On Global Error Estimation and Control 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 Verver [SIAM J. Sci. Comput., 2007] for initial value problems to parabolic partial differential equations. The classical ODE approach based on the first variational equation is combined with an estimation for the PDE spatial truncation error to estimate the overall error in the computed solution. Control is achieved through tolerance proportionality and uniform mesh refinement. Numerical examples are used to illustrate the reliability of the estimation and control strategies.

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1 Introduction

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

$$\partial_t u(t,x) = f(t,x,u(t,x),\partial_x u(t,x),\partial_{xx}u(t,x))\,, \quad t\in(0,T]\,,\ x\in\Omega\subset\mathbb{R}^d\,, \tag{1.1}$$

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

$$u(0,x) = u_0(x)\,, \quad x\in\overline{\Omega}. \tag{1.2}$$

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

The method of lines is used to solve (1.1) numerically. We first discretize the PDE in space by means of finite differences or finite elements on a spatial mesh Ω_h with characteristic length 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

$$\begin{aligned} M_h\, U_h'(t) &= F_h(t, U_h(t))\,, \qquad t \in (0, T]\,, \\ U_h(0) &= U_{h,0}\,, \end{aligned} \tag{1.3}$$

with a unique solution vector $U_h(t)$ representing the spatial degrees of freedom. When finite differences are applied then M_h is the identity matrix and the initial condition is defined by evaluating the function $u_0(x)$ at the spatial mesh points. In the case of finite elements, M_h represents the well-known (regular) mass matrix and the initial vector $U_{h,0}$ is derived from a projection of $u_0(x)$ to the finite element space considered.

To solve the initial value problem (1.3), we apply a numerical integration method at a certain time grid

$$0 = t_0 < t_1 < \cdots < t_n < \cdots < t_{M-1} < t_M = T\,, \tag{1.4}$$

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

$$e_h(t) = V_h(t) - U_h(t)\,. \tag{1.5}$$

Numerical experiments in [7] 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. In order for the method of lines to be used efficiently, it is necessary to take also into account the spatial discretization error.

Let $R_h : u(t,\cdot) \to R_h u(t)$ be the restriction operator which maps $u(t)$ to its spatial degrees of freedom. Defining the spatial discretization error by

$$\eta_h(t) = U_h(t) - R_h u(t)\,, \tag{1.6}$$

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,

$$E_h(t) = e_h(t) + \eta_h(t)\,. \tag{1.7}$$

It is the purpose of this paper to present a new error control strategy for the global errors $E_h(t)$. This is achieved 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 [7]. To estimate the global spatial error, we follow an approach proposed in [2] (see also [8]) and use Richardson extrapolation to set up a linearized error transport equation. Spatial mesh refinement based on expected convergence orders is applied to control the global spatial error. In order to keep the description of the whole algorithm as clear as possible we consider only uniform meshes, however our estimates can be also used as a basis for adaptive mesh refinements.

In recent years goal-oriented adaptive control, that is, control of relevant quantities, has gained popularity [1, 3, 4, 9, 10]. Understood as optimal control problem, this approach naturally includes the backwards dual (or adjoint) system of ODEs or PDEs. The solution of the dual problem can be used to find optimal meshes, however it requires the additional storage of the approximate solution, which can be very demanding in practice. Nevertheless this goal would clearly justify more computational work. On the other hand, our algorithm uses only forward computations to control the overall global error.

2 Spatial and time error

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

$$\alpha_h(t) = M_h\,(R_h u)'(t) - F_h(t, R_h u(t))\,. \tag{2.1}$$

From (1.3) and (2.1), 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

$$\begin{aligned} M_h\,\eta_h'(t) &= F_h(t, U_h(t)) - F_h(t, R_h u(t)) - \alpha_h(t)\,, \qquad t \in (0,T]\,, \\ \eta_h(0) &= U_{h,0} - R_h u_0 \end{aligned} \tag{2.2}$$

Here and subsequently we use $U_{h,0} = R_h u_0$, which bears no restriction. Assuming F_h to be continuously differentiable, the mean value theorem for vector functions yields

$$\begin{aligned} M_h\,\eta_h'(t) &= \partial_{U_h} F_h(t, U_h(t))\,\eta_h(t) - \alpha_h(t) + \mathcal{O}(\eta_h(t)^2), \qquad t \in (0,T], \\ \eta_h(0) &= 0\,. \end{aligned} \tag{2.3}$$

