An improved local error estimator for symmetric time-stepping schemes[1]

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Abstract

We propose a symmetrized version of the defect to be used in the estimation of the local time-stepping error of symmetric one-step methods for the time propagation of linear autonomous evolution equations. Using the anti-commutator of the numerical flow and the right-hand side operator in the definition of the defect of the numerical approximation, a local error estimator is obtained which has higher accuracy asymptotically than an established version using the common defect. This theoretical result is illustrated for a splitting method applied to a linear Schrödinger equation.

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1. Introduction

Consider the evolution equation

$$u'(t) = H\,u(t), \quad u(0) = u_0, \tag{1}$$

defined on a Banach space $\mathcal{X}$, with a generally unbounded time-independent operator $H\colon \mathcal{D}(H) \subset \mathcal{X} \to \mathcal{X}$ which generates a semigroup. We assume that the problem is well-defined with a sufficiently regular solution u, and denote the fundamental solution by $\mathcal{E} = \mathcal{E}(t) = \mathrm{e}^{\,t\,H}$, such that

$$\mathcal{E}' = H\,\mathcal{E} = \mathcal{E}\,H = \tfrac{1}{2}\,\mathcal{E}\,H + \tfrac{1}{2}\,H\,\mathcal{E} = \tfrac{1}{2}\{\mathcal{E}, H\}, \tag{2}$$

where $\{U, V\} = U\,V + V\,U$ denotes the anti-commutator of two operators. Observe that the symmetrized problem (2) is a special case of a Sylvester-type differential equation.

Let $\mathcal{S}(t)$ denote the numerical flow generated by a one-step integration scheme of order p, with $\mathcal{S} \approx \mathcal{E}$. The local error of the integrator is denoted by $\mathcal{L} = \mathcal{S} - \mathcal{E}$.

In computational practice, the error estimator $\tilde{\mathcal{L}} \approx \mathcal{L}$ discussed below will be applied in a finite-dimensional setting after (spatial) discretization of the given evolution equation and can serve as a reliable basis for the adaptive choice of optimal time step-sizes for efficient large-scale computations. In our reasoning below we tacitly assume all the appearing quantities to be as smooth as required.

2. Defect-based local error estimation

2.1. Classical version

We consider (w.l.o.g.) a single step of the one-step method represented by $\mathcal{S}$ starting from $t = 0$. An asymptotically correct computable local error estimator based on the (classical) defect $\mathcal{D}_c$ of the numerical solution,

$$\mathcal{D}_c(t) = \mathcal{S}'(t) - H\,\mathcal{S}(t), \tag{3}$$

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has been successfully employed particularly for the adaptive integration of time-dependent Schrödinger equations by splitting methods in a series of papers [1, 2, 3]. Here the local error is approximated on the basis of the relation

$$\mathcal{L}(t) = \int_0^t \mathrm{e}^{\,(t-\tau)H}\, \mathcal{D}_c(\tau)\, \mathrm{d}\tau = \tfrac{1}{p+1}\, t\, \mathcal{D}_c(t) + \mathscr{O}(t^{p+2}). \tag{4}$$

This represents the approximation of the local error integral by Hermite quadrature, involving a single evaluation at $\tau = t$ and exploiting the fact that, due to convergence order p, the derivatives of the integrand vanish at $\tau = 0$ up to order $p-1$. The resulting a posteriori error estimator is denoted by $\tilde{\mathcal{L}}_c(t) := \frac{1}{p+1}\, t\, \mathcal{D}_c(t)$.

2.2. Symmetrized version

Self-adjoint one-step schemes (also called time-reversible or symmetric) are characterized by the property $\mathcal{S}(-t)\mathcal{S}(t) = \mathrm{Id}$. We stress that self-adjoint schemes have even order p, see [4, Theorem II.3.2].

