A generalized multiscale finite element method for numerical solution of neutron transport problems in SP_3 approximation

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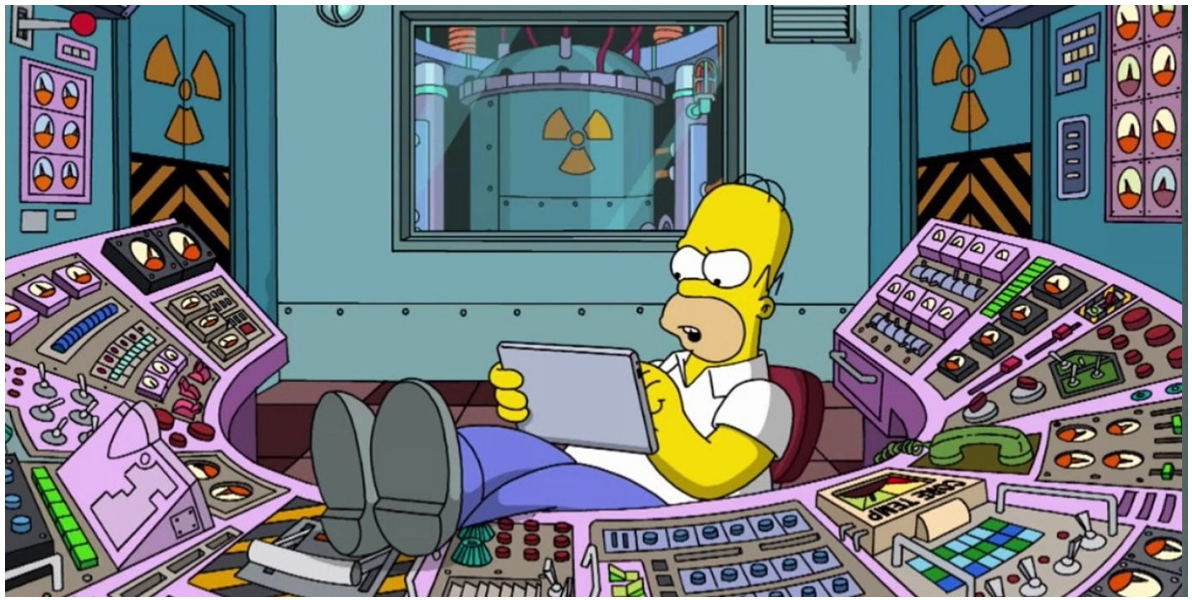
Introduction

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.

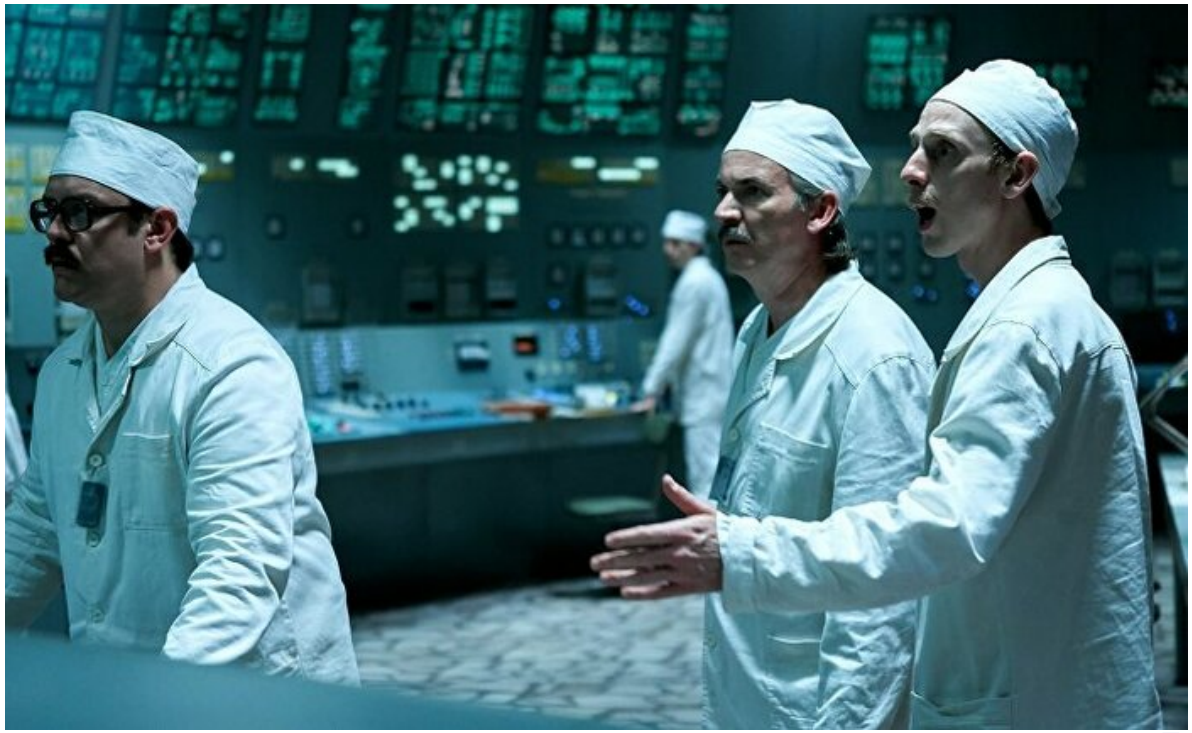


When solving these problems, it is common to use numerical averaging techniques or different multiscale methods that can significantly reduce the number of unknowns, through the construction of coarse-scale model.

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 with a convex boundary $\partial\Omega$. The neutron transport is described by the system of equations

$$\begin{aligned}
\frac{1}{v_g}\frac{\partial \phi_{0,g}}{\partial t} - \frac{2}{v_g}\frac{\partial \phi_{2,g}}{\partial t} - \nabla \cdot D_{0,g}\nabla\phi_{0,g} + \Sigma_{r,g}\phi_{0,g} - 2\Sigma_{r,g}\phi_{2,g} &= (1-\beta)\chi_{n,g}S_n + S_{s,g} + \chi_{d,g}S_d, \\
-\frac{2}{v_g}\frac{\partial \phi_{0,g}}{\partial t} + \frac{9}{v_g}\frac{\partial \phi_{2,g}}{\partial t} - \nabla \cdot D_{2,g}\nabla\phi_{2,g} + 5\Sigma_{t,g} + 4\Sigma_{r,g})\phi_{2,g} - 2\Sigma_{r,g}\phi_{0,g} &= -2(1-\beta)\chi_{n,g}S_n - 2S_{s,g} - 2\chi_{d,g}S_d,
\end{aligned}$$

where

$$S_n = \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'}, \quad S_{s,g} = \sum_{g\neq g'=1}^{G} \Sigma_{s,g'\to g}\phi_{g'}, \quad S_d = \sum_{m=1}^{M} \lambda_m c_m,$$

$$\phi_{0,g} = \phi_g + 2\phi_{2,g}, \quad D_{0,g} = \frac{1}{3\Sigma_{tr,g}}, \quad D_{2,g} = \frac{9}{7\Sigma_{t,g}}, \quad g = 1, 2, \ldots, G.$$