With $V_h(t)$ being the continuous extension of the numerical approximation to (1.3), the residual time error is defined by

$$r_h(t) = M_h V_h'(t) - F_h(t, V_h(t))\,. \tag{2.4}$$

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

$$\begin{aligned} M_h\,e_h'(t) &= F_h(t, V_h(t)) - F_h(t, U_h(t)) + r_h(t)\,, \qquad t \in (0,T]\,, \\ e_h(0) &= 0\,. \end{aligned} \tag{2.5}$$

Again, the mean value theorem yields

$$\begin{aligned} M_h\,e_h'(t) &= \partial_{U_h} F_h(t, V_h(t))\,e_h(t) + r_h(t) + \mathcal{O}(e_h(t)^2), \qquad t \in (0,T], \\ e_h(0) &= 0\,. \end{aligned} \tag{2.6}$$

Apparently, by implementing proper choices of the defects $\alpha_h(t)$ and $r_h(t)$, solving (2.3) and (2.6) 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 (1.3) is of order $p \le 3$. Following the approach proposed in [7] 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

$$V_h(t) = V_{h,n} + A_n(t - t_n) + B_n(t - t_n)^2 + C_n(t - t_n)^3, \qquad t_n \le t \le t_{n+1}, \tag{3.1}$$

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

$$V_h(t_n + \theta\tau_n) = v_0(\theta) V_{h,n} + v_1(\theta) V_{h,n+1} + \tau_n w_0(\theta) M_h^{-1} F_{h,n} + \tau_n w_1(\theta) M_h^{-1} F_{h,n+1} \tag{3.2}$$

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

$$v_0(\theta) = (1-\theta)^2(1+2\theta),\ v_1(\theta) = \theta^2(3-2\theta),\ w_0(\theta) = (1-\theta)^2\theta,\ w_1(\theta) = \theta^2(\theta-1). \quad (3.3)$$

Now let $Y_h(t)$ be the (sufficiently smooth) solution of the ODE (1.3) 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

$$le_{n+1} = V_{h,n+1} - Y_h(t_{n+1}) = \mathcal{O}(\tau_n^{p+1}). \quad (3.4)$$

Combining (3.2) and (3.4) gives

$$\begin{aligned} V_h(t_n+\theta\tau_n) - Y_h(t_n+\theta\tau_n) \; = \; & \\ & v_1(\theta) le_{n+1} - Y_h(t_n+\theta\tau_n) + v_0(\theta)Y_h(t_n) + v_1(\theta)Y_h(t_{n+1}) \\ & +\tau_n w_0(\theta) M_h^{-1} F_h(t_n, Y_h(t_n)) + \tau_n w_1(\theta) M_h^{-1} F_h(t_{n+1}, Y_h(t_{n+1})) \\ & +\tau_n w_1(\theta) M_h^{-1}(F_h(t_{n+1}, V_{h,n+1}) - F_h(t_{n+1}, Y_h(t_{n+1}))), \end{aligned} \quad (3.5)$$

and by Taylor expansion we obtain

$$V_h(t_n+\theta\tau_n) - Y_h(t_n+\theta\tau_n) = v_1(\theta) le_{n+1} + \frac{1}{24}(2\theta^3-\theta^2-\theta^4)\tau_n^4 Y_h^{(4)}(t_n) + \mathcal{O}(\tau_n^{p+2}). \quad (3.6)$$

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

$$r_h(t) = M_h\, V_h'(t_n+\theta\tau_n) - M_h\, Y_h'(t_n+\theta\tau_n) + F_h(t, Y_h(t)) - F_h(t, V_h(t)), \quad (3.7)$$

with $\theta = (t-t_n)/\tau_n$, we find by differentiating the right hand side of (3.6)

$$r_h(t_n+\theta\tau_n) = 6(\theta-\theta^2)\frac{M_h\, le_{n+1}}{\tau_n} + \frac{1}{12}(3\theta^2-\theta-2\theta^3)\tau_n^3 M_h Y_h^{(4)}(t_n) + \mathcal{O}(\tau_n^{p+1}). \quad (3.8)$$

Here we have assumed that F_h is Lipschitz. Setting $\theta = 1/2$ in (3.8) will reveal

$$r_h(t_{n+1/2}) = \frac{3}{2}\frac{M_h\, le_{n+1}}{\tau_n} + \mathcal{O}(\tau_n^{p+1}). \quad (3.9)$$

