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ON GLOBAL ERROR ESTIMATION AND CONTROL OF FINITE DIFFERENCE SOLUTIONS FOR PARABOLIC EQUATIONS

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Abstract. The aim of this paper is to extend the global error estimation and control addressed in Lang and Verwer [SIAM J. Sci. Comput. 29, 2007] for initial value problems to finite difference solutions of parabolic partial differential equations. The classical ODE approach based on the first variational equation is combined with an estimation of the PDE spatial truncation error to estimate the overall error in the computed solution. Control in a discrete L_2-norm is achieved through tolerance proportionality and mesh refinement. A numerical example illustrates the reliability of the estimation and control strategies.

1 Introduction

We consider initial boundary value problems of parabolic type, which can be written as

$$\partial_t u(t,x) = f(t,x,u(t,x),\partial_x u(t,x),\partial_{xx} u(t,x))\,, \quad t \in (0,T]\,,\ x \in \Omega \subset \mathbb{R}^d\,, \tag{1}$$

equipped with an appropriate system of boundary conditions and with the initial condition

$$u(0,x) = u_0(x)\,, \quad x \in \overline{\Omega}. \tag{2}$$

The PDE is assumed to be well posed and to have a unique continuous solution $u(t,x)$ which has sufficient regularity.

The method of lines is used to solve (1) numerically. We first discretize the PDE in space by means of finite differences on a (possibly non-uniform) spatial mesh Ω_h and solve the resulting system of ODEs using existing time integrators. For simplicity, we shall assume that this system of time-dependent ODEs can be written in the general form

$$\begin{aligned} U_h'(t) &= F_h(t, U_h(t))\,, \qquad t \in (0,T]\,, \\ U_h(0) &= U_{h,0}\,, \end{aligned} \tag{3}$$

with a unique solution vector $U_h(t)$ being a grid function on Ω_h. Let

$$R_h : \, u(t,\cdot) \to R_h u(t) \tag{4}$$

be the usual restriction operator defined by $R_h u(t) = (u(t,x_1),\ldots,u(t,x_N))^T$, where $x_i \in \Omega_h$ and N is the number of all mesh points. Then we take as initial condition $U_{h,0} = R_h u(0)$.

To solve the initial value problem (3), we apply a numerical integration method at a certain time grid

$$0 = t_0 < t_1 < \cdots < t_n < \cdots < t_{M-1} < t_M = T\,, \tag{5}$$

using local control of accuracy. This yields approximations $V_h(t_n)$ to $U_h(t_n)$, which may be calculated for other values of t by using a suitable interpolation method provided by the integrator. The global time error is then defined by

$$e_h(t) = V_h(t) - U_h(t)\,. \tag{6}$$

Numerical experiments in [5] for ODE systems have shown that classical global error estimation based on the first variational equation is remarkably reliable. In addition, having the property of tolerance proportionality, that is, there exists a linear relationship between the global time error and the local accuracy tolerance, $e_h(t)$ can be successfully controlled by a second run with an adjusted local tolerance. Numerous techniques to estimate global errors are described in [9].

In order for the method of lines to be used efficiently, it is necessary to take also into account the spatial discretization error. Defining the spatial discretization error by

$$\eta_h(t) = U_h(t) - R_h u(t)\,, \tag{7}$$

the vector of overall global errors $E_h(t) = V_h(t) - R_h u(t)$ may be written as sum of the global time and spatial error, that is,

$$E_h(t) = e_h(t) + \eta_h(t)\,. \tag{8}$$

It is the purpose of this paper to present a new error control strategy for the global errors $E_h(t)$. We will mainly focus on reliability. So our aim is to provide error estimates

$\tilde{E}_h(t) \approx E_h(t)$ which are not only asymptotically exact, but also work reliably for moderate tolerances, that is for relatively coarse discretizations.

The global errors are measured in discrete L_2-norms. A priori bounds for the global error in such norms are well known, see e.g. [6, 10]. However, reliable a posteriori error estimation and efficient control of the accuracy of the solution numerically computed to an imposed tolerance level are still challenging. We achieve global error control by iteratively improving the temporal and spatial discretizations according to estimates of $e_h(t)$ and $\eta_h(t)$. The global time error is estimated and controlled along the way fully described in [5]. To estimate the global spatial error, we follow an approach proposed in [1] (see also [7]) and use Richardson extrapolation to set up a linearised error transport equation.