Boundary and initial conditons

The density of sources of delayed neutrons

$$\frac{\partial c_m}{\partial t} + \lambda_m c_m = \beta_m S_n, \quad m = 1, 2, \ldots, M, \quad \beta = \sum_{m=1}^{M} \beta_m.$$

The Marshak-type boundary conditions ($\partial\Omega$)

$$\begin{bmatrix} J_{0,g}(\boldsymbol{x}) \\ J_{2,g}(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{3}{8} \\ -\frac{3}{8} & \frac{21}{8} \end{bmatrix} \begin{bmatrix} \phi_{0,g}(\boldsymbol{x}) \\ \phi_{2,g}(\boldsymbol{x}) \end{bmatrix},$$

$$J_{i,g}(\boldsymbol{x}) = -D_{i,g} \nabla \phi_{i,g}(\boldsymbol{x}), \quad i = 0, 2.$$

The initial conditions

$$\phi_g(\boldsymbol{x}, 0) = \phi_g^0(\boldsymbol{x}), \quad g = 1, 2, \ldots, G,$$

$$c_m(\boldsymbol{x}, 0) = c_m^0(\boldsymbol{x}), \quad m = 1, 2, \ldots, M.$$

Time approximation

We assume that at the initial time t = 0, the reactor is in steady-state critical condition.

We discretize the time derivatives of equation using finite-difference scheme. We use a fully implicit scheme with time step τ for the time approximation.
For delayed neutron source equation, we use numerical-analytical method

$$c_m^{n+1} = e^{-\lambda_m \tau} c_m^n + \beta_m \int_{t_n}^{t_{n+1}} e^{\lambda_m (t - t^{n+1})} \sum_{g=1}^{G} \nu \Sigma_{fg} \phi_g \, dt, \quad m = 1, 2, \ldots, M.$$

Varitional formulation

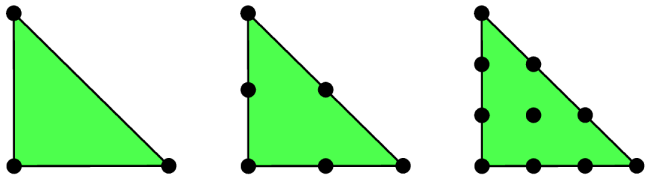
Let's $H^1(\Omega)$ – Sobolev space, $q \in H^1$: q^2 and $|\nabla q|^2$ have a finite integral in Ω. Find $\phi_g^{n+1} \in V^G = [H^1(\Omega)]^G$ such that

$$\int_\Omega \left(\frac{\phi_{0,g}^{n+1} - \phi_{0,g}^n}{v_g \tau} - \frac{2(\phi_{2,g}^{n+1} - \phi_{2,g}^n)}{v_g \tau} \right) q_{2g-1} d\boldsymbol{x} - \int_\Omega D_{0,g} \nabla \phi_{0,g}^{n+1} \nabla q_{2g-1} d\boldsymbol{x}$$
$$+ \int_{\partial\Omega} J_{0,g}^{n+1} q_{2g-1} d\boldsymbol{s} + \int_\Omega (\Sigma_{r,g} \phi_{0,g}^{n+1} - 2\Sigma_{r,g} \phi_{2,g}^{n+1}) q_{2g-1} d\boldsymbol{x}$$
$$= \int_\Omega ((1-\beta)\chi_{n,g} S_n^{n+1} + S_{s,g}^{n+1} + \chi_{d,g} S_d^{n+1}) q_{2g-1} d\boldsymbol{x},$$

$$\int_\Omega \left(-\frac{2(\phi_{0,g}^{n+1} - \phi_{0,g}^n)}{v_g \tau} + \frac{9(\phi_{2,g}^{n+1} - \phi_{2,g}^n)}{v_g \tau} \right) q_{2g} d\boldsymbol{x} - \int_\Omega D_{2,g} \nabla \phi_{2,g}^{n+1} \nabla q_{2g} d\boldsymbol{x}$$
$$+ \int_{\partial\Omega} J_{2,g}^{n+1} q_{2g} d\boldsymbol{s} + \int_\Omega ((5\Sigma_{t,g} + 4\Sigma_{r,g}) \phi_{2,g}^{n+1} - 2\Sigma_{r,g} \phi_{0,g}^{n+1}) q_{2g} d\boldsymbol{x}$$
$$= \int_\Omega (-2(1-\beta)\chi_{n,g} S_n^{n+1} - 2S_{s,g}^{n+1} - 2\chi_{d,g} S_d^{n+1}) q_{2g} d\boldsymbol{x}.$$

Discrete problem

Further, it's necessary to pass from the continuous variational problem to the discrete problem. We introduce finite-dimensional space of finite elements $V_h^G \subset V^G$ 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

$$A_f \phi = b_f,$$

where operator A_f corresponds to the bilinear form, and the vector b_f corresponds to the linear form.

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.