In the following we assume that $\mathcal{S}$ is self-adjoint, and thus the parameter p, denoting the order of the scheme, is an even integer. For this case, a modified construction employing a symmetrized defect,

$$\mathcal{D}_s(t) := \mathcal{S}'(t) - \tfrac{1}{2}\{\mathcal{S}(t), H\}, \tag{5}$$

yields a local error estimator with higher asymptotical accuracy, as we reason below. We will show that, in contrast to (4), we even have

$$\mathcal{L}(t) = \int_0^t \mathrm{e}^{\,(t-\tau)(\frac{1}{2}H)}\, \mathcal{D}_s(\tau)\, \mathrm{e}^{\,(t-\tau)(\frac{1}{2}H)} \mathrm{d}\tau = \tfrac{1}{p+1}\, t\, \mathcal{D}_s(t) + \mathscr{O}(t^{p+3}). \tag{6}$$

The error estimator $\tilde{\mathcal{L}}_s(t) := \frac{1}{p+1}\, t\, \mathcal{D}_s(t)$ with symmetrized defect $\mathcal{D}_s$ is based on Hermite quadrature formula as for the classical version, but now applied to (6).

Theorem 1. *Consider a selfadjoint one-step scheme of (even) order $p \geq 2$, represented by $\mathcal{S}(t)$, applied to a linear evolution equation* (1)*. Let $\mathcal{E}(t) = \mathrm{e}^{tH}$, and*

$$\widehat{\mathcal{S}}(t) = \mathcal{S}(t) - \tilde{\mathcal{L}}_s(t) = \mathcal{S}(t) - \tfrac{1}{p+1}\, t\, \mathcal{D}_s(t), \quad \mathcal{D}_s(t) \text{ from } (5).$$

Then the local error operator $\widehat{\mathcal{L}}(t) = \widehat{\mathcal{S}}(t) - \mathcal{E}(t)$ of the corrected scheme represented by $\widehat{\mathcal{S}}(t)$ satisfies

$$\widehat{\mathcal{L}}(t) = \mathscr{O}(t^{p+3}), \tag{7}$$

i.e., the corrected scheme has even order $p+2$.

Proof: By assumption on $\mathcal{S}$ we have $\mathcal{S}(-t)\,\mathcal{S}(t) = I$. By construction of $\mathcal{D}_s$ we have $\mathcal{D}_s(t) = \mathscr{O}(t^p)$, and the corrected scheme is of order $p+1$ at least (cf. e.g. [2]). It will have even order $p+2$ if it is again selfadjoint or sufficiently close to selfadjoint. Thus, let us consider $\widehat{\mathcal{S}}(-t)\,\widehat{\mathcal{S}}(t)$:

$$\begin{aligned}\widehat{\mathcal{S}}(-t)\,\widehat{\mathcal{S}}(t) &= \big(\mathcal{S}(-t) + \tfrac{1}{p+1}\, t\, \mathcal{D}_s(-t)\big)\,\big(\mathcal{S}(t) - \tfrac{1}{p+1}\, t\, \mathcal{D}_s(t)\big) \\ &= \underbrace{\mathcal{S}(-t)\,\mathcal{S}(t)}_{=\,I} - \tfrac{1}{p+1}\, t\,\big(\mathcal{S}(-t)\,\mathcal{D}_s(t) - \mathcal{D}_s(-t)\,\mathcal{S}(t)\big) - \tfrac{1}{(p+1)^2}\, t^2\, \mathcal{D}_s(-t)\,\mathcal{D}_s(t)\,.\end{aligned}$$

Here, $\mathcal{S}(-t)\,\mathcal{D}_s(t) - \mathcal{D}_s(-t)\,\mathcal{S}(t)$ is the critical term. With

$$\begin{aligned}\mathcal{D}_s(t) &= \mathcal{S}'(t) - \tfrac{1}{2}\{\mathcal{S}(t), H\}, \\ \mathcal{D}_s(-t) &= \mathcal{S}'(-t) - \tfrac{1}{2}\{\mathcal{S}(-t), H\}\end{aligned}$$

we have

$$\begin{aligned}\mathcal{S}(-t)\,\mathcal{D}_s(t) &= \mathcal{S}(-t)\,\mathcal{S}'(t) - \mathcal{S}(-t)\,\tfrac{1}{2}\{\mathcal{S}(t), H\} \\ &= \mathcal{S}(-t)\,\mathcal{S}'(t) - \tfrac{1}{2}H - \tfrac{1}{2}\mathcal{S}(-t)\,H\,\mathcal{S}(t),\end{aligned}$$

and

$$\begin{aligned}\mathcal{D}_s(-t)\,\mathcal{S}(t) &= \mathcal{S}'(-t)\,\mathcal{S}(t) - \tfrac{1}{2}\{\mathcal{S}(-t), H\}\,\mathcal{S}(t)\\ &= \mathcal{S}'(-t)\,\mathcal{S}(t) - \tfrac{1}{2}\mathcal{S}(-t)\,H\,\mathcal{S}(t) - \tfrac{1}{2}H\,.\end{aligned}$$