2 Spatial and time error

By making use of the restriction operator R_h, the spatial truncation error is defined by

$$\alpha_h(t) = (R_h u)'(t) - F_h(t, R_h u(t)) \,. \tag{9}$$

From (3) and (9), it follows that the global spatial error $\eta_h(t)$ representing the accumulation of the spatial discretization error is the solution of the initial value problem

$$\begin{aligned} \eta_h'(t) &= F_h(t, U_h(t)) - F_h(t, R_h u(t)) - \alpha_h(t)\,, \qquad t \in (0,T]\,, \\ \eta_h(0) &= 0\,. \end{aligned} \tag{10}$$

Assuming F_h to be continuously differentiable, the mean value theorem for vector functions yields

$$\begin{aligned} \eta_h'(t) &= \partial_{U_h} F_h(t, U_h(t))\, \eta_h(t) - \alpha_h(t) + \mathcal{O}(\eta_h(t)^2), \qquad t \in (0,T], \\ \eta_h(0) &= 0\,. \end{aligned} \tag{11}$$

With $V_h(t)$ being the continuous extension of the numerical approximation to (3), the residual time error is defined by

$$r_h(t) = V_h'(t) - F_h(t, V_h(t)) \,. \tag{12}$$

Thus the global time error $e_h(t)$ fulfills the initial value problem

$$\begin{aligned} e_h'(t) &= F_h(t, V_h(t)) - F_h(t, U_h(t)) + r_h(t)\,, \qquad t \in (0,T]\,, \\ e_h(0) &= 0\,. \end{aligned} \tag{13}$$

Again, the mean value theorem yields

$$\begin{aligned} e_h'(t) &= \partial_{U_h} F_h(t, V_h(t))\, e_h(t) + r_h(t) + \mathcal{O}(e_h(t)^2), \qquad t \in (0,T], \\ e_h(0) &= 0\,. \end{aligned} \tag{14}$$

Apparently, by implementing proper choices of the defects $\alpha_h(t)$ and $r_h(t)$, solving (11) and (14) will in leading order provide approximations to the true global error. The issue of how to approximate the spatial truncation error and the residual time error will be discussed in the next sections.

3 Estimation of the residual time error

We assume that the time integration method used to approximate the general ODE system (3) is of order $p \leq 3$. Following the approach proposed in [5] we define the interpolated solution $V_h(t)$ by piecewise cubic Hermite interpolation. Let $V_{h,n} = V_h(t_n)$ and $F_{h,n} = F_h(t_n, V_{h,n})$ for all $n = 0, 1, \ldots, M$. Then at every subinterval $[t_n, t_{n+1}]$ we form

$$V_h(t) = V_{h,n} + A_n(t-t_n) + B_n(t-t_n)^2 + C_n(t-t_n)^3, \qquad t_n \leq t \leq t_{n+1}, \tag{15}$$

and choose the coefficients such that $V_h'(t_n) = F_{h,n}$ and $V_h'(t_{n+1}) = F_{h,n+1}$. This gives

$$V_h(t_n + \theta\tau_n) = v_0(\theta)V_{h,n} + v_1(\theta)V_{h,n+1} + \tau_n w_0(\theta)F_{h,n} + \tau_n w_1(\theta)F_{h,n+1} \tag{16}$$

with $0 \leq \theta \leq 1$, $\tau_n = t_{n+1} - t_n$, and

$$v_0(\theta) = (1-\theta)^2(1+2\theta),\ v_1(\theta) = \theta^2(3-2\theta),\ w_0(\theta) = (1-\theta)^2\theta,\ w_1(\theta) = \theta^2(\theta-1). \tag{17}$$

Now let $Y_h(t)$ be the (sufficiently smooth) solution of the ODE (3) with initial value $Y(t_n) = V_{h,n}$. Then the local error of the time integration method at time t_{n+1} is given by

$$le_{n+1} = V_{h,n+1} - Y_h(t_{n+1}) = \mathcal{O}(\tau_n^{p+1}). \tag{18}$$

Combining (16) and (18) and applying a Taylor expansion gives

$$V_h(t_n + \theta\tau_n) - Y_h(t_n + \theta\tau_n) = v_1(\theta)le_{n+1} + \frac{1}{24}(2\theta^3 - \theta^2 - \theta^4)\tau_n^4 Y_h^{(4)}(t_n) + \mathcal{O}(\tau_n^{p+2})\,. \tag{19}$$

