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 MHPCMP, September 9-12, 2020 Sochi

Introduction

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

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

Here $\phi(\boldsymbol{x}, t)$ is the neutron flux at point $\boldsymbol{x}$ and time t, v is the effective neutron velocity, $D(\boldsymbol{x})$ is the diffusion coefficient, $\Sigma_r(\boldsymbol{x}, t)$ is the removal cross-section, $\Sigma_f(\boldsymbol{x}, t)$ 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 $\partial\Omega$:

$$D\frac{\partial \phi}{\partial n} + \gamma\phi = 0, \qquad (2)$$

where n is an outer normal to the boundary $\partial\Omega$, γ is the albedo constant. Let's propose that at the initial time $\mathrm{t} = 0$, the reactor is in steady-state critical condition

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

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

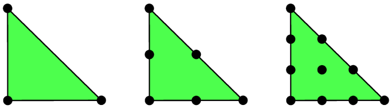
To specify the variational formulation, we multiply equations by the test function q and integrate over the domain Ω. Using the integration by parts, we obtain the following variational formulation: let's find $\phi^{n+1} \in V$ such that

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

where $V = H^1(\Omega)$ is the Sobolev space consisting of scalar functions υ such that υ^2 and $|\nabla \upsilon^2|$ 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.



Time step selection algorithm

1. Predictable time step: $\widetilde{\tau}^{n+1} = \gamma \tau^n$ (eg $\gamma = 1.25$)
2. Predictive solution $\widetilde{y}^{n+1}$: an explicit scheme, $\widetilde{t}^{n+1} = t^n + \widetilde{\tau}^{n+1}$
3. Estimation of approximation error: by found $\widetilde{y}^{n+1}$ from an implicit scheme
4. Step selection τ^{n+1}: $\|\psi^{n+1}\| \approx \delta$
5. Solution on a new time layer y^{n+1}: an implicit scheme, $t^{n+1} = t^n + \tau^{n+1}$

Neutron diffusion equation

One group diffusion approximation with one group delayed neutron sources

$$\frac{1}{v}\frac{\partial \phi}{\partial t} - \nabla \cdot D\nabla\phi + \Sigma_a\phi = (1-\beta)\nu\Sigma_f\phi + \lambda c,$$
$$\frac{\partial c}{\partial t} + \lambda c = \beta\nu\Sigma_f\phi.$$

Boundary condition

$$D\frac{\partial \phi}{\partial n} + \gamma_a\phi = 0.$$

Initial conditions

$$\phi(0) = \phi^0, \; c(0) = c^0.$$

Calculated formulas

Denote vectors and matrix $\boldsymbol{\varphi} = \{\varphi, s\}$, $\boldsymbol{\psi} = \{\psi_1, \psi_2\}$,

$$A = \begin{pmatrix} -\nabla \cdot D\nabla + \Sigma_a - (1-\beta)\nu\Sigma_f - \lambda & 0 \\ 0 & \lambda - \beta\nu\Sigma_f \end{pmatrix}.$$

The approximation error

$$\begin{aligned} \widetilde{\boldsymbol{\psi}}^{\boldsymbol{n+1}} &= (A^{n+1} - A^n)\boldsymbol{\varphi}^{\boldsymbol{n}} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{\boldsymbol{n+1}} - \boldsymbol{\varphi}^{\boldsymbol{n}}) \\ &= \widetilde{\tau}^{n+1}\left(\frac{A^{n+1} - A^n}{\widetilde{\tau}^{n+1}}\boldsymbol{\varphi}^{\boldsymbol{n}} + A^{n+1}\frac{\widetilde{\boldsymbol{\varphi}}^{\boldsymbol{n+1}} - \boldsymbol{\varphi}^{\boldsymbol{n}}}{\widetilde{\tau}^{n+1}}\right). \end{aligned}$$

We match error $\widetilde{\boldsymbol{\psi}}^{n+1}$ with step $\widetilde{\tau}^{n+1}$, and $\boldsymbol{\psi}^{n+1}$ with step τ^{n+1}:

$$\widetilde{\tau}^{n+1} = \gamma_{n+1}\tau^n, \quad \gamma_{n+1} = \frac{\delta}{\|\widetilde{\boldsymbol{\psi}}^{n+1}\|}\gamma.$$

The needed time step

$$\tau^{n+1} \le \bar{\tau}^{n+1}, \quad \tau^{n+1} \le \widetilde{\tau}^{n+1}, \quad \tau^{n+1} = \max\left\{\tau^0, \min\{\gamma_{n+1}, \gamma\}\tau^n\right\}.$$

The approximation error has the first order in time

$$\widetilde{\psi}^{\boldsymbol{n+1}} = \mathcal{O}(\widetilde{\tau}_{n+1}).$$

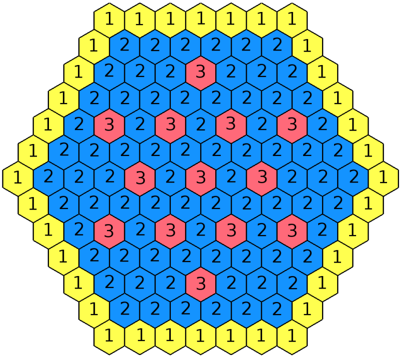
In view of this, we set

$$\|\widetilde{\psi}^{\boldsymbol{n+1}}\| \le \|(A^{n+1} - A^n)\boldsymbol{\varphi}^{\boldsymbol{n}} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{\boldsymbol{n+1}} - \boldsymbol{\varphi}^{\boldsymbol{n}})\|.$$