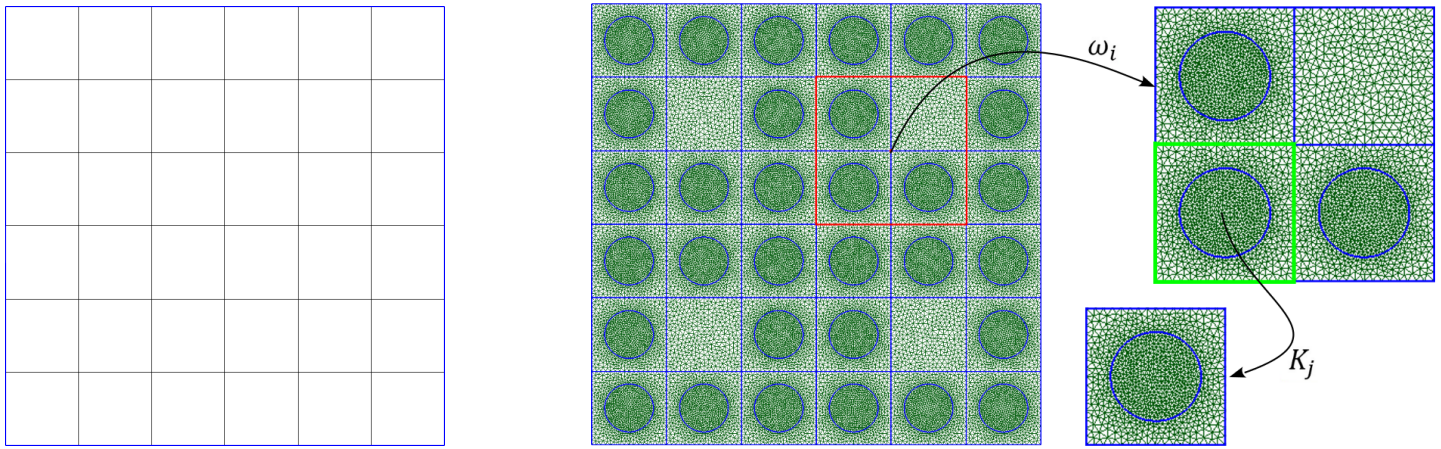


Figure: Coarse grid and local domain ω_i with K_j

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

$$A\varphi^i = \lambda S\varphi^i,$$

where $A = \{a_{ij}\}$ and $S = \{s_{ij}\}$ are defined as folows

$$a_{ij} = \int_{\omega_i} D_{0,g}\nabla\phi_{0,g}\nabla q_{2g-1}d\boldsymbol{x} - \int_{\omega_i}((1-\beta)\chi_{n,g}S_n + S_{s,g} + \chi_{d,g}S_d)q_{2g-1}d\boldsymbol{x} +$$
$$\int_{\omega_i} D_{2,g}\nabla\phi_{2,g}\nabla q_{2g}d\boldsymbol{x} - 2\int_{\omega_i}((1-\beta)\chi_{n,g}S_n + S_{s,g} + \chi_{d,g}S_d)q_{2g}d\boldsymbol{x} +$$
$$\int_{\omega_i}(\Sigma_{r,g}\phi_{0,g} - 2\Sigma_{r,g}\phi_{2,g})q_{2g-1}d\boldsymbol{x} + \int_{\omega_i}((5\Sigma_{t,g} + 4\Sigma_{r,g})\phi_{2,g} - 2\Sigma_{r,g}\phi_{0,g})q_{2g}d\boldsymbol{x},$$
$$s_{ij} = \int_{\omega_i} D_{0,g}\phi_{0,g}q_{2g-1}d\boldsymbol{x} + \int_{\omega_i} D_{2,g}\phi_{2,g}q_{2g}d\boldsymbol{x}.$$

Then, we choose eigenvectors corresponding to dominant M_i eigenvalues 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.

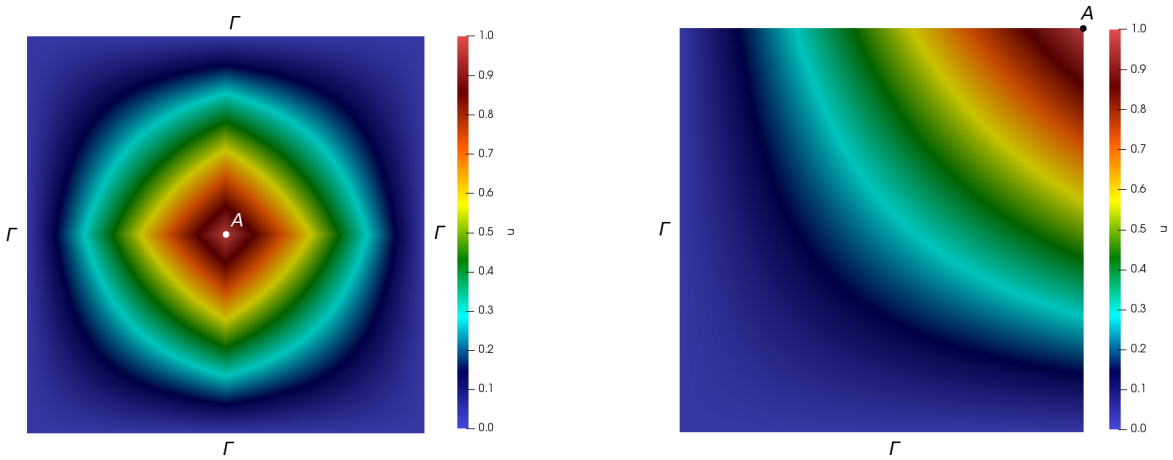


Figure: Partirion of unity functions on the ω_i (right) and K_j (left)

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, we construct the coarse grid approximation

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

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

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

Software

Small PWR 2D

Let's consider one-group 2D test problem for small PWR reactor.

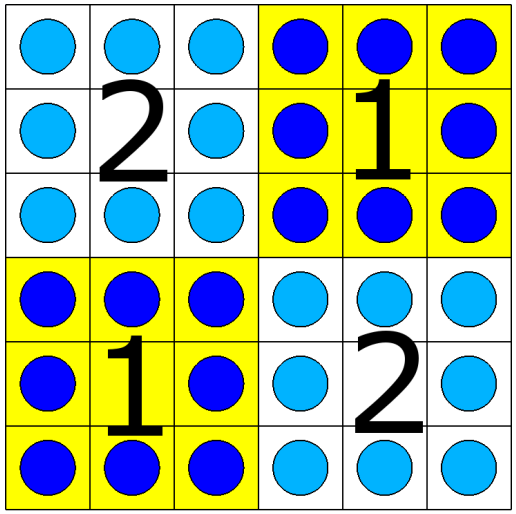


Figure: Geometrcial model of the small PWR-2D reactor core

The diameter of the fuel rod 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 condition is set. 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.

Scenario

Let's define the next scenario of the process:

- Solve the λ-spectral problem;
- As the initial condition, take the solution of the λ-spectral problem;
- At time $t = 0.1$ sec, change the removal cross-section Σ_r for fuel in zone 1 by $+2\%$ (simulation of immersion of control rods);
- At time $t = 0.3$ sec, change the removal cross-section Σ_r for fuel in zone 1 by -3% (simulation of withdrawal of control rods).

At each time step, we calculate the integrated power as

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

where a is the normalization coefficient.

Fine grid solution

The fine grid contains 115891 vertices. The calculation goes up to time $T = 0.4$ sec. The time step for both grids is $\tau = 0.001$. We take a fine-grid solution as an exact solution. The initial value of K_{eff} is 1.18398.

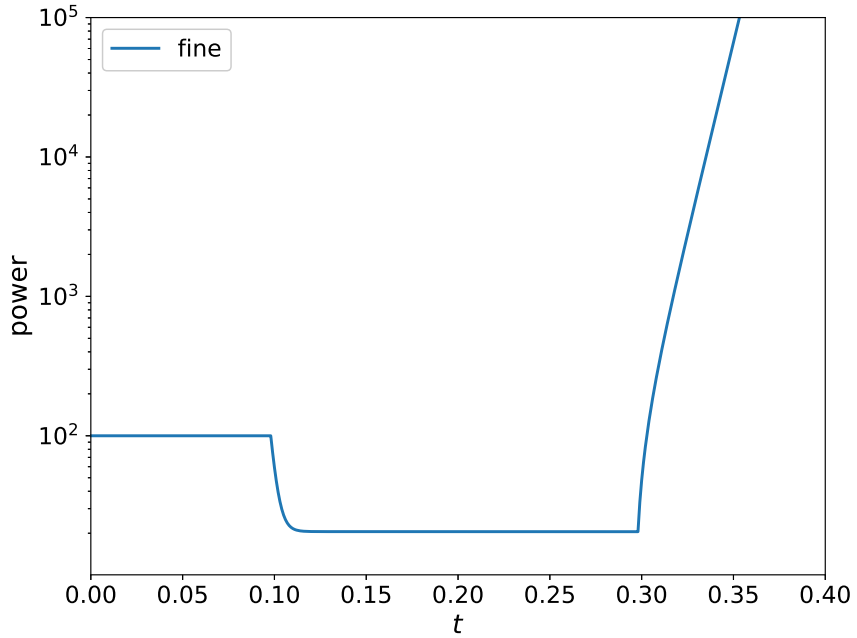


Figure: Integral power on the fine grid.