Recalling $Y_h'(t) = F_h(t, Y_h(t))$ for $t \in (t_n, t_{n+1}]$ and rewriting the residual time error as

$$r_h(t) = V_h'(t_n + \theta\tau_n) - Y_h'(t_n + \theta\tau_n) + F_h(t, Y_h(t)) - F_h(t, V_h(t))\,, \tag{20}$$

with $\theta = (t - t_n)/\tau_n$, we find by differentiating the right hand side of (19)

$$r_h(t_n + \theta\tau_n) = 6(\theta - \theta^2)\frac{le_{n+1}}{\tau_n} + \frac{1}{12}(3\theta^2 - \theta - 2\theta^3)\tau_n^3 Y_h^{(4)}(t_n) + \mathcal{O}(\tau_n^{p+1})\,. \tag{21}$$

Setting $\theta = 1/2$ in (21) will reveal

$$r_h(t_{n+1/2}) = \frac{3}{2}\frac{le_{n+1}}{\tau_n} + \mathcal{O}(\tau_n^{p+1})\,. \tag{22}$$

Thus the cubic Hermite defect halfway the step interval can be used to retrieve in leading order the local error of any one-step method of order $1 \le p \le 3$ (see also [5], Section 2.2). Following the arguments given in [5], Section 2.1, we consider instead of (14) the step size frozen version

$$\begin{aligned} \tilde{e}_h'(t) &= \partial_{U_h} F_h(t_n, V_{h,n})\, \tilde{e}_h(t) + \tfrac{2}{3} r_h(t_{n+\frac{1}{2}}),\ t \in (t_n, t_{n+1}],\ n = 0, \ldots, M-1, \\ \tilde{e}_h(0) &= 0 \end{aligned} \tag{23}$$

to approximate the global time error $e_h(t)$. Using

$$V_h(t_{n+1/2}) = \frac{1}{2}(V_{h,n} + V_{h,n+1}) + \frac{\tau}{8}(F_{h,n} - F_{h,n+1}) \tag{24}$$

and

$$V_h'(t_{n+1/2}) = \frac{3}{2\tau}(V_{h,n+1} - V_{h,n}) - \frac{1}{4}(F_{h,n} + F_{h,n+1}) \tag{25}$$

we can compute the residual time error halfway the step interval from (12)

$$\begin{aligned} r_h(t_{n+1/2}) \;=\; & \tfrac{3}{2\tau}(V_{h,n+1} - V_{h,n}) - \tfrac{1}{4}(F_{h,n} + F_{h,n+1}) \\ & -F_h\left(t_{n+\frac{1}{2}}, \tfrac{1}{2}(V_{h,n} + V_{h,n+1}) + \tfrac{\tau}{8}(F_{h,n} - F_{h,n+1})\right). \end{aligned} \tag{26}$$

Remark 3.1 From (21) we deduce

$$\frac{1}{\tau_n} \int_{t_n}^{t_{n+1}} r_h(t)\; dt = \frac{le_{n+1}}{\tau_n} + \mathcal{O}(\tau_n^{p+1}), \tag{27}$$

showing, in the light of (22), that $\frac{2}{3} r_h(t_{n+1/2})$ is in leading order equal to the time-averaged residual. Thus, we can justify the use of the error equation (23) without the link to the first variational equation. $\Diamond$

4 Estimation of the spatial truncation error

An efficient strategy to estimate the spatial truncation error by Richardson extrapolation is proposed in [1]. We will adopt this approach to our setting.