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 [7], Section 2.2). Following the arguments given in [7], Section 2.1, we consider instead of (2.6) the step size frozen version

$$\begin{aligned} M_h\, \tilde{e}_h'(t) &= \partial_{U_h} F_h(t_n, V_{h,n})\, \tilde{e}_h(t) + \tfrac{2}{3} r_h(t_{n+\frac{1}{2}}),\ t \in (t_n, t_{n+1}],\ n = 0,\ldots,M-1, \\ \tilde{e}_h(0) &= 0 \end{aligned} \quad (3.10)$$

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

$$V_h(t_{n+1/2}) = \frac{1}{2}(V_{h,n} + V_{h,n+1}) + \frac{\tau}{8} M_h^{-1}(F_{h,n} - F_{h,n+1}) \quad (3.11)$$

and

$$V_h'(t_{n+1/2}) = \frac{3}{2\tau}(V_{h,n+1} - V_{h,n}) - \frac{1}{4} M_h^{-1}(F_{h,n} + F_{h,n+1}) \quad (3.12)$$

we can compute the residual time error halfway the step interval from (2.4)

$$\begin{aligned} r_h(t_{n+1/2}) &= \tfrac{3}{2\tau} M_h (V_{h,n+1} - V_{h,n}) - \tfrac{1}{4}(F_{h,n} + F_{h,n+1}) \\ &\quad - F_h \left(t_{n+\frac{1}{2}}, \tfrac{1}{2}(V_{h,n} + V_{h,n+1}) + \tfrac{\tau}{8} M_h^{-1} (F_{h,n} - F_{h,n+1}) \right). \end{aligned} \tag{3.13}$$

Remark 3.1 From (3.8) we deduce

$$\frac{1}{\tau_n} \int_{t_n}^{t_{n+1}} r_h(t)\, dt = \frac{M_h le_{n+1}}{\tau_n} + \mathcal{O}(\tau_n^{p+1}), \tag{3.14}$$

showing, in the light of (3.9), that $\frac{2}{3} r_h(t_{n+1/2})$ is in leading order equal to the time-averaged residual. As long as this mean value is a sufficiently accurate approximation to $r_h(t)$ for $t \in [t_n, t_{n+1}]$, we can justify the use of the error equation (3.10) without the link to the first variational equation.

4 Estimation of the spatial truncation error

An efficient strategy to estimate the spatial truncation error by Richardson extrapolation was proposed in [2]. We will adopt this approach to our setting.

Suppose we are given a second semi-discretization of the PDE system (1.1), now with characteristic length $2h$,

$$\begin{aligned} M_{2h} U_{2h}'(t) &= F_{2h}(t, U_{2h}(t)), \qquad t \in (0, T], \\ U_{2h}(0) &= U_{2h,0}. \end{aligned} \tag{4.1}$$

The following two assumptions will be needed. (i) The solution $U_{2h}(t)$ to the discretised 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_{2h}^h from the fine grid Ω_h to the coarse grid Ω_{2h} by the identity $R_{2h} = R_{2h}^h R_h$ and set

$$\eta_h^c(t) = R_{2h}^h \eta_h(t), \quad U_h^c(t) = R_{2h}^h U_h(t), \quad V_h^c(t) = R_{2h}^h V_h(t). \tag{4.2}$$

From the second assumption it follows that

$$\eta_h^c(t) = 2^{-q} \eta_{2h}(t) + \mathcal{O}(h^{q+1}) \tag{4.3}$$

and therefore

$$R_{2h} u(t) = \frac{2^q}{2^q - 1} U_h^c(t) - \frac{1}{2^q - 1} U_{2h}(t) + \mathcal{O}(h^{q+1}). \tag{4.4}$$

The relation $U_h^c(t) - U_{2h}(t) = \eta_h^c(t) - \eta_{2h}(t)$ together with (4.3) gives

$$U_h^c(t) - U_{2h}(t) = \frac{1 - 2^q}{2^q} \eta_{2h}(t) + \mathcal{O}(h^{q+1}). \tag{4.5}$$