Coarse grid solution

The coarse grid contains 49 vertices. When using 4 or less multiscale basis functions, the error is more than 10% and for using 16 or more multiscale basis functions, the error it does not exceed 1%.

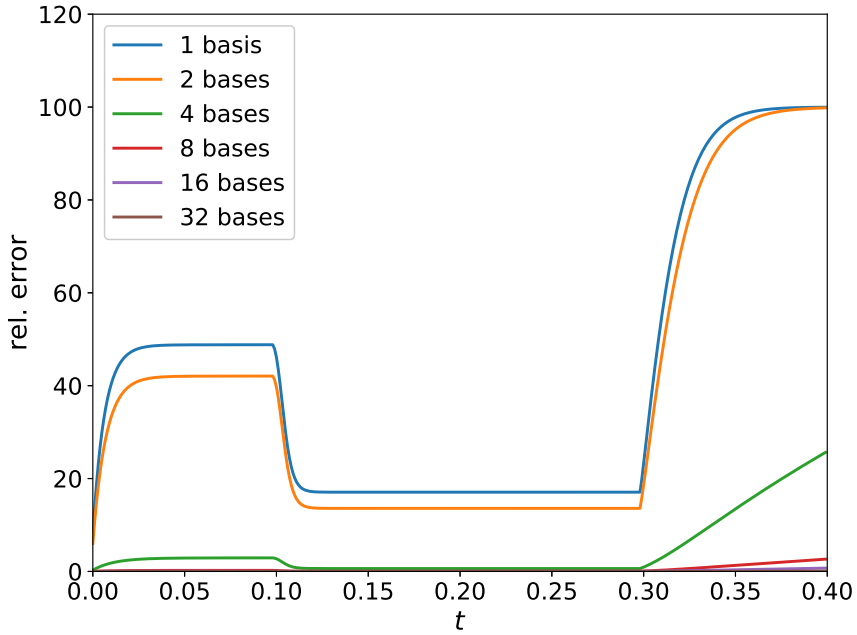
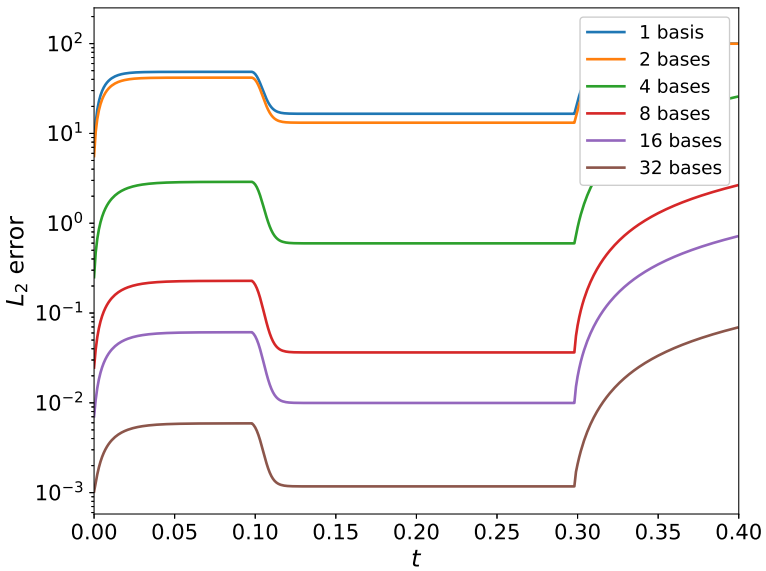
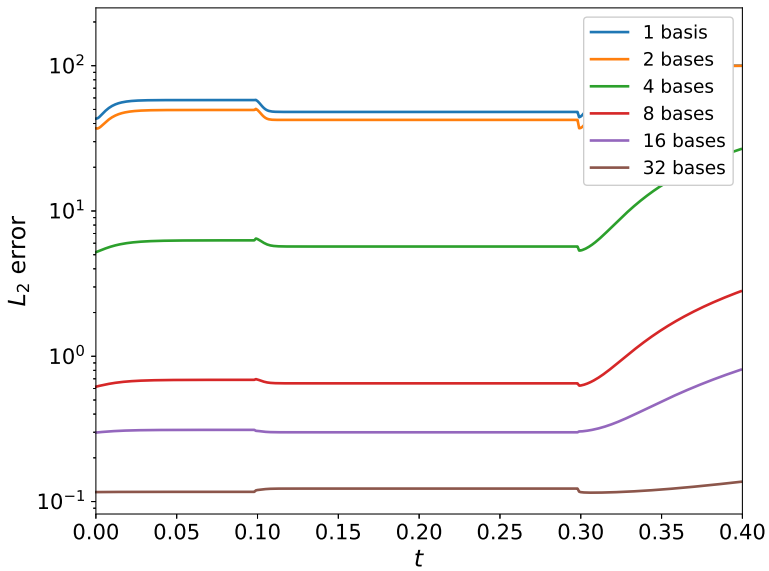


Figure: Relative errors (%) of the multiscale solution power.