Suppose we are given a second semi-discretization of the PDE system (1), now with doubled local mesh sizes $2h$,

$$\begin{aligned} U_{2h}'(t) &= F_{2h}(t, U_{2h}(t)), \qquad t \in (0, T], \\ U_{2h}(0) &= U_{2h,0}. \end{aligned} \tag{28}$$

In practice, one first chooses Ω_{2h} and constructs then Ω_h through uniform refinement. The following two assumptions will be needed. (i) The solution $U_{2h}(t)$ to the discretized PDE on the coarse mesh Ω_{2h} exists and is unique. (ii) The spatial discretization error

$\eta_h(t)$ is of order q with respect to h. We define the restriction operator R^h_{2h} from the fine grid Ω_h to the coarse grid Ω_{2h} by the identity $R_{2h} = R^h_{2h}R_h$ and set

$$\eta^c_h(t) = R^h_{2h}\eta_h(t), \quad U^c_h(t) = R^h_{2h}U_h(t), \quad V^c_h(t) = R^h_{2h}V_h(t)\,. \tag{29}$$

From the second assumption it follows that

$$\eta^c_h(t) = 2^{-q}\eta_{2h}(t) + \mathcal{O}(h^{q+1}) \tag{30}$$

and therefore

$$R_{2h}u(t) = \frac{2^q}{2^q-1}U^c_h(t) - \frac{1}{2^q-1}U_{2h}(t) + \mathcal{O}(h^{q+1})\,. \tag{31}$$

The relation $U^c_h(t) - U_{2h}(t) = \eta^c_h(t) - \eta_{2h}(t)$ together with (30) gives

$$U^c_h(t) - U_{2h}(t) = \frac{1-2^q}{2^q}\eta_{2h}(t) + \mathcal{O}(h^{q+1})\,. \tag{32}$$

The spatial truncation error on the coarse mesh Ω_{2h} is analogously defined to (9) as

$$\alpha_{2h}(t) = (R_{2h}u)'(t) - F_{2h}(t, R_{2h}u(t))\,. \tag{33}$$

Substituting $R_{2h}u(t)$ from (31) into the right-hand side, using the ODE system (28) to replace $U'_{2h}(t)$, and manipulating the expressions with (32) we get after Taylor expansion

$$\alpha_{2h}(t) = \frac{2^q}{2^q-1}\Big((U^c_h)'(t) - F_{2h}(t, U^c_h(t))\Big) + \mathcal{O}(h^{q+1})\,. \tag{34}$$

Analogously to (6), we set $e^c_h(t) = V^c_h(t) - U^c_h(t)$. Substituting $(U^c_h)'(t)$ by $R^h_{2h}F_h(t, U_h(t))$ and using again Taylor expansion it follows that

$$\begin{aligned}\alpha_{2h}(t) \;&=\; \tfrac{2^q}{2^q-1}\Big(R^h_{2h}F_h(t, V_h(t)) - F_{2h}(t, V^c_h(t))\Big) + \mathcal{O}(h^{q+1})\\ &\quad -\tfrac{2^q}{2^q-1}\Big(R^h_{2h}\big(\partial_{U_h}F_h(t, V_h(t))\, e_h(t)\big) - \partial_{U_h}F_{2h}(t, V^c_h(t))e^c_h(t)\Big) + \mathcal{O}(e_h(t)^2)\,.\end{aligned} \tag{35}$$

Assuming the term on the right-hand side involving the global time error to be sufficiently small, we can use

$$\tilde\alpha_{2h}(t) = \frac{2^q}{2^q-1}\Big(R^h_{2h}F_h(t, V_h(t)) - F_{2h}(t, V^c_h(t))\Big) \tag{36}$$

as approximation for the spatial truncation error on the coarse mesh. To guarantee a suitable quality of the estimate (36) we shall first control the global time error for attempting that afterwards the overall error is dominated by the spatial truncation error (see Section 6).

An approximation $\tilde\alpha_h(t)$ of the spatial truncation error on the (original) fine mesh is obtained by interpolation respecting the order of accuracy (see Section 5). Thus, to approximate the global spatial error $\eta_h(t)$ we consider instead of (11) the step-size frozen version

$$\begin{aligned}\tilde\eta'_h(t) \;&=\; \partial_{U_h}F_h(t_n, V_{h,n})\,\tilde\eta_h(t) - \tilde\alpha_h(t), \quad t\in(t_n, t_{n+1}],\ n = 0,\ldots,M-1,\\ \tilde\eta_h(0) \;&=\; 0\,.\end{aligned} \tag{37}$$

5 The example discretization formulas

In order to keep the illustration as simple as possible we restrict ourselves to one space dimension. For the spatial discretization of (1) we use standard second-order finite differences. Hence we have $q=2$. The discrete L_2-norm on a non-uniform mesh

$$x_0 < x_1 < \ldots < x_N < x_{N+1}\,, \quad h_i = x_i - x_{i-1}\,, \quad i = 1, \ldots, N+1\,, \tag{38}$$

for a vector $y = (y_1, \ldots, y_N)^T \in \mathbb{R}^N$ is defined through

$$\|y\|^2 = \sum_{i=1}^{N} \frac{h_i + h_{i+1}}{2}\, y_i^2\,. \tag{39}$$

Here, the components y_0 and y_{N+1} which are given by the boundary values are not considered.

