Automatic Time Step Selection for Numerical Solution of Neutron Diffusion Problems

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Introduction

In computational practice two-layer schemes are mostly used, compared with three-layered and multilayered schemes which are not so often used. The problem of controlling the time step is relatively well worked out for an approximate solution of the Cauchy problem for systems of differential equations.

The main approach is that the error of the approximate solution is estimated at a new time step on the basis of additional calculations. The step is estimated from the theoretical asymptotic dependence of the accuracy on time step and after that correction of step is applied, if necessary, the calculations are repeated.

The algorithm takes into account the features of neutron diffusion problems, for instance, fast changes in the solution or instability with respect to the initial data.

Problem description

Consider second-order parabolic equation

$$\frac{\partial u}{\partial t} - \sum_{\alpha=1}^{m} \frac{\partial}{\partial x_\alpha}\left(k(\boldsymbol{x},t)\frac{\partial u}{\partial x_\alpha}\right) + s(\boldsymbol{x},t)u = f(\boldsymbol{x},t), \quad \boldsymbol{x} \in \Omega, \quad 0 < t \le T,$$

where $\underline{k} \le k(\boldsymbol{x}) \le \overline{k}$, $\boldsymbol{x} \in \Omega$, $\underline{k} > 0$.

Boundary condition

$$u(\boldsymbol{x},t) = g(\boldsymbol{x},t), \quad \boldsymbol{x} \in \partial\Omega, \quad 0 < t \le T.$$

Initial condition

$$u(\boldsymbol{x},0) = u^0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega.$$

Operator notation

Cauchy problem

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Assume $A(t) \geq 0$ in H then

$$\|u(t)\| \leq \|u_0\| + \int_0^t \|f(\theta)\| d\theta.$$

Solution evaluation

Introduce irregular time grid

$$t^0 = 0, \quad t^{n+1} = t^n + \tau^{n+1}, \quad n = 0, 1, ..., N-1, \quad t^n = T.$$

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$$\frac{y^{n+1} - y^n}{\tau^{n+1}} + A^{n+1} y^{n+1} = f^{n+1}, \quad n = 0, 1, ..., N-1,$$

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Layerwise estimate $(A^{n+1} \geq 0)$

$$\|y^{n+1}\| \leq \|y^n\| + \tau^{n+1} \|f^{n+1}\|.$$

Difference estimate

$$\|y^{n+1}\| \leq \|u^0\| + \sum_{k=0}^{n} \tau^{k+1} \|f^{k+1}\|.$$

Solution error

For $z^n = y^n - u^n$:

$$\frac{z^{n+1} - z^n}{\tau^{n+1}} + A^{n+1} z^{n+1} = \psi^{n+1}, \quad n = 0, 1, ..., N-1,$$

$$z^0 = 0.$$

Approximation error

$$\psi^{n+1} = f^{n+1} - \frac{u^{n+1} - u^n}{\tau^{n+1}} - A^{n+1} u^{n+1}.$$

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$$\|z^{n+1}\| \le \sum_{k=0}^{n} \tau^{k+1} \|\psi^{k+1}\|.$$

Then we obtain

$$\|z^{n+1}\| \le \delta t^{n+1}.$$

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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

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

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

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

The needed time step

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

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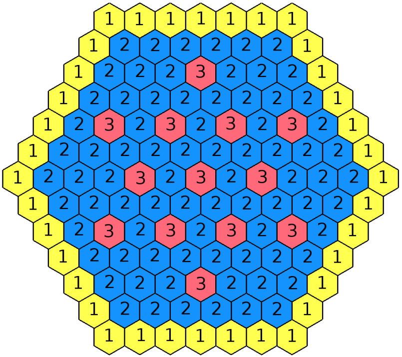
In view of this, we set

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

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);

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3. At a moment of 0.1 sec the value Σ_a for the zone 3 changes to $\pm$ 0.000625.

Software

gmsh

Software

gmsh

SLEPc

FEniCS project

Software

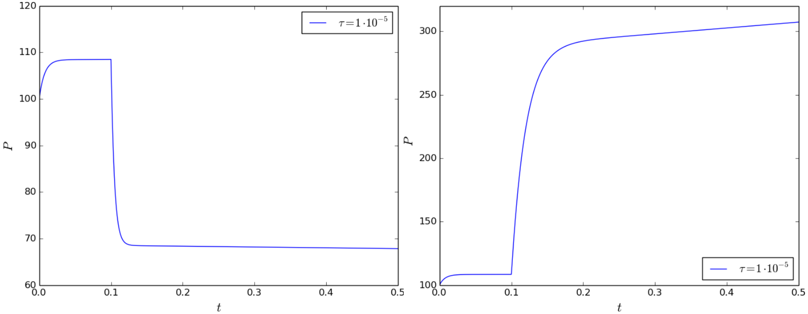
gmsh

SLEPc

FEniCS project

python™

Nuclear power

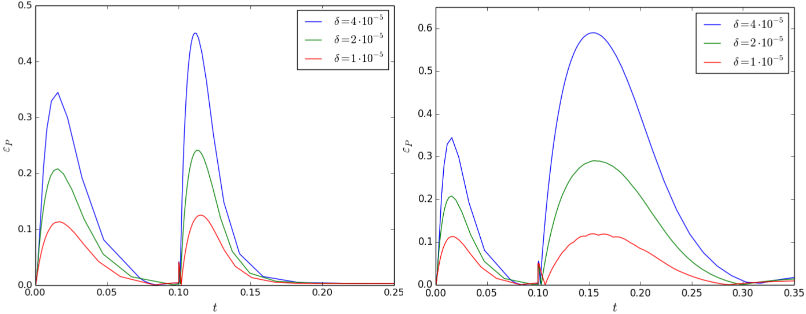


Nuclear power for immersion (left) and extraction (right).

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

where a – normalization factor.

Error

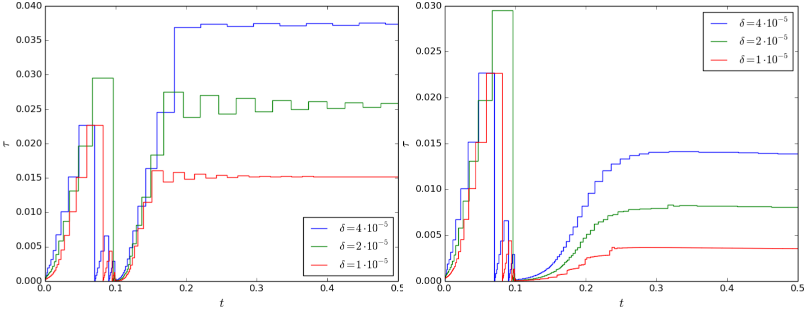


Error for immersion (left) and extraction (right).

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

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.

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.

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Thank you for your attention!