L_2 error



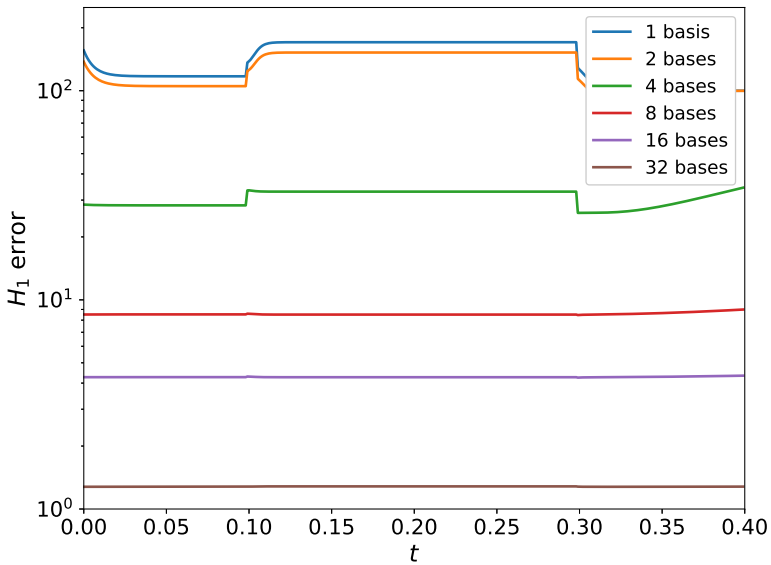
(a) pseudo 0th moment



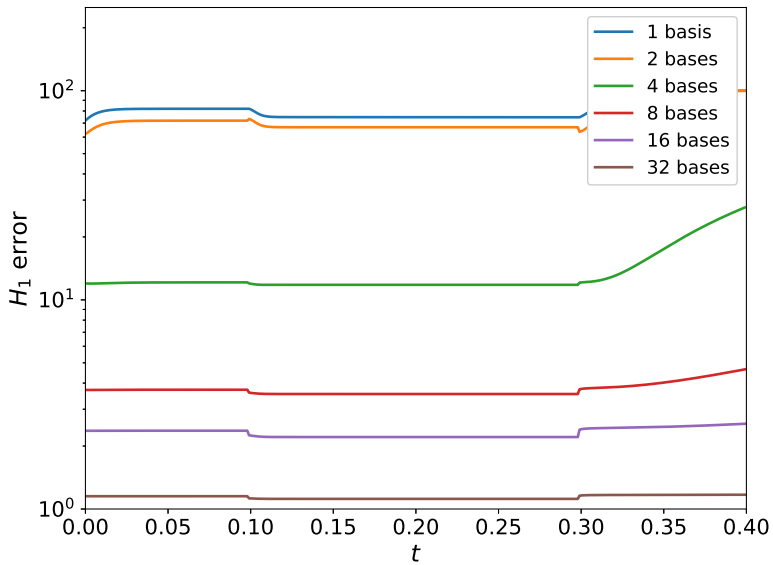
(b) second moment

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

H_1 error



(a) pseudo 0th moment



(b) second moment

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

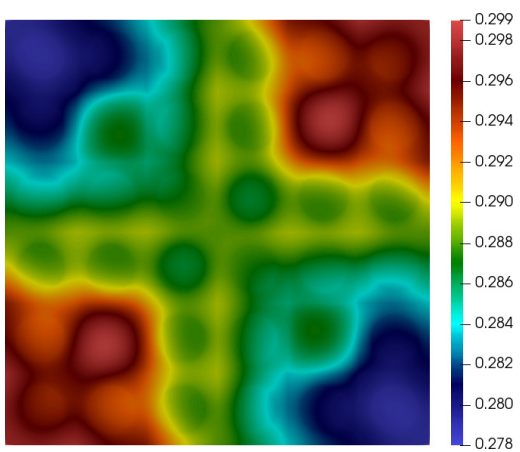
Errors at final time

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

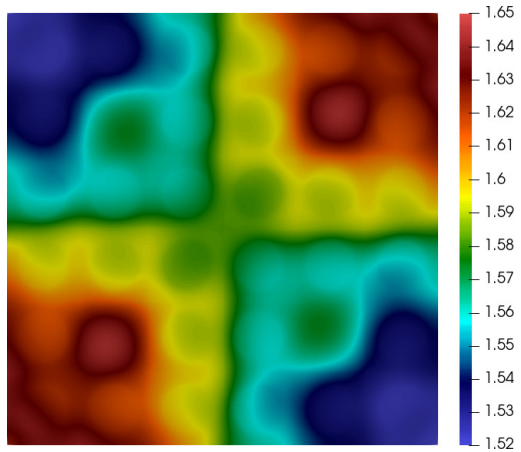
Bases	DOF	Pseudo 0th moment		Second moment		Calc time
		L_2 error	H_1 error	L_2 error	H_1 error	
1	49	99.97	99.99	99.97	99.99	0.03
2	98	99.83	99.90	99.84	99.90	0.05
4	196	25.61	34.38	26.65	27.64	0.10
8	392	2.64	8.99	2.80	4.65	0.35
16	784	0.71	4.34	0.81	2.56	1.15
32	1568	0.07	1.28	0.14	1.17	6.66
fine	115891	–	–	–	–	815.00

Calculations indicate that it is necessary to make use of 8 or more multiscale basis functions.

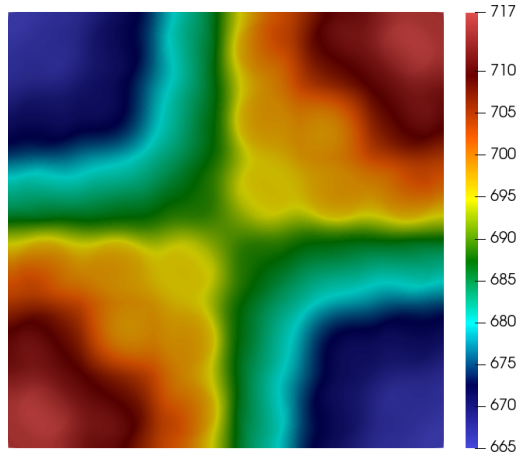
Multiscale solutions at final time $\phi_{ms_{0,1}}$



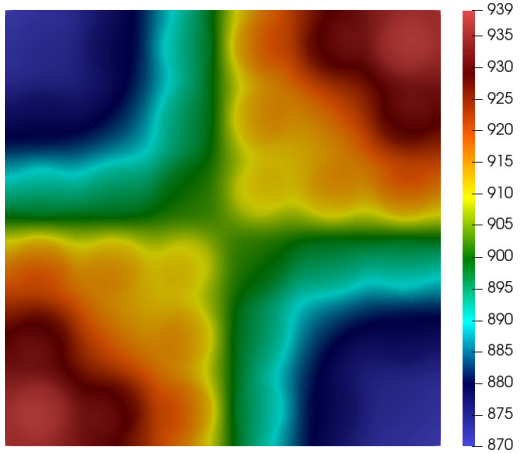
(a) 1 basis



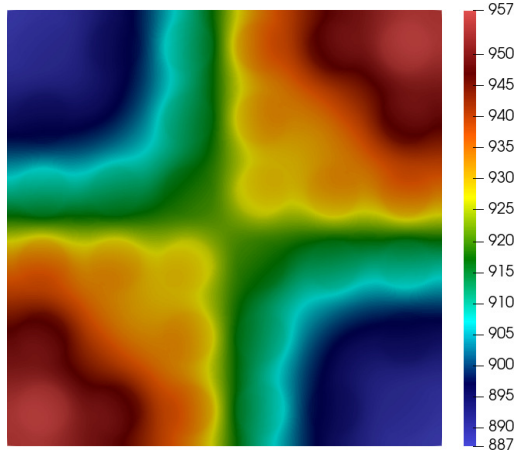
(b) 2 bases



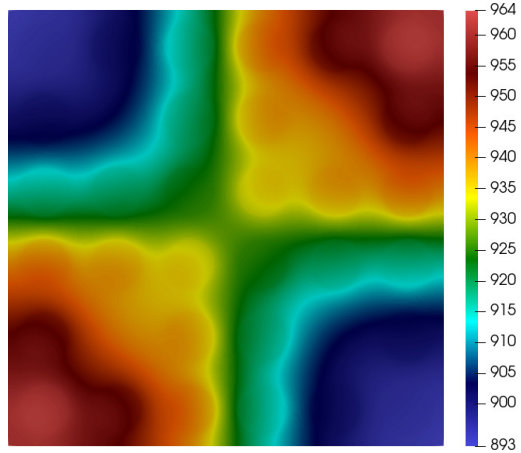
(c) 4 bases



(d) 8 bases



(e) 16 bases



(f) 32 bases

TWIGL 2D

The two-group transport test TWIGL-2D is considered.