The example time integration formulas are taken from [5]. For the sake of completeness we shall give a short summary of the implementation used. To generate the time grid (5) we use as an example integrator the 3rd-order, A-stable Runge-Kutta-Rosenbrock scheme ROS3P, see [3, 4] for more details. The property of tolerance proportionality [8] is asymptotically ensured through working for the local residual with

$$Est = \frac{2}{3}\,(I_h - \gamma\tau_n A_{h,n})^{-1} r_h(t_{n+1/2})\,, \qquad A_{h,n} = \partial_{U_h} F_h(t_n, V_{h,n})\,, \tag{40}$$

where γ is the stability coefficient of ROS3P. The common filter $(I_h - \gamma\tau_n A_{h,n})$ serves to damp spurious stiff components which would otherwise be amplified through the F_h-evaluations within $r_h(t_{n+1/2})$.

Let $D_n = \|Est\|$ and $Tol_n = Tol_A + Tol_R\|V_{h,n}\|$ with Tol_A and Tol_R given local tolerances. If $D_n > Tol_n$ the step is rejected and redone. Otherwise the step is accepted and we advance in time. In both cases the new step size is determined by

$$\tau_{new} = \min\big(1.5, \max(2/3, 0.9\,r)\big)\,\tau_n\,, \qquad r = (Tol_n/D_n)^{1/3}\,. \tag{41}$$

After each step size change we adjust τ_{new} to $\tau_{n+1} = (T - t_n)/\lfloor(1 + (T - t_n)/\tau_{new})\rfloor$ so as to guarantee to reach the end point T with a step of averaged normal length. The initial step size τ_0 is prescribed and is adjusted similarly.

The linear error transport equations (23) and (37) are simultaneously solved by means of the implicit midpoint rule, which gives approximations $\tilde{e}_{h,n}$ and $\tilde{\eta}_{h,n}$ to the global time and spatial error at time $t=t_n$. We use the implementations

$$(I_h - \frac{1}{2}\tau_n A_{h,n})\,\delta e_{n+1} = 2\tilde{e}_{h,n} + \frac{2}{3}\tau_n r(t_{n+1/2})\,, \qquad \tilde{e}_{h,n+1} = \delta e_{n+1} - \tilde{e}_{h,n}\,, \tag{42}$$

and

$$(I_h - \frac{1}{2}\tau_n A_{h,n})\,\delta\eta_{n+1} = 2\tilde{\eta}_{h,n} - \tau_n\tilde{\alpha}_h(t_{n+1/2})\,, \qquad \tilde{\eta}_{h,n+1} = \delta\eta_{n+1} - \tilde{\eta}_{h,n}\,. \tag{43}$$

Clearly, the matrices $A_{h,n}$ already computed within ROS3P can be reused. The spatial truncation error $\tilde{\alpha}_{2h}(t)$ at $t = t_{n+1/2}$ is given by

$$\tilde{\alpha}_{2h}(t_{n+1/2}) = \frac{4}{3}\left(R^h_{2h} F_h\left(t_{n+1/2}, V_h(t_{n+1/2})\right) - F_{2h}\left(t_{n+1/2}, R^h_{2h} V_h(t_{n+1/2})\right)\right). \tag{44}$$

Since $V_h(t_{n+1/2})$ and $F_h(t_{n+1/2}, V_h(t_{n+1/2})$ are available from the computation of $r_h(t_{n+1/2})$ in (26), this requires only one function evaluation on the coarse grid. The vector $\tilde{\alpha}_{2h}(t_{n+1/2})$ on the coarse mesh is prolongated to the fine mesh and is then divided by $2^q = 4$ if the neighboring fine grid points are equidistant, otherwise it is divided by $2^{q-1} = 2$. The remaining $\tilde{\alpha}_h(t_{n+1/2})$ on the fine mesh are computed by interpolation respecting the order of the neighboring spatial truncation errors.

