Algorithm of Time Step Selection for Numerical Solution of Boundary Value Problem for Parabolic Equations

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Introduction

The problem of the time step control is relatively well developed for the Cauchy problem solution of differential equations systems. (Gear 1971, Hairer Norsett Wanner 1987, Asher 1998, ...) 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.

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Additional calculations for estimating the error of the approximate solution can be carried out in different ways. The best-known strategy is connected with the solution of the problem on a separate time interval using the given step (the first solution) and with a step two times smaller (the second solution). The noted ways of selecting the time step are related to the class of a posteriori accuracy estimation methods. The decision as to suitable the time step or the re-calculation is accepted only after the calculation is completed.

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In this paper we consider in fact a priori choice of the time step in the approximate solution of boundary value problems for parabolic equations. The proposed algorithm allows a gain in CPU time with respect to the fine mesh calculation at the same calculation accuracy.

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 for linear equation

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

with following initial condition

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The problem is considered in a finite-dimensional Hilbert space H.

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Assume $A(t) \geq 0$ in H then, for the Cauchy problem we have a stability estimate with respect to the initial data and the right-hand side

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

Solution evaluation

Introduce irregular time grid

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

For an approximate solution the implicit scheme are used

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

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For an approximate solution under restriction $A^{n+1} \geq 0$:
Layerwise estimate

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

Difference estimate

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

Solution error

For the error of the approximate solution $z^n = y^n - u^n$:

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

$$z^0 = 0.$$

Where the approximation error is

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

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Similarly, we have an difference estimate for the error

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

Then we obtain

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

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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, $t^{n+1} = t^n + \tau^{n+1}$

Calculated formulas

The predictive solution $\widetilde{y}^{n+1}$ is defined from

$$\frac{\widetilde{y}^{n+1} - y^n}{\widetilde{\tau}^{n+1}} + A^n y^n = f^n.$$

The approximation error of predictive solution

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

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

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

Calculated formulas continued

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

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

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The approximation error has the first order in time

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In view of this, we set

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

Calculated formula for time step

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

Model

Consider the boundary problem for a 1D parabolic equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + p(t)u = f(t), \quad 0 < x < 1, \quad 0 < t \leq T,$$

with boundary and initial conditions

$$u(0,t) = 0, \quad u(1,t) = 0, \quad 0 < t \leq T,$$

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The operator $A(t)$ is given in the form

$$Au = -\frac{1}{h^2}(u(x+h) - 2u(x) + u(x-h)) + p(t)u(x), \quad x \in \omega.$$

The operator $A(t)$ is selfadjoint and for $p(t) \geq 0$ is positive definite in H. Thus, after space approximating, we arrive at the original problem.

Problem

The problem is considered for $T = 0.1$, $\tau^0 = 10^{-6}$ with a discontinuous coefficient $p(t)$ and discontinuous right-hand side $f(t)$:

$$p(t) = \begin{cases} \lambda t, & 0 < t \le 0.075, \\ 0, & 0.075 < t \le 0.1, \end{cases}$$

$$f(t) = \begin{cases} 0, & 0 < t \le 0.05, \\ \chi e^{-10(t-0.05)}, & 0.05 < t \le 0.1. \end{cases}$$

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We consider the case when the initial condition is taken in the form:

$$u^0(x) = \sin^\sigma(\pi x), \qquad 0 < x < 1.$$

For the basic variant, we set

$$\lambda = 100, \quad \chi = 10, \quad \sigma = 0.5.$$

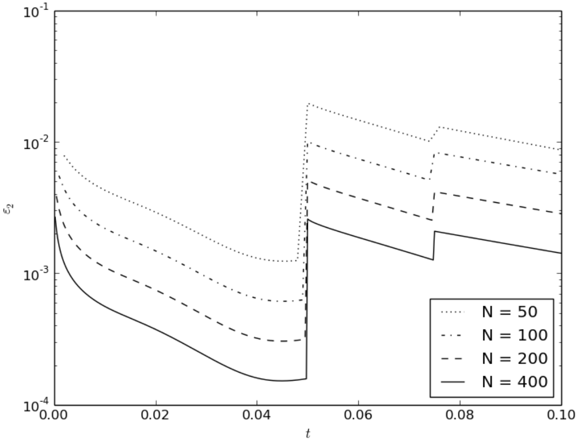
Comparing

The accuracy of the approximate solution was estimated from the reference solution, that a numerical solution on a fine grid in time ($\tau = 1 \cdot 10^{-7}$).