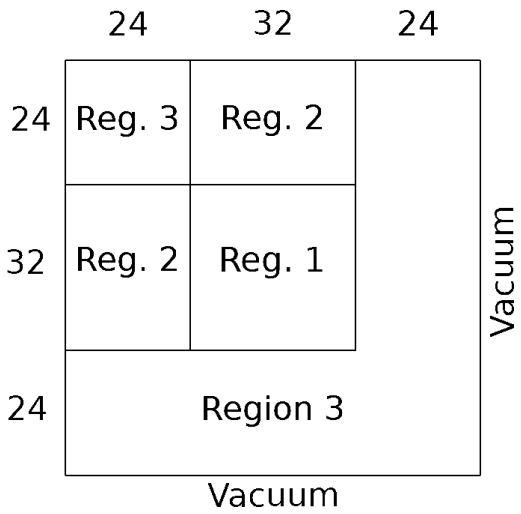


Figure: Geometrcial model of the small PWR-2D reactor core

One fourth of the reactor core is modeled. The fission spectrum $\chi_1 = 1$, $\chi_2 = 0$. One group of delayed neutrons with effective fraction $\beta = 0.0075$ and decay constant $\lambda = 0.08\ \mathrm{s}^{-1}$. Neutron velocity $v_1 = 10^7$ cm/s and $v_2 = 2 \cdot 10^5$ cm/s.

Scenario

Dynamic process scenario:

- Solve the λ-spectral problem;
- As the initial condition, take the solution of the λ-spectral problem;
- At time $t = 0$ sec, change the removal cross-section $\Sigma_{r,2}$ for region 1 by 0.0035 cm^{-1} (simulation of withdrawal of control rods).

Fine grid solution

The fine grid contains 25921 vertices. The calculation goes up to time $T = 0.5$ sec. The time step for both grids is $\tau = 0.0001$. As an exact solution, we take the fine-grid solution. The initial value of K_{eff} is 0.916075.

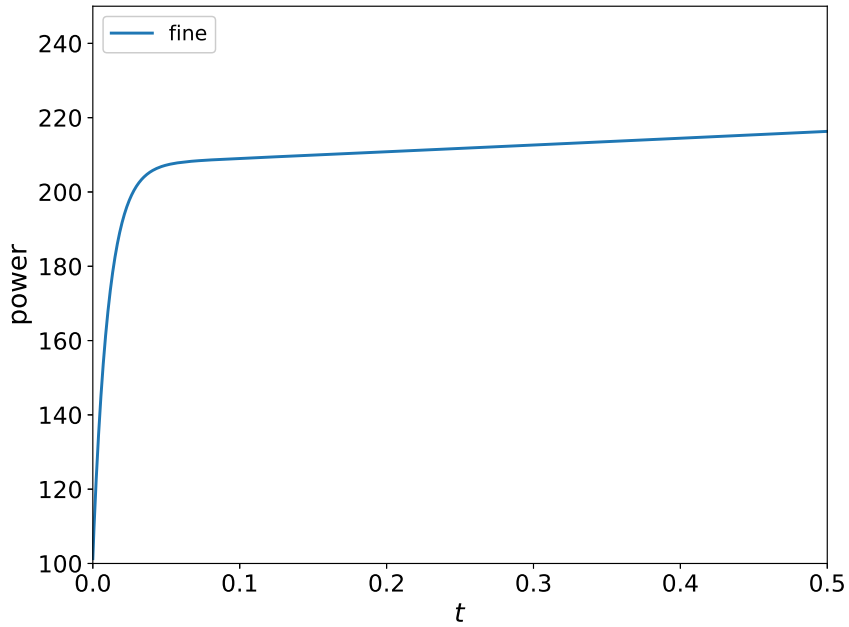


Figure: Integral power on the fine grid.

Coarse grid solution

The coarse grid contains 121 vertices. When using using 4 or more multiscale basis functions, the error it does not exceed 3%.

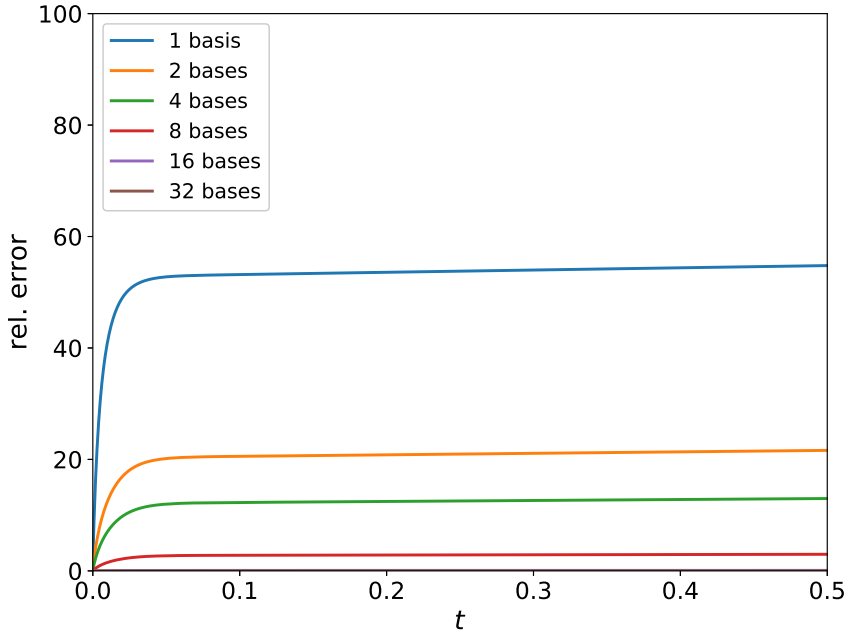
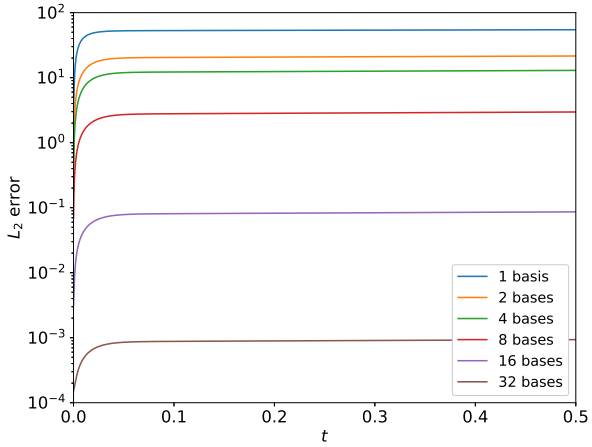
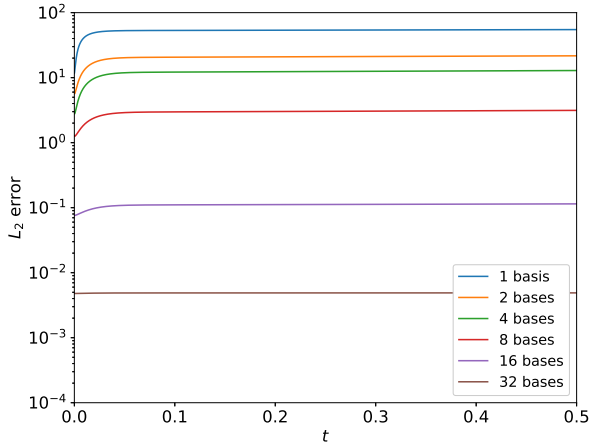


