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Time integration methods for coupled equations

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Summary. In this paper we discuss time integration methods designed for solving stiff-nonstiff problems. A tool for analysing the effect of using stepsizes larger than the time scale of the stiff subsystem is presented.

1 Introduction

In many applications we have to deal with time integration of coupled systems, with subsystems of different time scales. Over the years, several approaches have been developed to exploit the particular properties of each subsystem, like multirate methods, implicit-explicit methods and splitting methods. More recently, also exponential integrators are enjoying a renaissance. Most of these methods are well understood in terms of classical local error / order analysis. However, the desired modus operandi often gives stepsizes larger than the time scales of the rapid subsystems. In this case, the classical order analysis is of limited, although important, relevance.

The problem can be illustrated by the following simple example: Consider the equation

$$y' = \lambda y + y + \mathrm{e}^t, \qquad y(0) = 1, \qquad \mathrm{Re}(\lambda) << 0.$$

The linear term λy represents the fast subsystem, while $y + \mathrm{e}^t$ is the slow one. The problem is solved by two different explicit exponential integrators, both of order 3. Exponential integrators work such that the fast linear part is integrated exactly. Figure 1 shows the relative error after one step, using different stepsizes. The local error is measured for two values of t, at $t = 0$ where the solution is dominated by its transient, and at $t = 0.5$, in which the transient is completely damped. From these pictures, we can draw several conclusions. First, even if the two methods are both of classical order 3, they behave quite differently, in the nonstiff regime (for which λh is small) as well as in the stiff. We also observe that the error depends not only on the stepsize h,

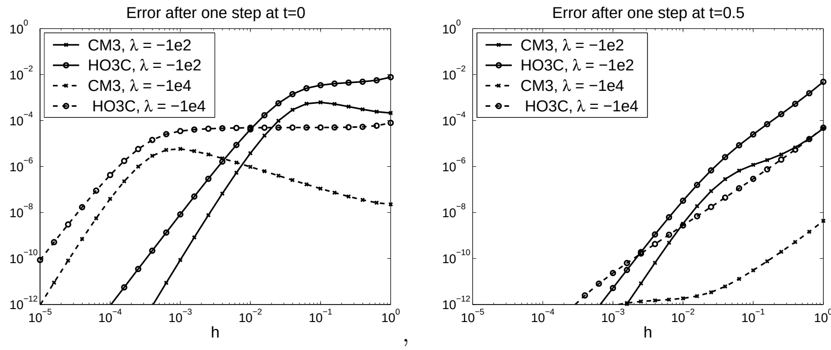

Fig. 1. Local error for two exponential integrators

but also of the stiffness parameter λ and of the initial values. Unfortunately, this behaviour can not be completely understood by a classical local error analysis, neither by a standard stability analysis.

In this paper, we will first describe two different strategies for solving stiff-nonstiff problems. In section 3 an alternative local error analysis is presented, although details are only given for the linear problems. A simple numerical test verifies the theoretical results.

2 Stiff-nonstiff problems

Given the problem

$$y' = f_S(t,y) + f_N(t,y), \qquad y(t_0) = y_0, \tag{1}$$

where f_S corresponds to the stiff term and f_N to the nonstiff. Such problems arise frequently from discretization of partial differential equations (PDEs) of advection-diffusion-reaction type, see e.g. [8]. In this paper we will put emphasis on semilinear problems

$$y' = Ly + f_N(t,y) \qquad y(t_0) = y_0, \tag{2}$$

coming from e.g. the discretization of semilinear parabolic equations or the Schrödinger equation. In the following, we will present two different strategies for solving such problems.

2.1 Implicit-explicit Runge-Kutta methods

The strategy of applying an implicit scheme for f_S and an explicit one for f_N is the idea behind implicit-explicit (IMEX) methods. Multistep methods as well as one-step methods have been constructed this way. In this paper,

Table 1. IMEX3: A third order, L-stable IMEX-RK method.