The spatial truncation error on the coarse mesh Ω_{2h} is analogously defined to (2.1) as

$$\alpha_{2h}(t) = M_{2h} (R_{2h} u)'(t) - F_{2h}(t, R_{2h} u(t)). \tag{4.6}$$

Substituting $R_{2h}u(t)$ from (4.4) into the right-hand side, using the ODE system (4.1) to replace $M_{2h}U'_{2h}(t)$, and manipulating the expressions with (4.5) we get

$$\begin{aligned}\alpha_{2h}(t) &= \tfrac{2^q}{2^q-1}\Big(M_{2h}(U_h^c)'(t) - F_{2h}\Big(t, U_h^c(t) - \tfrac{1}{2^q}\eta_{2h}(t) + \mathcal{O}(h^{q+1})\Big)\Big) \\ &\quad + \tfrac{1}{2^q-1}\Big(F_{2h}\Big(t, U_{2h}(t) - \eta_{2h}(t) + \mathcal{O}(h^{q+1})\Big) - F_{2h}(t, U_{2h}(t))\Big) + \mathcal{O}(h^{q+1}).\end{aligned} \tag{4.7}$$

Taylor expansions yield

$$\alpha_{2h}(t) = \frac{2^q}{2^q-1}\Big(M_{2h}(U_h^c)'(t) - F_{2h}(t, U_h^c(t))\Big) + \mathcal{O}(h^{q+1})\,. \tag{4.8}$$

Analogously to (1.5), we set $e_h^c(t) = V_h^c(t) - U_h^c(t)$. Substituting $U_h^c(t)$ and its time derivative into (4.8) it follows that

$$\begin{aligned}\alpha_{2h}(t) &= \tfrac{2^q}{2^q-1}\Big(M_{2h}(V_h^c)'(t) - F_{2h}(t, V_h^c(t))\Big) + \mathcal{O}(h^{q+1}) \\ &\quad - \tfrac{2^q}{2^q-1}\Big(M_{2h}(e_h^c)'(t) - \partial_{U_h}F_{2h}(t, V_h^c(t))e_h^c(t)\Big) + \mathcal{O}(e_h^c(t)^2)\,.\end{aligned} \tag{4.9}$$

From (2.6) we expect that the term on the right-hand side involving $e_h^c(t)$ is of the order of the residual time error, that is, $\mathcal{O}(\tau^p)$ for any one-step method of order p. Assuming this expression to be sufficiently small, we can use

$$\tilde{\alpha}_{2h}(t) = \frac{2^q}{2^q-1}\Big(M_{2h}(V_h^c)'(t) - F_{2h}(t, V_h^c(t))\Big) \tag{4.10}$$

as approximation for the spatial truncation error on the coarse mesh. Since R_{2h}^h is time-independent we have $(V_h^c)'(t) = R_{2h}^h M_h^{-1} F_h(t, V_h(t))$. To guarantee a suitable quality of the estimation (4.10) 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. Thus, to approximate the global spatial error $\eta_h(t)$ we consider instead of (2.3) the step-size frozen version

$$\begin{aligned} M_h\,\tilde{\eta}'_h(t) &= \partial_{U_h}F_h(t_n, V_{h,n})\,\tilde{\eta}_h(t) - \tilde{\alpha}_h(t), \quad t \in (t_n, t_{n+1}],\ n = 0, \ldots, M-1, \\ \tilde{\eta}_h(0) &= 0 \end{aligned} \tag{4.11}$$

Remark 4.1 If an approximation $\tilde{e}_h(t)$ of the global time error has already been computed, we could make use of $U_h^c(t) \approx V_h^c(t) + \tilde{e}_h^c(t)$ to obtain a better approximation of $\alpha_{2h}(t)$ from (4.8). However, we have found by experiments that even in the case when the global time error was not small, using the step size frozen equations (3.10) and (4.11) to approximate the global time and spatial error does not yield a significantly better approximation. Since in practise the use of formula (4.8) requires additional function evaluations, equation (4.10) appears to be more efficient.

Remark 4.2 We note that special care has to be taken in the handling with the spatial truncation error at the boundary when derivative boundary conditions are present. In general, this causes no problem for finite element methods but requests interpolation adopted to the correct order of accuracy in the case of finite differences (see [2]).

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 (1.1) we use standard linear finite elements. Hence we have $q=2$. As restriction operator R^h_{2h} from Ω_h to Ω_{2h} injection is applied.