The error is estimated in the norm of $L_2(\omega)$ ($\varepsilon_2 = \| \cdot \|$) or $L_\infty(\omega)$ ($\varepsilon_\infty = \| \cdot \|_\infty$), where

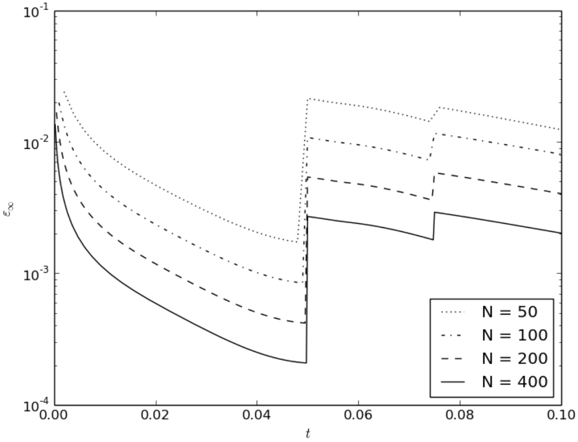
$$\|u\|_\infty = \max_{x \in \omega} |u(x)|.$$

Uniform grid



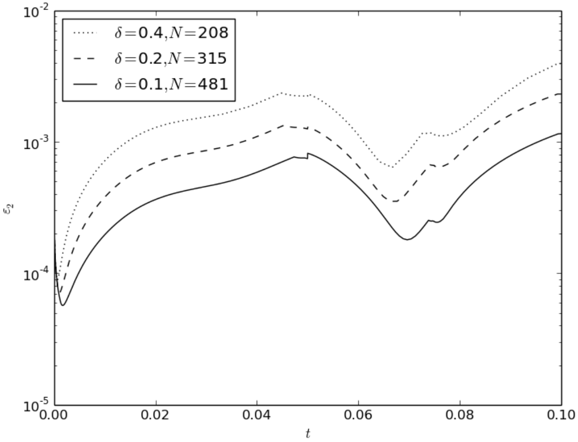
Error in $L_2(\omega)$.

Uniform grid



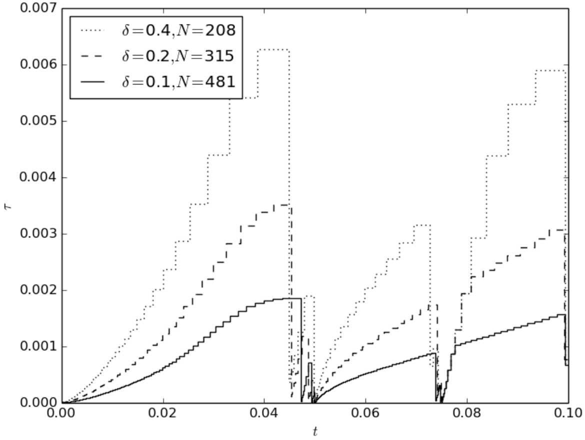
Error in $L_\infty(\omega)$.

Irregular grid



Error in $L_2(\omega)$.

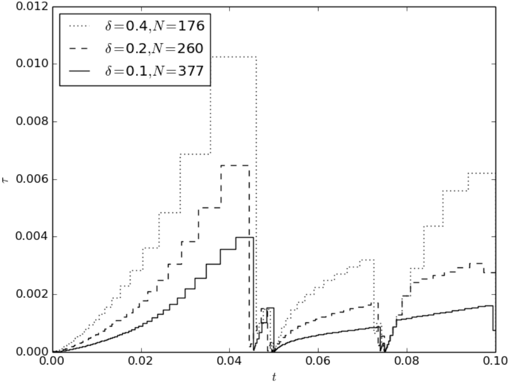
Irregular grid



Time steps.

Three layered scheme

We can also use more accurate difference schemes to find the predictive solution. The results of calculations using a three-layer explicit scheme.



