Automatic Time Step Selection for Numerical Solution of Neutron Diffusion Problems

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Abstract. An automatic algorithm of time step control for solving the boundary value problems for nonstationary parabolic equations is presented. The solution is obtained using complete stable implicit schemes, and the time step is evaluated using of the explicit scheme solution. The time step evaluation formulas are derived using the estimation of the approximation error at next time step. Calculation results obtained for several neutron diffusion problems demonstrate reliability of the proposed algorithm for time step control.

Keywords: Time step selection · Parabolic equation · Approximation error · Neutron diffusion

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1 Introduction

For the second order parabolic equations unconditionally stable schemes are constructed on the basis of implicit approximations [1]. 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 the time step control is relatively well developed for the Cauchy problem solution of differential equations systems [2]. The basic approach is to use additional calculations at a new time step to estimate the approximate solution. The time step is estimated using the theoretical asymptotic dependence of the accuracy on time step [3]. The algorithm takes into account the features of neutron diffusion problems [7], for instance, fast changes in the solution or instability with respect to the initial data. The proposed algorithm allows a gain in CPU time with respect to the fine mesh calculation at the same calculation accuracy.

2 Problem Description

Consider the Cauchy problem for the linear equation

$$\frac{du}{dt} + A(t)u = f(t), \quad 0 < t \leq T, \tag{1}$$

with initial condition $u(0) = u^0$.

The problem is considered in a finite-dimensional Hilbert space. We assume that $A(t) \geq 0$. Let's use an irregular time grid

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

For approximate solution the implicit scheme are used

$$\frac{y^{n+1} - y^n}{\tau^{n+1}} + A^{n+1}y^{n+1} = f^{n+1}, \quad n = 0, 1, ..., N-1, \tag{2}$$

and initial condition $y^0 = u^0$. For the approximate solution we can use the following estimate

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

Then we can obtain a difference analogue of the estimate

$$\|y^{n+1}\| \leq \|u^0\| + \sum_{k=0}^{n} \tau^{k+1}\|f^{k+1}\| \tag{3}$$

for problem (2). For the error of the approximate solution $z^n = y^n - u^n$ we have

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

Here ψ^{n+1} is approximation error

$$\psi^{n+1} = f^{n+1} - \frac{u^{n+1} - u^n}{\tau^{n+1}} - A^{n+1}u^{n+1}. \tag{4}$$

Similarly (3) we have an estimate for the error

$$\|z^{n+1}\| \leq \sum_{k=0}^{n} \tau^{k+1}\|\psi^{k+1}\|. \tag{5}$$

Checking the error we can focus on the total error $\delta\tau^{n+1}$ in interval $t^n < t < t^{n+1}$. Then from (5) we obtain $\|z^{n+1}\| \leq \delta t^{n+1}$. The error accumulates and increases linearly.

The solution is obtained using the unconditionally stable implicit scheme. The major part of computing costs is related with this scheme. The step control is performed using the explicit scheme solution. The algorithm stability is not violated and is determined by the implicit scheme properties.

The error accumulation from the time layer t^n to the new layer t^{n+1} is defined as

$$\|z^{n+1}\| \leq \|z^n\| + \tau^{n+1}\|\psi^{n+1}\|. \tag{6}$$

Therefore, we have to control the local error ψ^{n+1}. Comparing ψ^{n+1} with a given level of error δ we can control the time step choice. If ψ^{n+1} is significantly larger

(or smaller) then the δ - it means that the time step is too large (or small). Thereby

$$\tau^{n+1}: \ \|\psi^{n+1}\| \approx \delta. \tag{7}$$

Consider the basic algorithm to control the time step. We select the time step based on the analysis of the previous step solutions. The predicted time step is determined as following

$$\widetilde{\tau}^{n+1} = \gamma\tau^n, \tag{8}$$

where γ is numerical parameter. The default value of γ is 1.25 or 1.5. Using the explicit scheme we can obtain a solution $\widetilde{y}^{n+1}$ at time $\widetilde{t}^{n+1} = t^n + \widetilde{\tau}^{n+1}$. The calculation is performed only at single time step; therefore the possible computational instability does not appear. We estimate the approximation error using the calculated $\widetilde{y}^{n+1}$ by the implicit scheme. The τ^{n+1} is estimated by the proximity of the error norm to δ. The solution at a new time step t^{n+1} is calculated with a τ^{n+1} by the implicit scheme.