Due to freezing the coefficients in each time step, the second-order midpoint rule is a first-order method when interpreted for solving the linearised equations (14) (or likewise the first variational equation) and (11). Thus if all is going well, we asymptotically have $\tilde{e}_{h,n} = e_h(t_n) + \mathcal{O}(\tau^4_{max})$ and $\tilde{\eta}_{h,n} = \eta_h(t_n) + \mathcal{O}(\tau_{max} h^q_{max}) + \mathcal{O}(h^{q+1}_{max})$.

After computing the spatial truncation errors we can solve the discretized error transport equations (43) for all $\tilde{\eta}_{h,n}$. We restrict here to globally uniform refinement. A locally adaptive refinement strategy can be found in [2]. Although the uniform strategy may be less efficient, it is very easy to implement and therefore of special practical interest if software packages which do no allow dynamic adaptive mesh refinement are used.

Let Tol be a given tolerance. Then our aim is to guarantee $\|\eta_h(T)\| \leq Tol$. From (43), we get an approximate value $\tilde{\eta}_{h,M}$ for the spatial discretization error at T. If the desired accuracy is still not satisfied, i.e., $\|\tilde{\eta}_{h,M}\| > Tol$, we choose a new (uniform) spatial resolution

$$h_{new} = \sqrt[q]{\frac{Tol}{\|\tilde{\eta}_{h,M}\|}}\, h \tag{45}$$

to account for achieving $\|\eta_{h_{new}}(T)\| \approx Tol$. From h_{new} we determine a new number of mesh points. The whole computation is redone with the new spatial mesh.

6 The control rules

Like for the ODE case studied in [5] our aim is to provide global error estimates and to control the accuracy of the solution numerically computed to the imposed tolerance level. Let $GTol_A$ and $GTol_R$ be the global tolerances. Then we start with the local tolerances $Tol_A = GTol_A$ and $Tol_R = GTol_R$.

Suppose the numerical schemes have delivered an approximate solution $V_{h,M}$ and global estimates $\tilde{e}_{h,M}$ and $\tilde{\eta}_{h,M}$ for the time and spatial error at time $t_M = T$. We then verify whether

$$\|\tilde{e}_{h,M}\| \leq C_T C_{control} Tol_M, \quad Tol_M = GTol_A + GTol_R \|V_{h,M}\|, \tag{46}$$

where $C_{control} \approx 1$, typically > 1, and $C_T \in (0,1)$ denotes the fraction desired for the global time error with respect to the tolerance Tol_M. If (46) does not hold, the whole computation is redone over $[0,T]$ with the same initial step τ_0 and the adjusted local tolerances

$$Tol_A = Tol_A \cdot fac, \quad Tol_R = Tol_R \cdot fac, \quad fac = C_T Tol_M / \|\tilde{e}_{h,M}\|. \tag{47}$$

Based on tolerance proportionality, reducing the local error estimates with the factor *fac* will reduce $e_h(T)$ by *fac* [8].

If (46) holds, we check whether

$$\|\tilde{e}_{h,M} + \tilde{\eta}_{h,M}\| \leq C_{control} Tol_M. \tag{48}$$

If it is true, the overall error $E_h(T) = V_h(T) - R_h u(T) = e_h(T) + \eta_h(T)$ is considered small enough relative to the chosen tolerance and $V_{h,M}$ is accepted. Otherwise, the whole computation is redone with the (already) adjusted tolerances (47) and an improved spatial resolution.

We use the new mesh size computed from (45) with $Tol = (1 - C_T) Tol_M$. To check the convergence behaviour in space and therefore also the quality of the approximation of the spatial truncation error, we additionally compute the numerically observed order

$$q_{num} = \log\left(\frac{\|\tilde{\eta}_{h,M}\|}{\|\tilde{\eta}_{h_{new},M}\|}\right) / \log\left(\frac{h}{h_{new}}\right). \tag{49}$$

If q_{num} computed for the final run is not close to the expected value q used for our Richardson extrapolation, we reason that the approximation of the spatial truncation errors has failed due to a dominating global time error, which happens, e.g., if the initial spatial mesh is already too fine. Consequently, we coarsen the initial mesh by a factor two and start again. If the control approach stops without a mesh refinement, we perform an additional control run on the coarse mesh and compute q_{num} from (49) with $h_{new} = 2h$. It turns out that this simple strategy works quite robustly, provided that the meshes used are able to resolve the basic behaviour of the solution.