$$
\begin{array}{c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\
\frac{2}{3} & 0 & \frac{1}{6} & \frac{1}{2} & 0 & 0 \\
\frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\
1 & 0 & \frac{3}{2} & -\frac{3}{2} & \frac{1}{2} & \frac{1}{2} \\
\hline
1 & 0 & \frac{3}{2} & -\frac{3}{2} & \frac{1}{2} & \frac{1}{2}
\end{array},
\qquad
\begin{array}{c|ccccc}
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\
\frac{2}{3} & \frac{11}{18} & \frac{1}{18} & 0 & 0 & 0 \\
\frac{1}{2} & \frac{5}{6} & -\frac{5}{6} & \frac{1}{2} & 0 & 0 \\
1 & \frac{1}{4} & \frac{7}{4} & \frac{3}{4} & -\frac{7}{4} & 0 \\
\hline
1 & \frac{1}{4} & \frac{7}{4} & \frac{3}{4} & -\frac{7}{4} & 0
\end{array}
$$

we restrict ourself to IMEX Runge-Kutta (IMEX-RK) schemes as defined in [1, 9]. One step of an s-stage IMEX-RK scheme applied to (1) is given by

$$
\begin{aligned}
Y_1 &= y_0, \\
Y_i &= y_0 + h\sum_{j=1}^{i} a_{ij} f_S(t_0 + c_j h, Y_j) + h\sum_{j=1}^{i-1} \hat{a}_{ij} f_N(t_0 + c_j h, Y_j), \quad i = 2, \cdots, s, \\
y_1 &= y_0 + h\sum_{i=1}^{s} b_i f_S(t_0 + c_i h, Y_i) + h\sum_{i=1}^{s} \hat{b}_i f_N(t_0 + c_i h, Y_i),
\end{aligned}
\tag{3}
$$

where the coefficients are given in the following tableaux

$$
\begin{array}{c|ccccc}
0 & 0 & 0 & 0 & \cdots & 0 \\
c_2 & a_{21} & a_{22} & 0 & \cdots & 0 \\
c_3 & a_{31} & a_{32} & a_{33} & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & a_{s3} & \cdots & a_{ss} \\
\hline
 & b_1 & b_2 & b_3 & \cdots & b_s
\end{array},
\qquad
\begin{array}{c|ccccc}
0 & 0 & 0 & 0 & \cdots & 0 \\
c_2 & \hat{a}_{21} & 0 & 0 & \cdots & 0 \\
c_3 & \hat{a}_{31} & \hat{a}_{32} & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & \hat{a}_{s1} & \hat{a}_{s2} & \hat{a}_{s3} & \cdots & 0 \\
\hline
 & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_s
\end{array},
$$

or in short form as

$$
\begin{array}{c|c}
c & A \\
\hline
 & b^T
\end{array},
\qquad
\begin{array}{c|c}
c & \hat{A} \\
\hline
 & \hat{b}^T
\end{array}.
$$

A third order, L-stable scheme, proposed in [1] is given in Table 1. Sometimes it might be useful to write IMEX-RK methods applied to the semilinear problem (2) as

$$
\begin{aligned}
Y &= (I_{ms} - hA \otimes L)^{-1}(\mathbb{1}_s \otimes y_0) + (I_{ms} - hA \otimes L)^{-1} f_N(t_0 + ch, Y), \\
y_1 &= r(hL)y_0 + h(\hat{b}^T \otimes I_m + (b^T \otimes L)(I_{ms} - hA \otimes L)^{-1}) f_N(t_0 + ch, Y),
\end{aligned}
\tag{4}
$$

where $Y = [Y_1^T, \cdots, Y_s^T]^T$, $f_N(t_0 + ch, Y) = [f(t_0 + c_1 h, Y_1)^T, \cdots, f(t_0 + c_s h, Y_s)^T]^T$, $\mathbb{1} = [1, 1, \cdots, 1]^T$, s refers to the number of stages and m to the dimension of the problem (1). Further, $r(z) = 1 + zb^T(I_s - zA)^{-1}\mathbb{1}_s$ is the stability function for the implicit method.

2.2 Exponential integrators

Exponential integrators are mostly constructed to solve problems of the form (2). The idea behind these integrators dates back to the sixties, but has not been considered practical since the schemes involve computation of matrix exponential functions. Using modern techniques, such functions can now be computed quite efficiently, see [11] for a review. Today exponential integrators are enjoying a renaissance, numerical comparisons reveal several examples where they outperform standard integrators. A nice introduction to the idea of exponential integrators can be found in [3], see also [7].