3   Calculated Formulas

We present the calculated formulas for the time step control for neutron diffusion equation.

Neutron Diffusion Equation. Let's consider neutron diffusion equation in one-group approximation with one-group delayed neutron sources. Neutron flux dynamics is considered within a bounded 2D domain Ω ($\boldsymbol{x} = \{x_1, x_2\} \in \Omega$) with a convex boundary $\partial\Omega$.

$$\frac{1}{v}\frac{\partial\phi}{\partial t} - \nabla \cdot D\nabla\phi + \Sigma_a\phi = \ (1-\beta)\nu\Sigma_f\phi + \lambda c,$$
$$\frac{\partial c}{\partial t} + \lambda c = \beta\nu\Sigma_f\phi. \tag{9}$$

Here $\phi(\boldsymbol{x}, t)$ is the neutron flux at point $\boldsymbol{x}$ and time t, v is the neutron velocity, $D(\boldsymbol{x})$ is the diffusion coefficient, $\Sigma_a(\boldsymbol{x}, t)$ is the absorption cross-section, β is the effective fraction of delayed neutrons, $\nu\Sigma_{fg}(\boldsymbol{x}, t)$ is the generation cross-section, c is density of source of delayed neutrons, λ is decay constant of delayed neutrons source.

The conditions so-called albedo-type are set at the boundary $\partial\Omega$:

$$D\frac{\partial\phi}{\partial n} + \gamma\phi = 0. \tag{10}$$

where n is the outer normal to the boundary $\partial\Omega$. Let's consider problem (9) with boundary conditions (10) and initial conditions: $\phi(0) = \phi^0, c(0) = c^0$. Space discretization is performed using the standard Lagrange finite elements (for example, see [4]).

Time Step Estimate. In our case, the approximation error $\boldsymbol{\psi^{n+1}} = \{\psi_1^{n+1}, \psi_2^{n+1}\}$ is

$$
\begin{aligned}
\psi_1^{n+1} &= \frac{1}{v}\frac{\phi^{n+1} - \phi^n}{\tau^{n+1}} - \nabla \cdot D^{n+1}\nabla\phi^{n+1} + \Sigma_a^{n+1}\phi^{n+1} \\
&\quad - (1-\beta)\nu\Sigma_f^{n+1}\phi^{n+1} - \lambda c^{n+1}, \\
\psi_2^{n+1} &= \frac{c^{n+1} - c^n}{\tau^{n+1}} + \lambda c^{n+1} - \beta\nu\Sigma_f^{n+1}\phi^{n+1},
\end{aligned}
\tag{11}
$$

where $\boldsymbol{\phi^{n+1}} = \{\phi^{n+1}, c^{n+1}\}$ is exact solution. The predictive solution is

$$
\begin{aligned}
\frac{1}{v}\frac{\widetilde{\varphi}^{n+1} - \varphi^n}{\widetilde{\tau}^{n+1}} - \nabla \cdot D^n\nabla\varphi^n + \Sigma_a^n\varphi^n &= (1-\beta)\nu\Sigma_f^n\varphi^n + \lambda s^n, \\
\frac{\widetilde{s}^{n+1} - s^n}{\widetilde{\tau}^{n+1}} + \lambda s^n &= \beta\nu\Sigma_f^n\varphi^n.
\end{aligned}
\tag{12}
$$

This solution is used to estimate the approximation error of the implicit scheme in the transition from time t^n to time $\widetilde{t}^{n+1}$.