Calculated formula for time step

$$\gamma_{n+1} = \frac{\delta}{\|(A^{n+1} - A^n)\boldsymbol{\varphi}^{\boldsymbol{n}} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{\boldsymbol{n+1}} - \boldsymbol{\varphi}^{\boldsymbol{n}})\|}\gamma.$$

IAEA-2D benchmark



- Without reflector
- One group of *instantaneous* and *delayed* neutrons
- Modeling effect of *immersion* or *extraction* of control rods

Scenario

Define the scenario of process:

1. The spectral problem is solved (initial condition);
2. Calculation for the non-stationary model in the range 0 to 0.5 sec;
3. At a moment of 0.1 sec the value Σ_a for the zone 3 changes to $\pm$ 0.000625.

Software

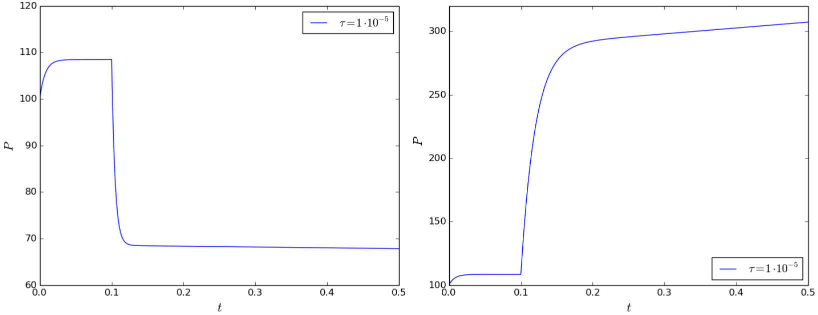
gmsh

SLEPc

FEniCS project

python™

Nuclear power

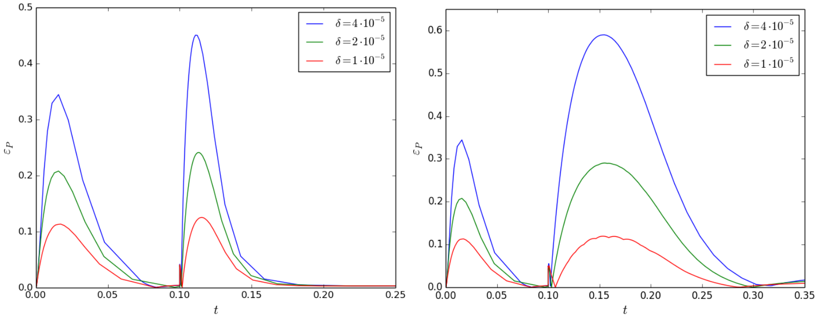


Nuclear power for immersion (left) and extraction (right).

$$P(t) = a \sum_{g=1}^{G} \int_{\Omega} \Sigma_{fg} \phi_g d\boldsymbol{x},$$

where a – normalization factor.

Error

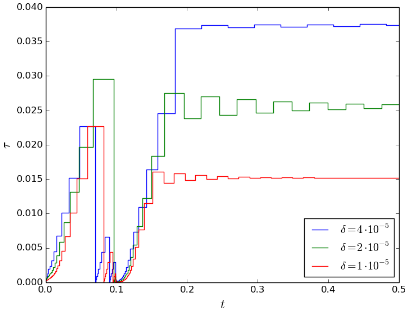


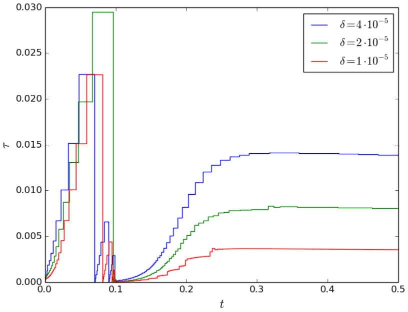
Error for immersion (left) and extraction (right).

$$\epsilon_P(t) = |P_{ref} - P|,$$

where P_{ref} – reference solution.

Time step





Time steps for immersion (left) and extraction (right).

Counting time and number of steps

	immersion			extraction		
δ	$\max(\epsilon_P)$	n	t, sec	$\max(\epsilon_P)$	n	t, sec
$4 \cdot 10^{-5}$	0.450	136	16	0.590	241	35
$2 \cdot 10^{-5}$	0.241	159	20	0.290	373	62
$1 \cdot 10^{-5}$	0.125	270	37	0.120	773	145

Reference solution: fixed time step 10^{-5}, number of steps – 50000, counting time – 2130 sec.

Acknowledgements

This work was supported by the Russian Foundation for Basic Research (grants 16-08-01215 and 18-31-00315) and by the grant of the Russian Federation Government 14.Y26.31.0013.

Conclusion

- An algorithm for automatic time step selection for numerical solution of neutron diffusion problems has been developed.
- The solution is obtained using guaranteed stable implicit schemes, and the step choice is performed with the use of the solution obtained by an explicit scheme.
- Calculation results obtained for a neutron diffusion problems demonstrate reliability of the proposed algorithm for time step choice.

Thank you for your attention!