In the presentation of exponential integrators, we will frequently use the following function

$$\phi_q(hL) = \frac{1}{(q-1)!}\,\frac{1}{h^q}\,\mathrm{e}^{hL}\int_0^h \mathrm{e}^{-\tau L}\tau^{q-1}d\tau,$$

or

$$\phi_q(z) = \frac{1}{z^q}\left(\mathrm{e}^z - \sum_{j=0}^{q-1}\frac{z^j}{j!}\right), \qquad q = 1, 2, \cdots. \tag{5}$$

Note that ϕ_q is an analytic function of z and $\phi_q(0) = \frac{1}{q!}$.

Exponential integrators can be considered as approximations of the variation-of-constants formula, which gives the exact solution of (2) as

$$y(t_0 + h) = \mathrm{e}^{hL}y_0 + \mathrm{e}^{hL}\int_0^h \mathrm{e}^{-\tau L} f_N(t_0 + \tau, y(t_0 + \tau))d\tau. \tag{6}$$

A first order method can be derived by using $f_N \approx f_N(t_0, y_0)$. Inserting this into (6) gives an exponential forward Euler method

$$y_1^{fe} = \mathrm{e}^{hL}y_0 + h\phi_1(hL)f(t_0, y_0). \tag{7}$$

This result can be improved by using

$$f_N \approx f_N(t_0, y_0) + \frac{t - t_0}{h}(f_N(t_0 + h, y_1^{fe}) - f_N(t_0, y_0))$$

which, when inserted into (6) gives

$$\begin{aligned} y_1^{imp} &= \mathrm{e}^{hL}y_0 + h\phi_1(hL)f_N(t_0, y_0) \\ &\quad + h\phi_2(hL)(f_N(t_0 + h, y_1^{fe}) - f_N(t_0, y_0)). \end{aligned} \tag{8}$$

In general, explicit exponential Runge-Kutta integrators are given by

$$\begin{aligned} Y_i &= \mathrm{e}^{c_i hL}y_0 + h\sum_{j=1}^{i-1} a_{ij}(hL)f_N(t_0 + c_j h, Y_j), \quad i = 1, 2, \cdots, s, \\ y_1 &= \mathrm{e}^{hL}y_0 + h\sum_{i=1}^{s} b_i(hL)f_N(t_0 + c_i h, Y_i). \end{aligned} \tag{9}$$

where the method coefficients are exponential functions evaluated at hL. Table 2 presents two third order exponential RK methods. The first, called CM3, was proposed by Cox and Matthew in [3]. The second, HO3C, was presented in a talk by Hochbruck and Ostermann, [6].

By comparing (4) and (9) we observe that both IMEX-RK and explicit exponential RK methods can be written in the general form

$$
\begin{aligned}
Y_i &= \chi_i(hL)y_0 + h\sum_{j=1}^{i-1}\alpha_{ij}(hL)f_N(t_0+c_jh, Y_j), \quad i=1,2,\cdots,s,\\
y_1 &= r(hL)y_0 + h\sum_{i=1}^{s}\beta_i(hL)f_N(t_0+c_ih, Y_i). \qquad (10)
\end{aligned}
$$

where the coefficients are given in the tableau

$$
\begin{array}{c|c|ccccc}
0 & \chi_1(z) & & & & & \\
c_2 & \chi_2(z) & \alpha_{21}(z) & & & & \\
c_3 & \chi_3(z) & \alpha_{31}(z) & a_{32}(z) & & & \\
\vdots & \vdots & \vdots & \vdots & \ddots & & \\
c_s & \chi_s(z) & \alpha_{s1}(z) & \alpha_{s2}(z) & \cdots & \alpha_{s,s-1}(z) & \\
\hline
 & r(z) & \beta_1(z) & \beta_2(z) & \cdots & \beta_{s-1}(z) & \beta_s(z)
\end{array}
\quad \text{or short as} \quad
\begin{array}{c|c|c}
c & \chi(z) & \mathcal{A}(z) \\
\hline
 & r(z) & \beta^T(z)
\end{array}.
$$