In accordance with (11), the approximation error is calculated from the exact solution for two time moments: in our case, for t^n and $\widetilde{t}^{n+1}$. To estimate the error we take $\boldsymbol{\varphi^n} = \{\varphi^n, s^n\}$ instead of $\boldsymbol{\phi}(t^n)$. An exact solution at a new time step $\boldsymbol{\phi}(\widetilde{t}^{n+1})$, is matched by an approximate solution $\widetilde{\boldsymbol{\varphi}}^{n+1} = \{\widetilde{\varphi}^{n+1}, \widetilde{s}^{n+1}\}$, which is obtained by the explicit scheme. By virtue of this, we set

$$
\begin{aligned}
\widetilde{\psi}_1^{n+1} &= \frac{1}{v}\frac{\widetilde{\varphi}^{n+1} - \varphi^n}{\widetilde{\tau}^{n+1}} - \nabla \cdot D^{n+1}\nabla\widetilde{\varphi}^{n+1} + \Sigma_a^{n+1}\widetilde{\varphi}^{n+1} \\
&\quad - (1-\beta)\nu\Sigma_f^{n+1}\widetilde{\varphi}^{n+1} - \lambda\widetilde{s}^{n+1}, \\
\widetilde{\psi}_2^{n+1} &= \frac{\widetilde{s}^{n+1} - s^n}{\widetilde{\tau}^{n+1}} + \lambda\widetilde{s}^{n+1} - \beta\nu\Sigma_f^{n+1}\widetilde{\varphi}^{n+1}.
\end{aligned}
\tag{13}
$$

We match the approximation error $\widetilde{\boldsymbol{\psi}}^{n+1} = \{\widetilde{\psi}_1^{n+1}, \widetilde{\psi}_2^{n+1}\}$ at the time step $\widetilde{\tau}^{n+1}$ and $\boldsymbol{\psi^{n+1}}$ at the time step τ^{n+1}. Taking into account (7), we set

$$
\bar{\tau}^{n+1} = \gamma_{n+1}\tau^n, \quad \gamma_{n+1} = \frac{\delta}{\|\widetilde{\boldsymbol{\psi}}^{n+1}\|}\gamma.
\tag{14}
$$

The needed time step can not exceed the predicted time step, therefore

$$
\tau^{n+1} \leq \bar{\tau}_{n+1}, \quad \tau^{n+1} \leq \widetilde{\tau}_{n+1}.
$$

We limit the allowable time step by the minimum step τ^0:

$$
\tau^{n+1} = \max\left\{\tau^0, \min\{\gamma_{n+1}, \gamma\}\tau^n\right\}.
\tag{15}
$$

Let's determine the calculation formulas for the step selection algorithm in accordance with (12)–(15):

$$
\begin{aligned}
\widetilde{\psi}_1^{n+1} &= (-\nabla \cdot D^{n+1}\nabla + \Sigma_a^{n+1} - (1-\beta)\nu\Sigma_f^{n+1} + \nabla \cdot D^n\nabla - \Sigma_a^n + (1-\beta)\nu\Sigma_f^n)\varphi^n \\
&\quad + (-\nabla \cdot D^{n+1}\nabla + \Sigma_a^{n+1} - (1-\beta)\nu\Sigma_f^{n+1})(\widetilde{\varphi}^{n+1} - \varphi^n) - \lambda(\widetilde{s}^{n+1} - s^n). \\
\widetilde{\psi}_2^{n+1} &= (-\beta\nu\Sigma_f^{n+1} + \beta\nu\Sigma_f^n)\varphi^n + \lambda(\widetilde{s}^{n+1} - s^n) - \beta\nu\Sigma_f^{n+1}(\widetilde{\varphi}^{n+1} - \varphi^n).
\end{aligned}
$$

For convenience, rewrite it in the operator notation

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

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

where

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

Thus, the approximation error has the first order for time variable: $\widetilde{\psi}^{n+1} = \mathcal{O}(\widetilde{\tau}_{n+1})$. By virtue of this, we set

$$\|\widetilde{\psi}^{n+1}\| \le \|(A^{n+1} - A^n)\boldsymbol{\varphi^n} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{n+1} - \boldsymbol{\varphi^n})\|. \tag{16}$$

Taking into account (16) from (14), we obtain the calculated formula for time step (15), in which

$$\gamma_{n+1} = \frac{\delta}{\|(A^{n+1} - A^n)\boldsymbol{\varphi^n} + A^{n+1}(\widetilde{\boldsymbol{\varphi}}^{n+1} - \boldsymbol{\varphi^n})\|}\gamma. \tag{17}$$

This formula (the denominator of the expression) clearly shows the corrective actions, which are associated with the change of the problem operator (the first part), with the dynamics of the solution (second part).