Figure: Relative errors (%) of the multiscale solution power.

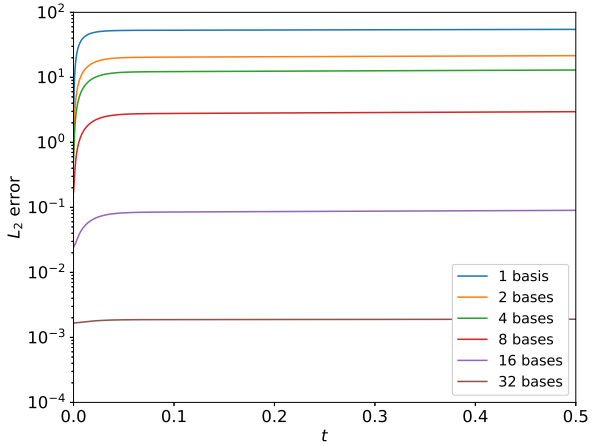
L_2 error



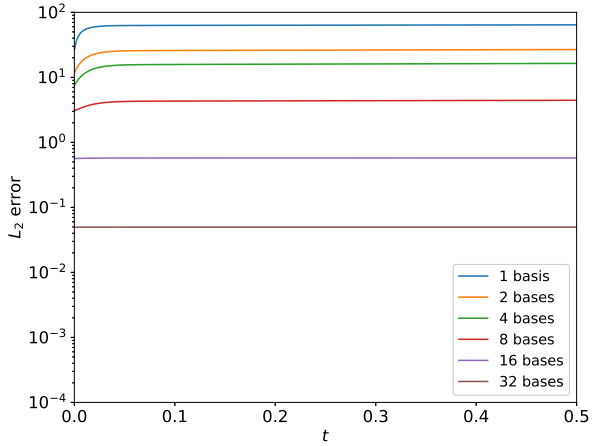
(a) $\phi ms_{0,1}$



(b) $\phi ms_{2,1}$



(c) $\phi ms_{0,2}$



(d) $\phi ms_{2,2}$

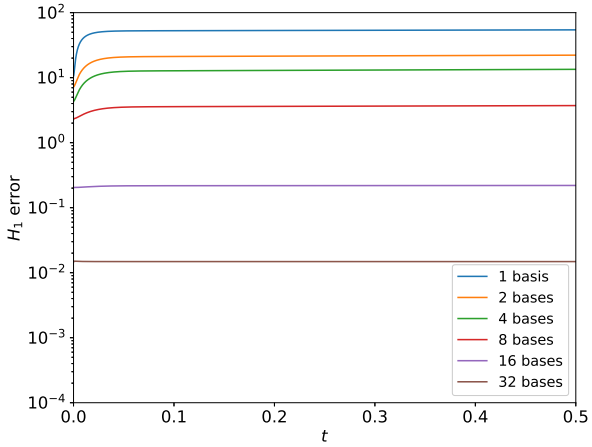
L_2 errors at final time

Table: Relative L_2 errors (%) of the solution at final time.

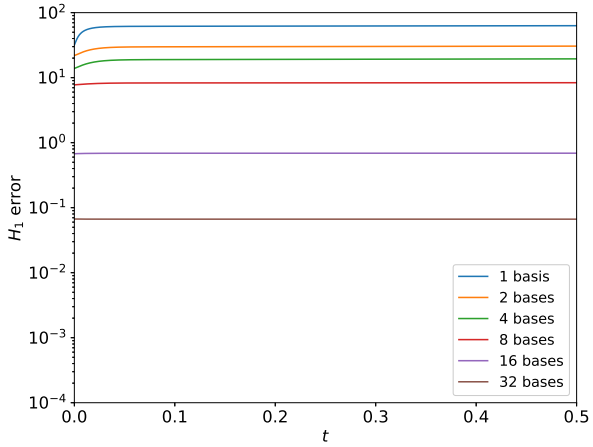
Bases	DOF	L_2 error				Calc time
		$\phi_{ms_{0,1}}$	$\phi_{ms_{2,1}}$	$\phi_{ms_{0,2}}$	$\phi_{ms_{2,2}}$	
1	121	54.64	54.88	54.70	64.23	1.70
2	242	21.55	21.69	21.55	26.80	4.15
4	484	12.93	12.88	12.96	16.39	12.61
8	968	2.97	3.14	2.96	4.44	45.12
16	1936	0.09	0.11	0.09	0.06	165.36
32	3872	0.00	0.00	0.00	0.05	690.30
fine	25921	–	–	–	–	6590.00

Calculations indicate that it is necessary to make use of 8 or more multiscale basis functions.

