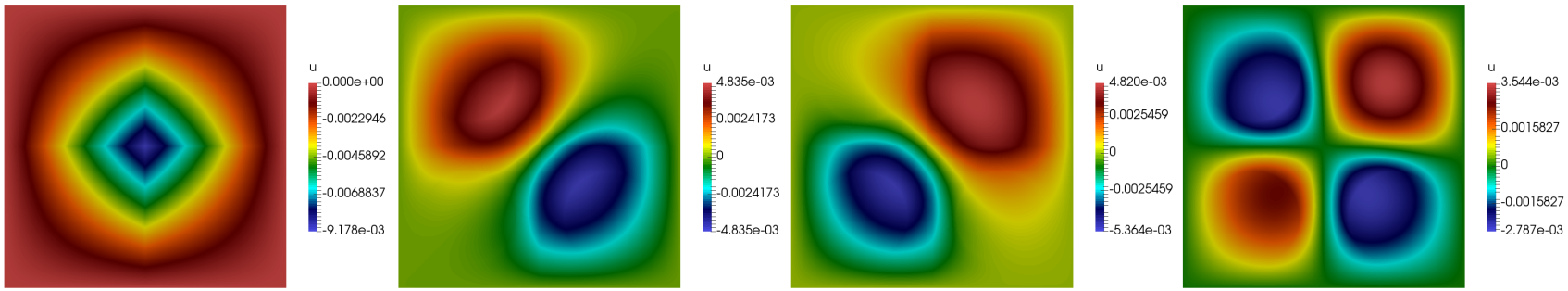


Figure: The first four multiscale basis functions.

Neutron flux

The fine-grid solution and the multiscale solution (16 basis functions on each local domain) ω_i are shown in Figure. Relative errors are 0.13% for L_2 and 4.43% for H_1.

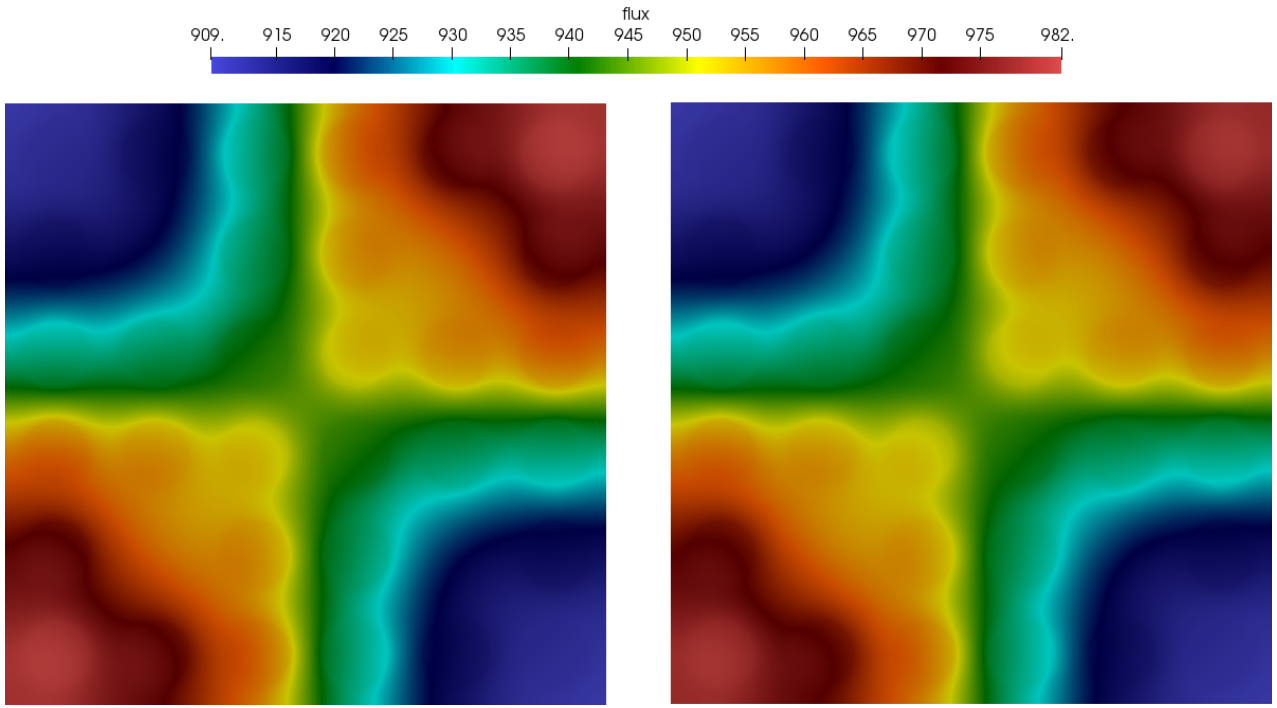


Figure: Fine grid (left) and multiscale solutions (right).

Conclusion and future work

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

In the current work, we considered the 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 neutron transport, such as SP_3 approximation.


Thank you for your attention!