Summarizing, the first check (46) and the possibly second control computation serve to significantly reduce the global time error. This enables us to make use of the approximation (36) for the spatial truncation error, which otherwise could not be trusted. The second step based on suitable spatial mesh improvement attempts to bring the overall error down to the imposed tolerance. Using the sum of the approximate global time and spatial error inside the norm in (48), we take advantage of favourable effects of error cancellation. These two steps are successively repeated until the second check is successful. Additionally, we take into account the numerically observed order in space to assess the approximation of the spatial truncation error.

7 Numerical illustration

To illustrate the performance of the global error estimators and the control strategy, we consider the Allen-Cahn equation modelling a diffusion-reaction problem. For results on further test problems and adaptive mesh refinement, see [2].

The bi-stable Allen-Cahn equation is defined by

$$\partial_t u = 10^{-2}\,\partial_{xx} u + 100u\,(1-u^2)\,, \quad 0<x<2.5\,, \qquad 0<t\leq T=0.5\,, \tag{50}$$

with the initial function and Dirichlet boundary values taken from the exact wave front solution $u(x,t) = (1+e^{\lambda\,(x-\alpha\,t)})^{-1}$, $\lambda = 50\sqrt{2}$, $\alpha = 1.5\sqrt{2}$. This problem was also used in [5].

We set $GTol_A = GTol_R = GTol$ for $GTol = 10^{-l}, l = 2,\dots,7$ and start with one and the same initial step size $\tau_0 = 10^{-5}$. Equally spaced meshes of 25, 51, 103, 207, 415, 831, and 1663 points are used as initial mesh. The control parameters introduced above for the control rules are $C_T = 1/3$ and $C_{control} = 1.2$. All runs were performed, but for convenience we only select a representative set of them for our presentation, which can be found in Table 1.

Table 1: Selected data for the Allen-Cahn problem.

Tol	N	Tol_M	$\Vert\tilde{E}_{h,M}\Vert$	$\Vert\tilde{e}_{h,M}\Vert$	$\Vert\tilde{\eta}_{h,M}\Vert$	Θ_{est}	Θ_{ctr}	q_{num}
1.00e-2	103	2.05e-2	1.84e-0	1.45e-1	1.98e-0	9.89	0.11	
4.69e-4	103	2.05e-2	5.78e-1	1.26e-3	5.79e-1	2.69	0.10	
4.69e-4	677	2.02e-2	6.04e-3	1.11e-3	7.15e-3	1.19	3.98	2.34
1.00e-2	415	2.02e-2	7.69e-2	1.44e-1	6.73e-2	3.05	0.80	
4.66e-4	415	2.02e-2	1.86e-2	1.11e-3	1.97e-2	1.23	1.34	
4.66e-4	207	2.03e-2	9.17e-2	1.15e-3	9.29e-2	1.47	0.32	2.24
1.00e-3	207	2.03e-3	9.82e-2	2.97e-3	1.01e-1	1.60	0.03	
2.27e-4	207	2.03e-3	8.80e-2	4.93e-4	8.85e-2	1.39	0.03	
2.27e-4	1683	2.02e-3	6.14e-4	4.71e-4	1.09e-3	1.11	3.67	2.10
1.00e-3	831	2.02e-3	2.26e-3	2.87e-3	5.12e-3	1.33	1.19	
2.35e-4	831	2.02e-3	4.01e-3	4.91e-4	4.50e-3	1.12	0.57	
2.35e-4	1521	2.02e-3	8.42e-4	4.90e-4	1.33e-3	1.12	2.68	2.02
1.00e-4	1663	2.02e-4	8.89e-4	1.86e-4	1.08e-3	1.07	0.24	
3.63e-5	1663	2.02e-4	9.88e-4	6.14e-5	1.05e-3	1.05	0.21	
3.63e-5	4643	2.02e-4	7.30e-5	6.14e-5	1.34e-4	1.04	2.89	2.00

Table 1 contains the following quantities, $Tol = Tol_A = Tol_R$ from (47), the number of mesh points N, $Tol_M = GTol\,(1+\Vert V_{h,M}\Vert)$ from (46), the estimated global error $\tilde{E}_{h,M} = \tilde{e}_{h,M} + \tilde{\eta}_{h,M}$ at time $t = T$, the estimated time error $\tilde{e}_{h,M}$, and the estimated spatial truncation error $\tilde{\eta}_{h,M}$. Note that we always start with $Tol = GTol$ in the first run.