Together with $\mathcal{S}(-t)\,\mathcal{S}(t) = I$, whence

$$0 = \tfrac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{S}(-t)\,\mathcal{S}(t)\big) = -\mathcal{S}'(-t)\,\mathcal{S}(t) + \mathcal{S}(-t)\,\mathcal{S}'(t),$$

we obtain

$$\mathcal{S}(-t)\,\mathcal{D}_s(t) - \mathcal{D}_s(-t)\,\mathcal{S}(t) = 0\,.$$

Thus,

$$\widehat{\mathcal{S}}(-t)\,\widehat{\mathcal{S}}(t) = I - \tfrac{1}{(p+1)^2}t^2\,\mathcal{D}_s(-t)\,\mathcal{D}_s(t) = I + \mathscr{O}(t^{2\,p+2}),$$

i.e., $\widehat{\mathcal{S}}$ is very close to selfadjoint. Now we reason in a similar way as in the proof of [4, Theorem II.3.2], proceeding from the local error structure (asymptotic expansion) for $\widehat{\mathcal{S}}(t)$,

$$\widehat{\mathcal{S}}(t) = \mathcal{E}(t) + t^{p+2}\,C + \mathscr{O}(t^{p+3})\,.$$

Then,

$$\begin{aligned}I + \mathscr{O}(t^{2\,p+2}) &= \widehat{\mathcal{S}}(-t)\,\widehat{\mathcal{S}}(t)\\ &= \big(\mathcal{E}(-t) + t^{p+2}\,C + \mathscr{O}(t^{p+3})\big)\big(\mathcal{E}(t) + t^{p+2}\,C + \mathscr{O}(t^{p+3})\big)\\ &= \underbrace{\mathcal{E}(-t)\,\mathcal{E}(t)}_{=\,I} + t^{p+2}\,\big(\mathcal{E}(-t)\,C + C\,\mathcal{E}(t)\big) + \mathscr{O}(t^{p+3}).\end{aligned}$$

Due to $\mathcal{E}(\pm t) = I \pm t\,H + \mathscr{O}(t^2)$ this implies $C = 0$. □

Theorem 1 also implies that the symmetrized defect-based local error estimator is of a better asymptotic quality than the classical one, with a deviation $\tilde{\mathcal{L}}(t) - \mathcal{L}(t) = \mathscr{O}(t^{p+3})$ and not only $\mathscr{O}(t^{p+2})$.

Remark 1. *An inspection of the proof of Theorem 1 shows that the argument remains valid under the weaker assumption*

$$\mathcal{S}(-t)\,\mathcal{S}(t) = I + \mathscr{O}(t^q) \quad \textit{with} \quad q > p + 2\,. \tag{8}$$

This also shows that Theorem 1 can be applied to the corrected scheme $\widehat{\mathcal{S}}(t)$, with order $p+2 \geq 4$ instead of p, satisfying (see proof above)

$$\widehat{\mathcal{S}}(-t)\,\widehat{\mathcal{S}}(t) = I + \mathscr{O}(t^q) \quad \textit{with} \quad q = 2\,p + 2,$$

since for $p \geq 4$ we have $q = 2\,p + 2 > (p + 2) + 2$, and therefore (8) is satisfied (mutatis mutandis) for the scheme of order $p + 2$. This argument can be repeated inductively.
However, this method of increasing the order by defect correction will usually not be practically very relevant due to a prohibitive computational effort as compared to a straightforward higher-order method.