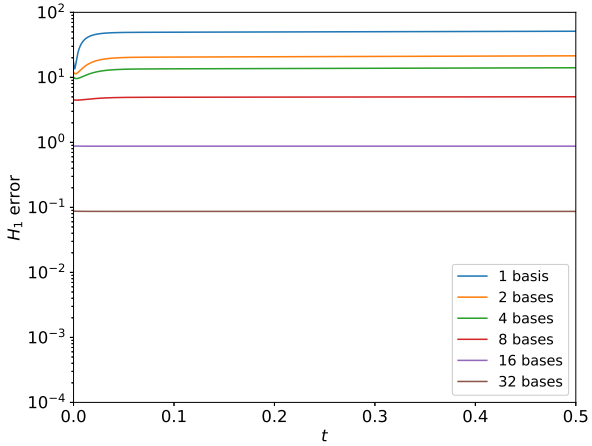
H_1 error



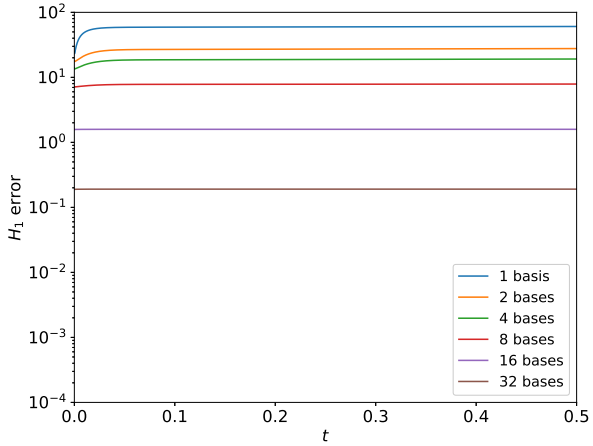
(a) $\phi ms_{0,1}$



(b) $\phi ms_{2,1}$



(c) $\phi ms_{0,2}$



(d) $\phi ms_{2,2}$

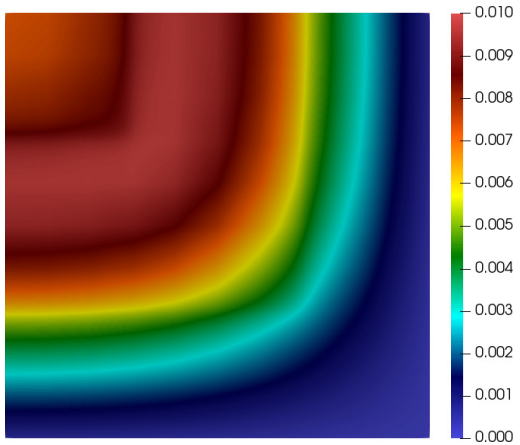
H_1 errors at final time

Table: Relative H_1 errors (%) of the solution at final time.

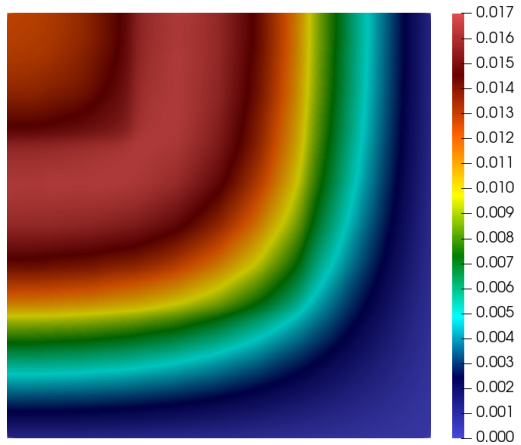
Bases	DOF	H_1 error				Calc time
		$\phi_{ms_{0,1}}$	$\phi_{ms_{2,1}}$	$\phi_{ms_{0,2}}$	$\phi_{ms_{2,2}}$	
1	121	54.38	63.02	51.19	60.59	1.70
2	242	22.19	30.57	21.44	27.71	4.15
4	484	13.43	19.46	14.05	19.14	12.61
8	968	3.72	8.36	5.03	7.88	45.12
16	1936	0.22	0.69	0.87	1.59	165.36
32	3872	0.01	0.07	0.09	0.19	690.30
fine	25921	–	–	–	–	6590.00

Calculations indicate that it is necessary to make use of 8 or more multiscale basis functions.

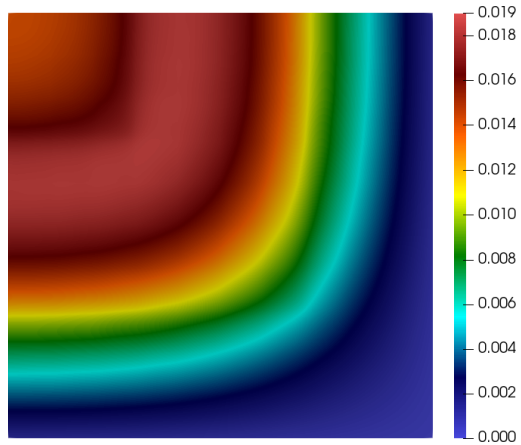
Multiscale solutions at final time ($\phi_{ms_{0,1}}$)



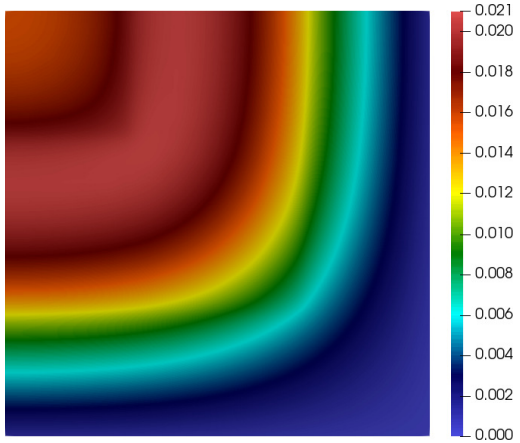
(a) 1 basis



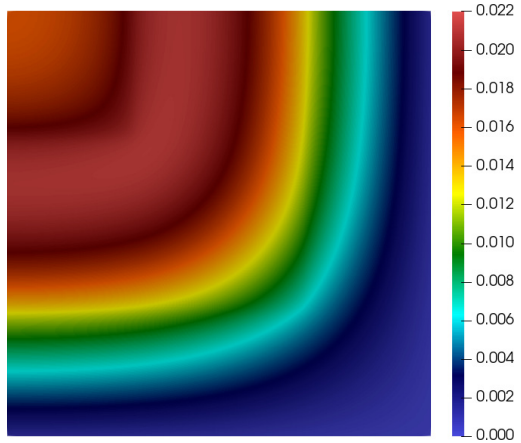
(b) 2 bases



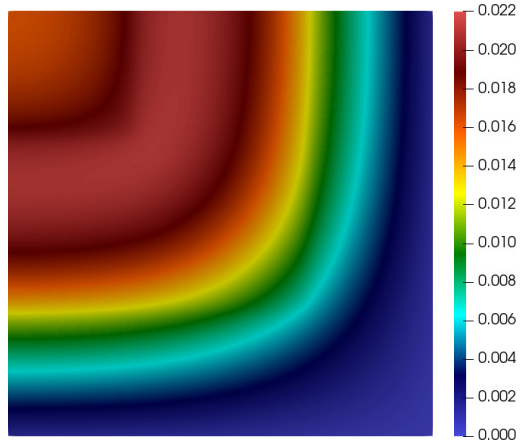
(c) 4 bases



(d) 8 bases



(e) 16 bases



(f) 32 bases

Conclusion and future work

A Generalized Multiscale Finite Element method was developed successfully for modelling neutron transport in SP_3 approximation. 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 a popular and simple 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 P_N approximation.


Thank you for your attention!