The example time integration formulas are taken from [7]. For the sake of completeness we shall give a short summary of the implementation used. To generate the time grid (1.4) we have used as an example integrator the 3rd-order, A-stable Runge-Kutta-Rosenbrock scheme ROS3P, see [5, 6] for more details. The property of tolerance proportionality [11] is asymptotically ensured through working for the local error with

$$Est = \frac{2}{3}\,(M_h - \gamma\tau_n A_{h,n})^{-1} r_h(t_{n+1/2})\,, \qquad A_{h,n} = \partial_{U_h} F_h(t_n, V_{h,n})\,, \tag{5.1}$$

where γ is the stability coefficient of ROS3P. The common filter $(M_h - \gamma\tau_n A_{h,n})$ 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 tolerances and the weighted L_2-norm $\|v_h\|^2 = v_h^T M_h v_h$. 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

$$\tau_{new} = \min\big(1.5, \max(2/3, 0.9\,r)\big)\,\tau_n\,, \qquad r = (Tol_n/D_n)^{1/3}\,. \tag{5.2}$$

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 (3.10) and (4.11) 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

$$\begin{aligned} (M_h - \tfrac{1}{2}\tau_n A_{h,n})\,\delta e_{n+1} &= 2M_h\tilde{e}_{h,n} + \tfrac{2}{3}\tau_n r(t_{n+1/2})\,, \\ \tilde{e}_{h,n+1} &= \delta e_{n+1} - \tilde{e}_{h,n}\,, \end{aligned} \tag{5.3}$$

and

$$\begin{aligned} (M_h - \tfrac{1}{2}\tau_n A_{h,n})\,\delta \eta_{n+1} &= 2M_h\tilde{\eta}_{h,n} - \tau_n\tilde{\alpha}_h(t_{n+1/2})\,, \\ \tilde{\eta}_{h,n+1} &= \delta \eta_{n+1} - \tilde{\eta}_{h,n}\,. \end{aligned} \tag{5.4}$$

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

$$\tilde{\alpha}_{2h}(t_{n+1/2}) = \frac{4}{3}\,\left(R^h_{2h}M_h^{-1}F_h\left(t_{n+1/2}, V_h(t_{n+1/2})\right) - F_{2h}\left(t_{n+1/2}, R^h_{2h}V_h(t_{n+1/2})\right)\right)\,. \tag{5.5}$$

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 (3.13), this requires only one linear solve with M_h and 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 by linear interpolation of the coarse grid values and is then divided by 2. Note that since a weak formulation is used for the finite element method we have $\alpha_h(t)=\mathcal{O}(h)$.

Due to freezing the coefficients in each time step, the second-order midpoint rule is a first-order method when interpreted for solving the linearized equations (2.6) (or likewise the first variational equation) and (2.3). Thus if all is going well, we asymptotically have $\tilde{e}_{h,n}=e_h(t_n)+\mathcal{O}(\tau_{max}^4)$ and $\tilde{\eta}_{h,n}=\eta_h(t_n)+\mathcal{O}(\tau_{max}h^q)+\mathcal{O}(h^{q+1})$.

6 The control rules

Like for the ODE case studied in [7] our aim is to provide global error estimations and to control the accuracy of the solution numerically computed to the imposed tolerance level. 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

$$\|\tilde{e}_{h,M}\| \leq C_T C_{control} Tol_M, \qquad Tol_M = Tol_A + Tol_R \|V_{h,M}\|, \tag{6.1}$$

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 (6.1) does not hold, the whole computation is redone over $[0,T]$ with the same initial step τ_0 and the adjusted tolerances

$$Tol_A = Tol_A \cdot fac, \qquad Tol_R = Tol_R \cdot fac, \qquad fac = C_T Tol_M / \|\tilde{e}_{h,M}\|. \tag{6.2}$$

Based on tolerance proportionality, reducing the local error estimates with the factor *fac* will reduce $e_h(T)$ by *fac* [11].

If (6.1) holds, we check whether

$$\|\tilde{e}_{h,M} + \tilde{\eta}_{h,M}\| \leq C_{control} Tol_M. \tag{6.3}$$

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 adjusted tolerances (6.2) and the new (uniform) spatial resolution

$$h_{new} = \sqrt[q]{\frac{(1 - C_T) Tol_M}{\|\tilde{\eta}_{h,M}\|}}\, h \tag{6.4}$$

to account for achieving $\eta_{h_{new}}(T) \approx (1 - C_T) Tol_M$. To check the convergence behavior in space and therefore also the quality of the approximation of the spatial truncation error, we compute the numerically observed order

$$q_{num} = \log\left(\frac{\|\tilde{\eta}_{h,M}\|}{\|\tilde{\eta}_{h_{new},M}\|}\right) \Big/ \log\left(\frac{h}{h_{new}}\right). \tag{6.5}$$

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 (6.5) with $h_{new} = 2h$. It turned out that this simple strategy works quite robust, provided that the meshes used are able to resolve the basic behavior of the solution.