4   Test Problem

The test problem for reactor IAEA-2D without a reflector in a one-dimensional approximation (Ω—is the reactor core area) is considered [5]. The geometrical model of the IAEA-2D reactor core is presented in Fig. 1. The fuel assembly pitch equals 20 cm. Diffusion neutronics constants in the common notations are given in Table 1. The boundary conditions (2) are used at $\gamma_g = 0.5$. The following delayed neutrons parameters are used: $\beta = 6.5 \cdot 10^3$, $\lambda = 0.08$ s^{-1} and $v = 1.0 \cdot 10^6$ cm/s. Modeling effect of insersion or withdrawal of control rods (depending on the sign of the perturbation). Define the scenario of the process:

1. The spectral problem is solved [6], the solution is taken as the initial condition;
2. Calculation for the non-stationary model at the time range 0 to 0.1 s;
3. At a moment of 0.1 s the value Σ_a for the zone 3 changes to ± 0.000625;
4. The dynamic regime is calculated starting from 0.1 s to 0.5 s.

At each time the integrated power is calculated

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

where a is the normalization coefficient by a given value of the integrated power.

Table 1. Diffusion neutronics constants for IAEA-2D test problem

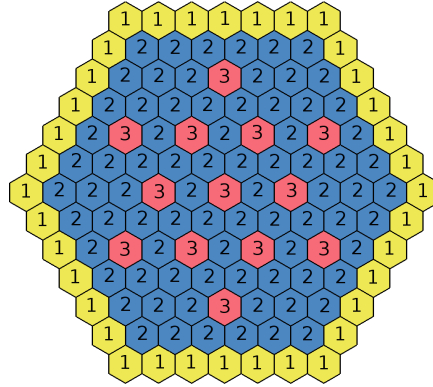| Zone	1	2	3
D, cm	1.03	1.03	1.03
Σ_a, cm^{-1}	0.02	0.02125	0.02625
$\nu\Sigma_f$, cm^{-1}	0.0225	0.0225	0.0225

Fig. 1. Geometrcial model of the IAEA-2D reactor core

Computational Results. The accuracy of the solution was evaluated by a reference solution, which uses a numerical solution on a sufficiently detailed grid in time ($\tau_{ref} = 1\cdot10^{-5}$) by the implicit scheme with a fixed time step. The initial value of k_{eff} was 1.0005063. Figure 2 show the integral powers for insersion or withdrawal of the control rods respectively.
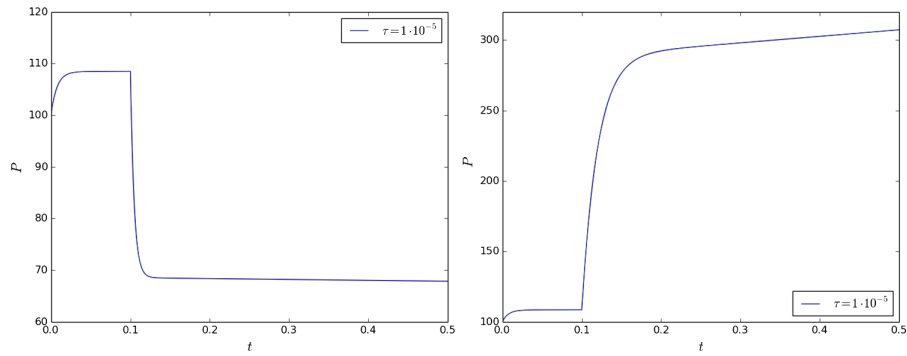

Fig. 2. The integral powers.

The error is estimated as $\varepsilon_P(t) = |P_{ref} - P|$, where P_{ref} is the reference solution, P is the solution obtained by using the time stepping algorithm. We took a minimum time step $\tau_0 = \tau_{ref}$.