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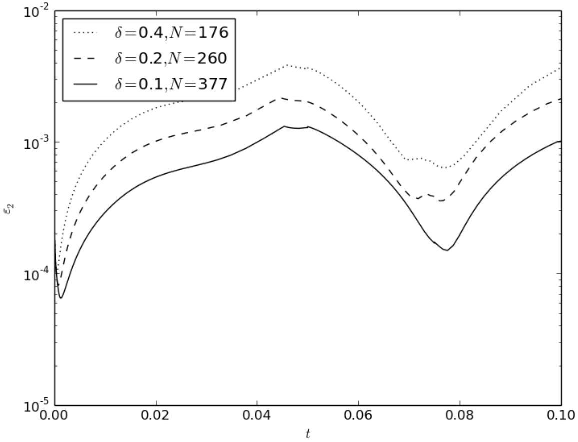
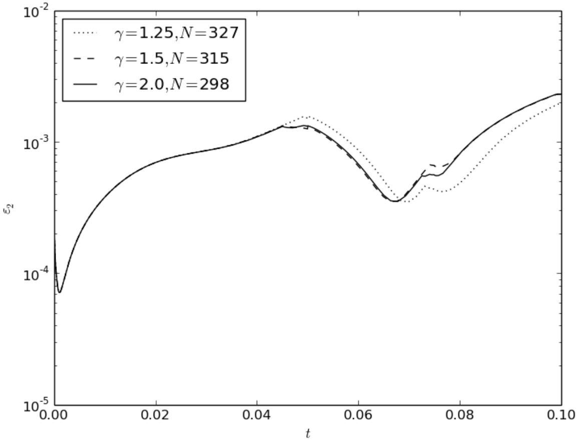


Error on irregular grid.

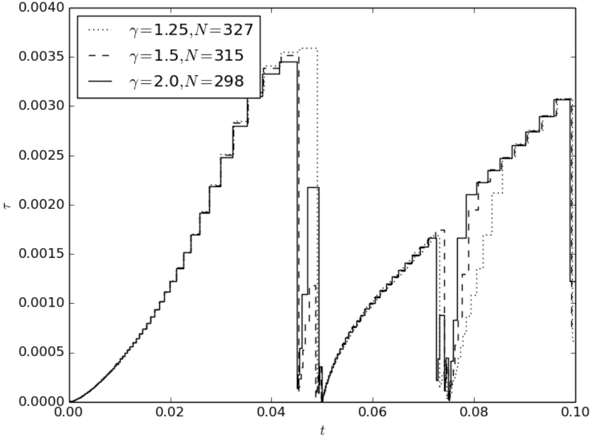
Gamma



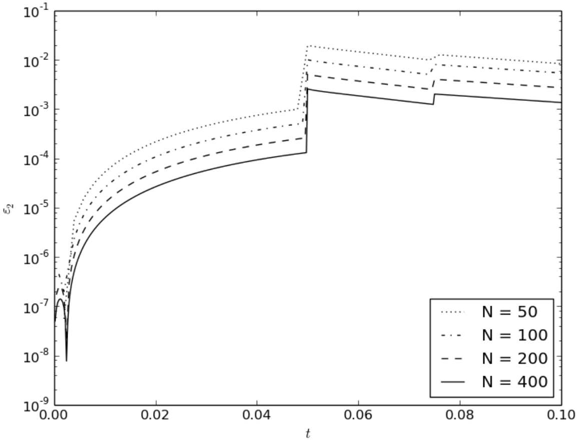
Error in $L_2(\omega)$.

Gamma

The effect of increase of the time step parameter is insignificant.