Summarizing, the first check (6.1) and the possibly second control computation serve to significantly reduce the global time error. This enables us to make use of the approximation (4.10) for the spatial truncation error, which otherwise could no be trusted. The second step based on suitable spatial mesh improvement attempts to bring the overall error down to the imposed tolerance. This is controlled by the spatial order of convergence numerically computed from (6.5). Using the sum of the approximate global time and spatial error inside the norm in (6.3), we take advantage of favorable effects of error cancelation. 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 illustrations

To illustrate the performance of the global error estimators and the control strategy, we consider three test problems: (i) the Allen-Cahn equation modelling a diffusion-reaction problem [7] , (ii) the highly stable heat equation with nonhomogeneous Neumann boundary conditions [2], and (iii) the nonlinear convection-dominated Burgers' equation [2, 8]. Analytic solutions are known for all three problems.

We set $Tol_A = Tol_R = Tol$ for $Tol = 10^{-l}, l = 2, \ldots, 7$ 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.

We define the estimated global error $\tilde{E}_{h,M} = \tilde{e}_{h,M} + \tilde{\eta}_{h,M}$ at time $t = T$ and set indicators $\Theta_{est} = \|\tilde{E}_{h,M}\| / \|E_h(T)\|$ for the ratio of the estimated global error and the true global error, and $\Theta_{ctr} = Tol_M / \|E_h(T)\|$ for the ratio of the desired tolerance and the true global error. Thus, $\Theta_{ctr} \geq 1/C_{control} = 5/6$ indicates control of the true global error.

The tables of results contain the following quantities, $Tol_M = Tol\,(1 + \|V_{h,M}\|)$ from (6.1), the estimated global error $\tilde{E}_{h,M}$, the estimated time error $\tilde{e}_{h,M}$, and the estimated spatial truncation error $\tilde{\eta}_{h,M}$. The ratios Θ_{est} and Θ_{ctr} serve to illustrate the quality of the global error estimation and the control. In addition, the numerically observed order q_{num} for the spatial error is given. It will be clear from the tables of results whether a tolerance-adapted run to control the global time error, a spatial mesh adaption step or an additional control run on a coarser grid was necessary.

7.1 The Allen-Cahn equation

The first problem is the bi-stable Allen-Cahn equation which is defined by

$$\partial_t u = 10^{-2}\,\partial_{xx} u + 100u\,(1 - u^2)\,, \quad 0 < x < 2.5\,, \qquad 0 < t \leq T = 0.5\,, \tag{7.1}$$

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 [7].

Table 7.1 reveals a high quality of the global error estimation and also the control process works quite well. The ratios for $\Theta_{est} = \|\tilde{E}_{h,M}\| / \|E_h(T)\|$ lie between 1.04 and 1.21, 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 improved for finer initial meshes. This results from a better approximation of the spatial truncation error in this case, which yields a more favourable h_{new} from (6.4). Also observe that for the extremely coarse or fine initial meshes chosen for the tolerance $Tol = 1.0e-4$, the approach performs excellent with respect to estimation and control. Similar results are obtained for other combinations of tolerances and initial spatial meshes.