Figure 3 show the error ε_P when the control rods are taken for immersion and extraction, respectively, for different values of the parameter δ. Here we see that the error converges as the parameter δ decreases.
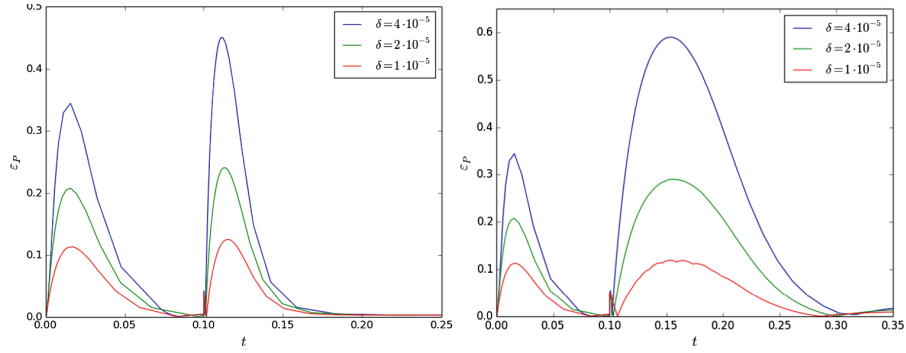

Fig. 3. Error by time.

Figure 4 shows the time steps for insertion or withdrawal of rods, respectively. It is seen that first there is a rapid growth of the time step with a specified accuracy of δ. Then the *catch* of a sudden change in power occurs with a strong decrease in the time step. Further, the time step grows to a certain point and remains at the same level, which is controlled by the error δ.
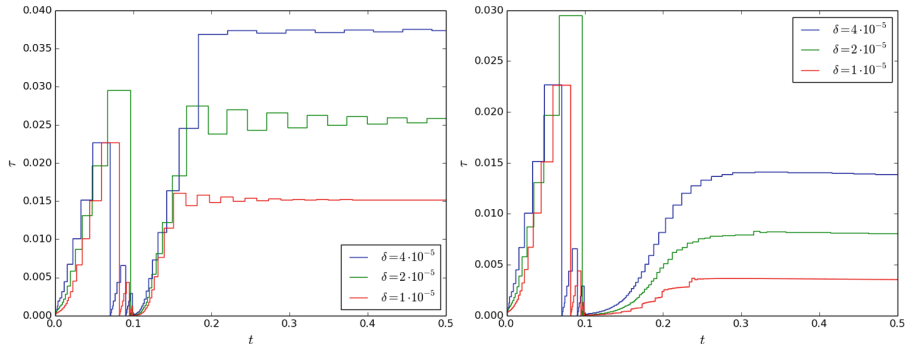

Fig. 4. Steps by time.

Table 2 shows the various output data for different values of the parameter δ, where $\max(\epsilon_P)$ is the maximum power error, n is the number of steps in time,

and t is the calculation time in seconds. The reference solution: the number of steps in time is 50000, the counting time is 2130 s.

Table 2. Counting time and number of steps.

δ	Insersion			Withdrawal		
	$\max(\epsilon_P)$	n	t	$\max(\epsilon_P)$	n	t
$4 \cdot 10^{-5}$	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

References

1. Samarskii, A.A., Matus, P.P., Vabishchevich, P.N.: Difference Schemes with Operator Factors. Kluwer, Dordrecht (2002)
2. Ascher, U.M.: Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations. Society for Industrial Mathematics, Philadelphia (1998)
3. Vabishchevich, P.N.: A priori estimation of a time step for numerically solving parabolic problems. Math. Model. Anal. **20**(1), 94–111 (2015)
4. Avvakumov, A.V., et al.: Numerical modeling of neutron diffusion non-stationary problems. Matematicheskoe Modelirovanie **29**(7), 44–62 (2017)
5. Chao, Y.A., Shatilla, Y.A.: Conformal mapping and hexagonal nodal methods-II: Implementation in the ANC-H Code. Nucl. Sci. Eng. **121**, 210–225 (1995)
6. Avvakumov, A.V., et al.: Spectral properties of dynamic processes in a nuclear reactor. Ann. Nucl. Energy **99**, 68–79 (2017)
7. Avvakumov, A.V., Strizhov, V.F., Vabishchevich, P.N., Vasilev, A.O.: Algorithms for numerical simulation of non-stationary neutron diffusion problems. In: Dimov, I., Faragó, I., Vulkov, L. (eds.) NAA 2016. LNCS, pp. 212–219. Springer, Cham (2017). https://doi.org/10.1007/978-3-319-57099-0_21