Remark 2. *A modification of the approach presented here also applies to nonlinear and/or nonautonomous problems. Its practical efficiency remains to be investigated, however, and corresponding results and applications will be reported elsewhere.*

3. Splitting methods

For problems (1) with a partitioned operator $H = A + B$, exponential splitting methods are commonly used because of their favorable computational properties [1, 2, 3, 4]. As an example to illustrate the general considerations above, we resort to a symmetric 3-stage splitting method

$$\mathcal{S} = \mathcal{S}(t) = \mathrm{e}^{\,tA_1}\,\mathrm{e}^{\,tB_1}\,\mathrm{e}^{\,tA_2}\,\mathrm{e}^{\,tB_1}\,\mathrm{e}^{\,tA_1}, \tag{9}$$

where we denote $A_j = a_j\,A$, $B_j = b_j\,B$. For a consistent scheme we have $2\,A_1 + A_2 = A$ and $2\,B_1 = B$.

Practical evaluation of the defect. In this situation, the defect can be evaluated efficiently, see [2]: With

$$v_1 = \mathrm{e}^{tB_1}\,\mathrm{e}^{tA_1}\,u, \quad v_2 = \mathrm{e}^{tB_1}\,\mathrm{e}^{tA_2}\,v_1, \quad v_3 = \mathrm{e}^{tA_1}\,v_2,$$

the classical defect (3) evaluates to

$$\begin{aligned}\mathcal{D}_c\,u = \mathrm{e}^{tA_1}\,\Big(B_1\,v_2 + \mathrm{e}^{tB_1}\,\mathrm{e}^{tA_2}\,\Big((A_2+B_1)\,v_1 + \mathrm{e}^{tB_1}\,\mathrm{e}^{tA_1}\,A_1\,u\Big)\Big)\\ - (A_1+A_2+B)\,v_3.\end{aligned}$$

Similarly for the symmetrized defect (5),

$$\begin{aligned}\mathcal{D}_s\,u = \mathrm{e}^{tA_1}\,\Big(B_1\,v_2 + \mathrm{e}^{tB_1}\,\mathrm{e}^{tA_2}\,\Big(\big(A_2+B_1\big)\,v_1 + \mathrm{e}^{tB_1}\,\mathrm{e}^{tA_1}\,\Big(-\big(\tfrac{1}{2}A_2+B_1\big)\,u\Big)\Big)\Big)\\ - \tfrac{1}{2}(A_2+B)\,v_3.\end{aligned}$$

Thus, the additional effort for the evaluation of $\mathcal{D}_s\,u$ only amounts to one more matrix-vector product. For an arbitrary number of stages the procedure is analogous.

4. Numerical example

To give a numerical illustration of the above considerations, we solve a linear Schrödinger equation

$$\mathrm{i}\,\partial_t\,\psi(x,t) = -\tfrac{1}{2}\,\partial_x^2\,\psi(x,t) + V(x)\,\psi(x,t), \tag{10a}$$

with harmonic potential

$$V(x) = \tfrac{1}{2}\,\omega^2\,x^2, \tag{10b}$$

and exact solution

$$\psi(x,t) = \big(\tfrac{\omega}{\pi}\big)^{\frac{1}{4}}\,\exp\big(-\tfrac{\omega}{2}(\mathrm{i}\,t + x^2)\big). \tag{10c}$$

We choose $\omega = 1$ and impose periodic boundary conditions on the interval $x \in [-H, H]$ with $H = 10$. We use the 5-stage 4th-order splitting scheme 'Emb 4/3 AK s' ($p = 4$) from the collection [5], with the potential $V(x)$ playing the role of A and the kinetic term playing the role of B. The latter is discretized in space using pseudospectral Fourier-type collocation using 512 subintervals. Table 1 shows the local splitting error after a single step with stepsize t together with the deviation of the local error estimates based on the classical and symmetrized defect, respectively.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\tilde{\mathcal{L}}_c\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order	$\|\tilde{\mathcal{L}}_s\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order
0.40	1.77 e-05		1.42 e-06		6.31 e-08	
0.20	5.57 e-07	5.0	2.23 e-08	6.0	4.95 e-10	7.0
0.10	1.74 e-08	5.0	3.49 e-10	6.0	3.87 e-12	7.0
0.05	5.45 e-10	5.0	5.45 e-12	6.0	3.16 e-14	7.0

Table 1: Numerical results for example (10). The norm $\|\cdot\|_2$ is gauged in a way such that it is a discrete analog of the L_2-norm on $[-H, H]$.

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