Tol	N	Tol_M	$\|\tilde{E}_{h,M}\|$	$\|\tilde{e}_{h,M}\|$	$\|\tilde{\eta}_{h,M}\|$	Θ_{est}	Θ_{ctr}	q_{num}
1.00e−2	51	1.64e−2	1.84e+1	2.89e−1	1.81e+1	20.76	0.02	
1.89e−4	51	1.64e−2	2.22e+0	1.02e−3	2.22e+0	2.54	0.02	
1.89e−4	741	1.65e−2	3.84e−3	3.41e−4	3.50e−3	1.14	4.90	2.43
1.00e−2	207	1.63e−2	5.65e−1	2.03e−1	3.61e−1	7.75	0.22	
2.68e−4	207	1.64e−2	6.48e−2	4.96e−4	6.43e−2	1.69	0.43	
2.68e−4	505	1.64e−2	8.48e−3	5.12e−4	7.97e−3	1.21	2.35	2.35
1.00e−3	103	1.62e−3	5.83e−1	2.72e−3	5.80e−1	4.59	0.01	
1.99e−4	103	1.62e−3	5.88e−1	3.62e−4	5.88e−1	4.67	0.01	
1.99e−4	2425	1.65e−3	6.80e−4	3.62e−4	3.19e−4	1.11	2.69	2.39
1.00e−3	415	1.64e−3	1.69e−2	2.69e−3	1.42e−2	1.44	0.14	
2.04e−4	415	1.64e−3	1.23e−2	3.70e−4	1.20e−2	1.23	0.16	
2.04e−4	1375	1.65e−3	1.37e−3	3.72e−4	9.98e−4	1.12	1.35	2.08
1.00e−4	25	1.78e−4	6.19e−2	7.07e−7	6.19e−2	0.06	0.00	
1.00e−4	595	1.65e−4	5.52e−3	1.64e−4	5.36e−3	1.13	0.03	0.78
3.33e−5	595	1.65e−4	5.25e−3	4.91e−5	5.20e−3	1.10	0.03	
3.33e−5	4103	1.65e−4	1.54e−4	4.91e−5	1.04e−4	1.04	1.12	2.03
1.00e−4	1663	1.65e−4	8.23e−4	1.65e−4	6.58e−4	1.08	0.22	
3.33e−5	1663	1.65e−4	6.87e−4	4.91e−5	6.38e−4	1.05	0.25	
3.33e−5	4013	1.65e−4	1.58e−4	4.90e−5	1.09e−4	1.04	1.09	2.01

Table 7.1: Selected data for the Allen-Cahn problem.

7.2 Heat equation with Neumann boundary conditions

This heat equation provides an example with inhomogeneous Neumann boundary conditions:

$$\partial_t u = \partial_{xx} u\,, \quad 0 < x < 1.0\,, \qquad 0 < t \leq T = 0.2\,, \tag{7.2}$$

and boundary conditions $\partial_x u = \pi\, e^{-\pi^2 t}\cos(\pi x)$ at $x=0$ and $x=1$. The initial condition is consistent with the analytic solution $u(x,t)=e^{-\pi^2 t}\sin(\pi x)$. Although the solution is very stable, it is not easy to provide good error estimators as stated in [2, 8].

Due to the high stability of the problem the global time errors are much smaller than imposed local tolerances. So, control of the global time error is redundant here and control runs were only carried out in case of insufficient spatial resolutions. Table 7.2 shows results for various tolerances and initial meshes. The global error estimation and control appear to work very well for this problem, where the influence of the initial mesh points is less strong. This holds also for other combinations of tolerances and initial meshes. Note the high quality of the estimator $\tilde{E}_{h,M}$ (and therefore also of $\tilde{\eta}_{h,M}$), showing that the derivative boundary condition is well resolved within the Richardson extrapolation. For the runs with tolerances $Tol=10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$, the order of the spatial convergence was successfully checked with a second run on the coarse mesh, that is, we can trust the first run.

7.3 Burgers' equation

The third problem is the nonlinear Burgers' equation

$$\partial_t u = \varepsilon\, \partial_{xx} u - u\partial_x u\,, \quad 0 < x < 1.0\,, \qquad 0 < t \leq T = 1.0\,, \tag{7.3}$$

Tol	N	Tol_M	$\|\tilde{E}_{h,M}\|$	$\|\tilde{e}_{h,M}\|$	$\|\tilde{\eta}_{h,M}\|$	Θ_{est}	Θ_{ctr}	q_{num}
1.00e−2	25	1.09e−2	6.63e−4	1.06e−4	7.48e−4	0.99	16.35	
1.00e−2	13	1.09e−2	2.77e−3	1.01e−4	2.85e−3	0.98	3.86	1.93
1.00e−3	51	1.10e−3	1.62e−4	1.87e−5	1.77e−4	1.00	6.77	
1.00e−3	25	1.09e−3	7.34e−4	1.83e−5	7.49e−4	0.99	1.48	1.97
1.00e−4	103	1.10e−4	4.15e−5	1.93e−6	4.29e−5	1.00	2.64	
1.00e−4	51	1.10e−4	1.75e−4	1.89e−6	1.77e−4	1.00	0.62	1.99
1.00e−5	207	1.10e−5	1.05e−5	1.96e−7	1.06e−5	1.00	1.05	
1.00e−5	103	1.10e−5	4.28e−5	1.94e−7	4.29e−5	1.00	0.26	1.99
1.00e−6	415	1.10e−6	2.61e−6	1.80e−8	2.62e−6	1.00	0.42	
1.00e−6	787	1.10e−6	7.19e−7	1.81e−8	7.29e−7	1.00	1.53	2.00
1.00e−7	25	1.09e−7	7.50e−4	1.56e−9	7.50e−4	1.00	0.00	
1.00e−7	2637	1.10e−7	6.40e−8	1.59e−9	6.48e−8	1.00	1.72	1.99
1.00e−7	1663	1.10e−7	1.62e−7	1.59e−9	1.63e−7	1.00	0.68	
1.00e−7	2485	1.10e−7	7.22e−8	1.59e−9	7.30e−8	1.00	1.52	2.00