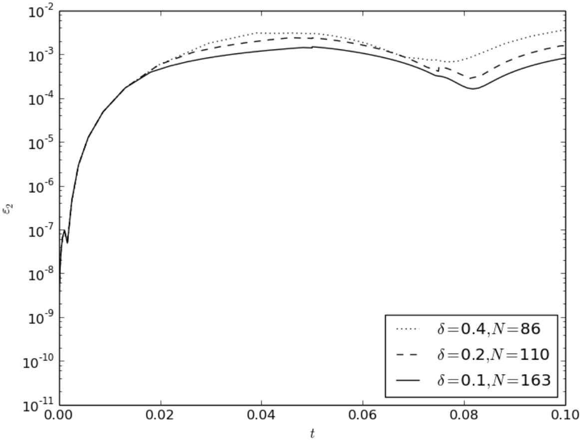


Initial condition parameter



Error on uniform grid at $\sigma = 1$

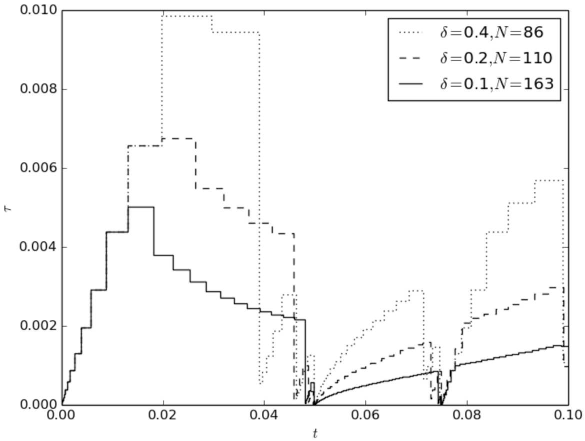
Initial condition parameter



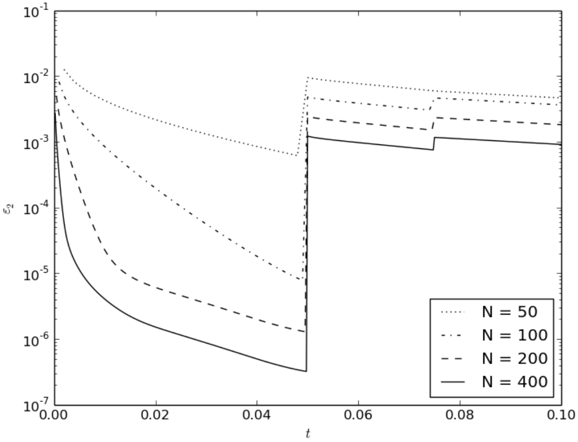
Error on irregular grid at $\sigma = 1$

Initial condition parameter

Other parameters do not affect.



Crank-Nicolson scheme



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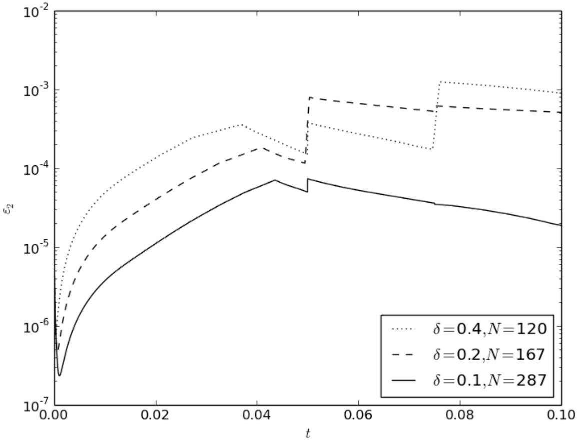

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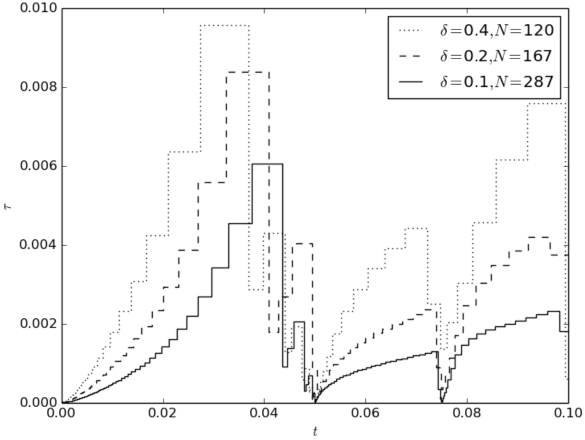

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Conclusion

- An algorithm of time step selection for numerical solution of boundary problem for parabolic equations 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 modal problem demonstrate reliability of the proposed algorithm for time step choice.

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Thank you for your attention!