The indicators $\Theta_{est} = \Vert\tilde{E}_{h,M}\Vert/\Vert E_h(T)\Vert$ for the ratio of the estimated global error and the true global error, and $\Theta_{ctr} = Tol_M/\Vert E_h(T)\Vert$ for the ratio of the desired tolerance and the true global error serve to illustrate the quality of the global error estimation and the control. $\Theta_{ctr} \geq 1/C_{control} = 5/6$ indicates control of the true global error.

The numerically observed order q_{num} for the spatial error is also given. From the table one can see whether a tolerance-adapted run to control the global time error, a spatial mesh adaptation step or an additional control run on a coarser grid was necessary. Especially, the latter is marked by a dashed line.

Table 1 reveals a high quality of the global error estimation and also the control process works quite well.

Let us pick one exemplary run out to explain the overall control strategy in more detail. Starting with $GTol = Tol = 10^{-3}$ and 831 mesh points, which corresponds to the fourth simulation, the numerical scheme delivers global error estimates $\|\tilde{e}_{h,M}\| = 2.87 \times 10^{-3}$ and $\|\tilde{\eta}_{h,M}\| = 5.12 \times 10^{-3}$ for the time and spatial error of the approximate solution $V_{h,M}$ at the final time $t_M = T$. The first check for the time error estimate $\|\tilde{e}_{h,M}\| \leq C_T C_{control} Tol_M = 8.08 \times 10^{-4}$ fails and we adjust the local tolerances by a factor $fac = C_T Tol_M / \|\tilde{e}_{h,M}\| = 2.35 \times 10^{-1}$, which yields the new $Tol = 2.35 \times 10^{-4}$. The computation is then redone. Due to the tolerance proportionality, in the second run the time error is significantly reduced and the inequality $\|\tilde{e}_{h,M}\| \leq 8.08 \times 10^{-4}$ is now valid. We proceed with checking $\|\tilde{E}_{h,M}\| \leq C_{control} Tol_M = 2.42 \times 10^{-3}$, which is still not true. From (45), we compute a new number of spatial mesh points $N = 1521$. Finally, the third run is successful and with the numerically observed spatial order $q_{num} = 2.02$ the numerical solution is accepted.

The ratios for $\Theta_{est} = \|\tilde{E}_{h,M}\| / \|E_h(T)\|$ lie between 1.04 and 1.23, after the control runs. Control of the global error, that is $\|E_h(T)\| \leq C_{control} Tol_M$, is in general achieved after two steps (one step to adjust the time grid and one step to control the space discretization), whereas the efficiency index $\Theta_{ctr} = Tol_M / \|E_h(T)\|$ is close to three. This results from a systematic cancellation effect between the global time and spatial error, which is not taken into account when computing h_{new} from (45).

8 Summary

We have developed an error control strategy for finite difference solutions of parabolic equations, involving both temporal and spatial discretization errors. The global time error strategy discussed in [5] appears to provide an excellent starting point for the development of such an algorithm. The classical ODE approach based on the first variational equation and the principle of tolerance proportionality is combined with an efficient estimation of the spatial error and mesh adaptation to control the overall global error. Inspired by [1], we have used Richardson extrapolation to approximate the spatial truncation error within the method of lines. Our control strategy aims at balancing the spatial and temporal discretization error in order to achieve an accuracy imposed by the user.

The key ingredients are: (i) linearised error transport equations equipped with sufficiently accurate defects to approximate the global time error and global spatial error and (ii) uniform or adaptive (see [2]) mesh refinement and local error control in time based on tolerance proportionality to achieve global error control. For illustration of the performance and effectiveness of our approach, we have implemented second-order finite differences in one space dimension and the example integrator ROS3P [4]. On the basis of the test problem in this article and two other test problems in [2] we could observe that our approach is very reliable, both with respect to estimation and control.

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