Automatic Time Step Selection for Numerical Solution of Neutron Diffusion Problems

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Introduction

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Problem description

Consider second-order parabolic equation

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

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

Boundary condition

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

Initial condition

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

Operator notation

Cauchy problem

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

with initial condition

$$u(0) = u_0.$$

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

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

Implicit scheme are used

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

and initial condition $y^0 = u^0$.
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

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

Layerwise estimate

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

Difference estimate

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

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

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

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

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

The approximation error has the first order in time

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

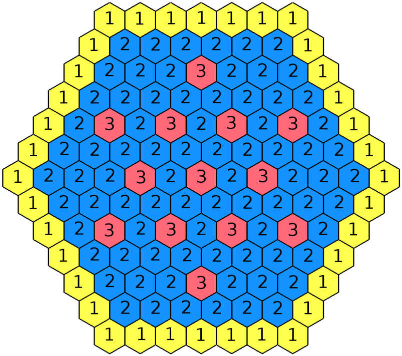
In view of this, we set

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

Calculated formula for time step

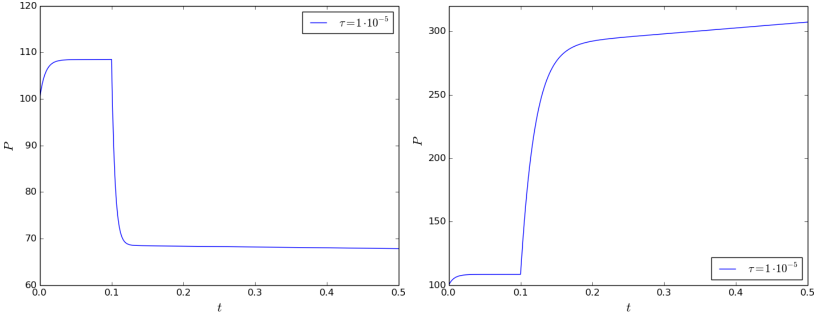
$$\gamma_{n+1} = \frac{\delta}{\|(A^{n+1} - A^n)\boldsymbol{\varphi}^{\boldsymbol{n}} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{\boldsymbol{n+1}} - \boldsymbol{\varphi}^{\boldsymbol{n}})\|}\gamma.$$

IAEA-2D benchmark



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

Nuclear power

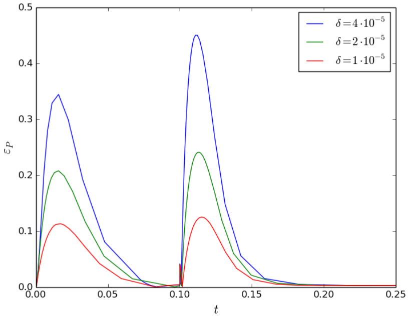


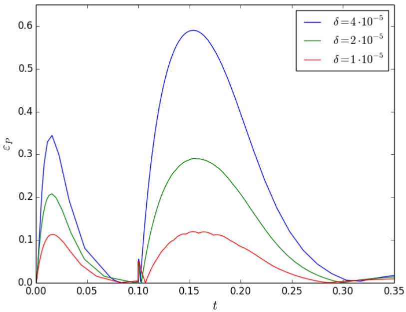
Nuclear power for immersion (left) and extraction (right).

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

where a – normalization factor.

Error



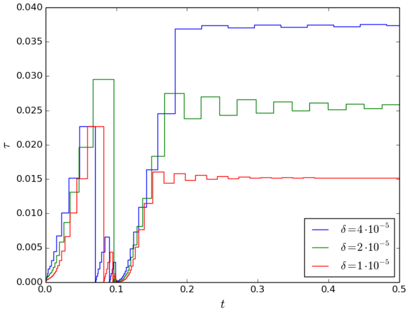


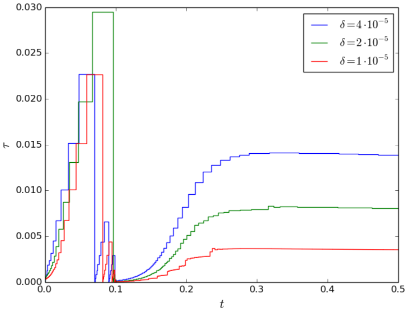
Error for immersion (left) and extraction (right).

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

where P_{ref} – reference solution.

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 .

Conclusion

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Thank you for your attention!