Table 7.2: Selected data for the heat equation with Neumann boundary conditions.

where $\varepsilon = 0.015$ as in [1] is used in the experiments. Dirichlet boundary conditions and initial conditions are consistent with the analytic solution defined by

$$u(x,t) = \frac{r_1 + 5r_2 + 10r_3}{10(r_1 + r_2 + r_3)} \tag{7.4}$$

where $r_1(x) = e^{0.45x/\varepsilon}$, $r_2(t,x) = e^{0.01(10+6t+25x)/\varepsilon}$, and $r_3(t) = e^{0.025(6.5+9.9t)/\varepsilon}$.

In Table 7.3 we present results for all tolerances used and the 51-point initial mesh. The use of a relatively coarse mesh at the beginning is the natural choice in practice. No adaptation in time is necessary, which is mainly due to the small first time step and the maximum factor 1.5 which is allowed in (5.2) for a step size enlargement. For the tolerances $Tol = 10^{-2}, 10^{-3}$, the numerical solution is accepted since the corresponding control run shows $q_{num} \approx 2$, the expected value. Remarkably excellent estimators are obtained for higher tolerances. Here, control is always achieved after one spatial mesh improvement.

8 Summary

We have developed an error control strategy for the solution of parabolic equations, involving both temporal and spatial discretization errors. The global time error strategy discussed in [7] 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 uniform refinement to control the overall global error. Inspired by [2], 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) linearized error transport equations equipped with sufficiently accurate defects to approximate the global time error and global spatial error and (ii) uniform

Tol	N	Tol_M	$\|\tilde{E}_{h,M}\|$	$\|\tilde{e}_{h,M}\|$	$\|\tilde{\eta}_{h,M}\|$	Θ_{est}	Θ_{ctr}	q_{num}
$1.00e-2$	51	$1.93e-2$	$2.82e-3$	$2.69e-3$	$3.27e-4$	1.26	8.59	
$1.00e-2$	25	$1.92e-2$	$3.06e-3$	$2.23e-3$	$1.29e-3$	1.21	7.63	1.99
$1.00e-3$	51	$1.93e-3$	$3.55e-4$	$1.22e-4$	$3.03e-4$	1.04	5.69	
$1.00e-3$	25	$1.92e-3$	$1.21e-3$	$1.19e-4$	$1.17e-3$	0.98	1.55	1.95
$1.00e-4$	51	$1.93e-4$	$3.02e-4$	$1.02e-5$	$3.00e-4$	1.01	0.65	
$1.00e-4$	79	$1.93e-4$	$1.28e-4$	$1.15e-5$	$1.26e-4$	1.01	1.52	2.02
$1.00e-5$	51	$1.93e-5$	$2.99e-4$	$9.91e-7$	$2.99e-4$	1.01	0.07	
$1.00e-5$	251	$1.94e-5$	$1.28e-5$	$1.02e-6$	$1.26e-5$	1.00	1.52	2.01
$1.00e-6$	51	$1.93e-6$	$2.99e-4$	$1.01e-7$	$2.99e-4$	1.01	0.01	
$1.00e-6$	791	$1.94e-6$	$1.29e-6$	$9.34e-8$	$1.28e-6$	1.00	1.51	2.00
$1.00e-7$	51	$1.93e-7$	$2.98e-4$	$9.94e-9$	$2.98e-4$	1.01	0.00	
$1.00e-7$	2503	$1.94e-7$	$1.29e-7$	$8.57e-9$	$1.28e-7$	1.00	1.51	2.00

Table 7.3: Selected data for Burgers' equation with 51 initial mesh points.

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 linear finite elements in one space dimension and the example integrator ROS3P [6]. On the basis of three different test problems we could observe that our approach is very reliable, both with respect to estimate and control. In forthcoming work we will also include adaptive mesh refinement in space, which is especially more efficient for solutions having a strongly nonuniform nature in space.

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