Automatic Time Step Selection for Numerical Solution of Neutron Diffusion Problems

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Introduction

Problem description

Consider second-order parabolic equation

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

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Initial condition

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

Operator notation

Cauchy problem

$$\frac{du}{dt} + A(t)u = f(t), \quad 0 < t \leq T,$$

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

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

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

Difference estimate

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

Solution error

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

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

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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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Difference estimate

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

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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

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

Initial conditions

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

Calculated formulas

The approximation error

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

Error $\widetilde{\boldsymbol{\psi}}^{n+1}$ compare with $\widetilde{\tau}^{n+1}$, and $\boldsymbol{\psi}^{n+1}$ with step τ^{n+1}:

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

Where $\boldsymbol{\varphi}^{\boldsymbol{n}} = \{\varphi^n, s^n\}$, $\boldsymbol{\psi}^{\boldsymbol{n+1}} = \{\psi_1^{n+1}, \psi_2^{n+1}\}$, $\widetilde{\boldsymbol{\psi}}^{\boldsymbol{n+1}} = \{\widetilde{\psi}_1^{n+1}, \widetilde{\psi}_2^{n+1}\}$,

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

The 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

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

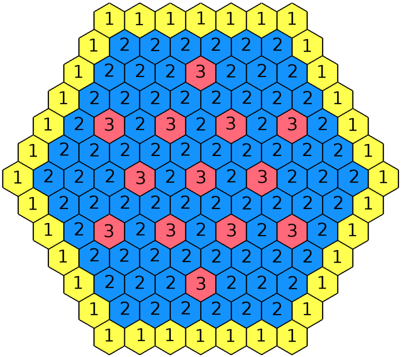
In view of this, we set

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

Calculated formula for time step

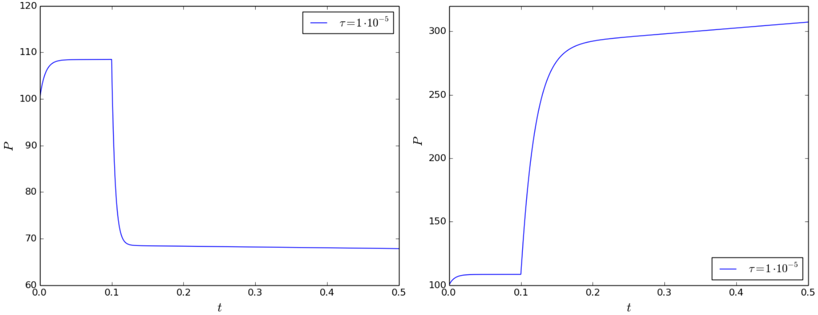
$$\gamma_{n+1} = \frac{\delta}{\|(A^{n+1} - A^n)\boldsymbol{\varphi}^{\boldsymbol{n}} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{\boldsymbol{n+1}} - \boldsymbol{\varphi}^{\boldsymbol{n}})\|}\gamma.$$

IAEA-2D benchmark



- One group of instantaneous neutrons
- One group of delayed neutrons
- Modeling effect of immersion or extraction of control rods

Nuclear power

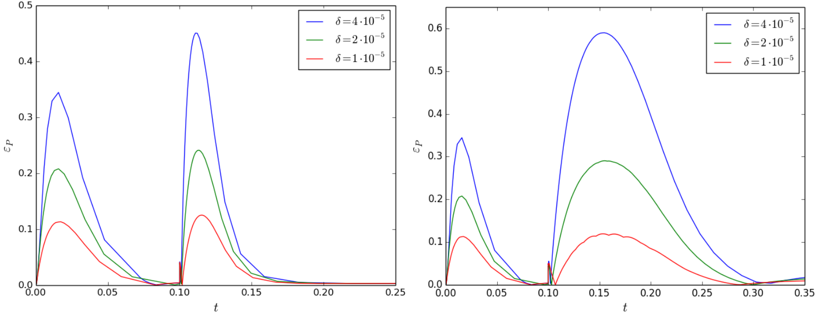


Nuclear power for immersion (left) and extraction (right).

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

where a – normalization factor.

Error



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

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

where P_{ref} – reference solution.

Software

gmsh

Software

gmsh

SLEPc

Software

gmsh

SLEPc

FEniCS project

Software

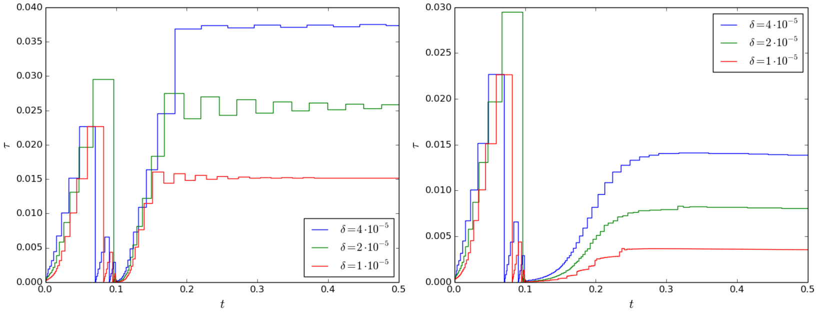
gmsh

SLEPc

FEniCS project

python™

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.

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Thank you for your attention!