The coefficients are either exponential or rational functions evaluated in hL. Other methods might fit into this formulation as well. For the two schemes in question, the coefficients are given by

$$
\begin{array}{rcl}
\text{IMEX} & & \text{ExpRK} \\
\chi(z) = (I_s - zA)^{-1}\mathbb{1}_s & & \chi(z) = \mathrm{e}^{cz} \\
r(z) = 1 + zb^T(I_s - zA)^{-1}\mathbb{1}_s & & r(z) = \mathrm{e}^{z} \\
\mathcal{A}(z) = (I_s - zA)^{-1}\hat{A} & & \mathcal{A}(z) = A(z) \\
\beta^T(z) = zb^T(I_s - zA)^{-1}\hat{A} + \hat{b}^T\ , & & \beta^T(z) = b(z)^T\ .
\end{array}
$$

This general formulation will be used in the local error analysis of the next section.

3 Local error analysis

Traditionally, local error analysis is done by comparing the Taylor expansions of the exact and the numerical solutions. For one-step methods it is useful to write these expansions in the form

Table 2. Exponential Runge-Kutta methods of order 3.

Cox and Matthew: CM3

$$
\begin{array}{c|c|ccc}
0 & 1 & 0 & & \\
\frac{1}{2} & \mathrm{e}^{z/2} & \frac{1}{2}\phi_1(\frac{z}{2}) & & \\
1 & \mathrm{e}^{z} & -\phi_1(z) & 2\phi_1(z) & \\
\hline
0 & \mathrm{e}^{z} & \phi_1(z)-3\phi_2(z)+4\phi_3(z) & 4\phi_2(z)-8\phi_3(z) & -\phi_2(z)+4\phi_3(z)
\end{array}
$$

Hochbruck and Ostermann: HO3C

$$
\begin{array}{c|c|ccc}
0 & 1 & 0 & & \\
\frac{1}{3} & \mathrm{e}^{z/3} & \frac{1}{3}\phi_1(\frac{z}{3}) & & \\
\frac{2}{3} & \mathrm{e}^{2z/3} & 0 & \frac{2}{3}\phi_1(\frac{2z}{3}) & \\
\hline
 & \mathrm{e}^{z} & \phi_1(z)-\frac{3}{2}\phi_2(z) & 0 & \frac{3}{2}\phi_2(z)
\end{array}
$$

$$
\begin{aligned}
y(t_0+h) &= \sum_{v\in V} \frac{h^{\rho(\tau)}}{\rho(v)!}\alpha(v)F(v)(t_0,y_0),\\
y_1 &= \sum_{v\in V} \varphi(v)\frac{h^{\rho(v)}}{\rho(v)!}\alpha(v)F(v)(t_0,y_0),
\end{aligned}
\tag{11}
$$

known as B-series for ordinary differential equations. The exact definition of the series depends on the problem in question. In any case, V is some index set, usually a set of rooted trees, $\rho(v)$ is the order of the tree, $\alpha(v)$ counts the number of times the same term appears, $F(v)$ is the elementary differential, evaluated at (t_0, y_0), and the term $\varphi(v)$ is method dependent. The terms $\alpha(v)$, $F(v)$ and $\varphi(v)$ are chosen such that

$$
y^{(p)}(t_0)= \sum_{\substack{v\in V\\ \rho(v)=p}} \alpha(v)F(v)(t_0,y_0), \qquad \left.\frac{\mathrm{d}^p y_1}{\mathrm{d}h^p}\right|_{h=0} = \sum_{\substack{v\in V\\ \rho(v)=p}} \varphi(v)\alpha(v)F(v)(t_0,y_0),
$$

so the relation to Taylor expansions is clear. The local truncation error is of local order $p+1$ if

$$
\varphi(v) = 1, \quad \forall v \in V, \quad \rho(v) \le p.
$$

For a thorough explanation of B-series for ordinary differential equations, as well as for other initial value problems, see [4, 5]. For exponential integrators, see [2, 7].

When applied to stiff problems, this approach is known to have severe limitations. The elementary differentials $F(v)(t_0, y_0)$ depend on the stiffness of the system, and might become very large. The truncated series will only describe the behaviour of the methods for quite small values of the stepsize h. To understand how methods behave for significantly larger stepsizes, it is instructive to study the evolution of a single Fourier-mode of (2), given by

$$y' = \lambda y + f(t,y), \qquad y(t_0) = y_0, \quad \lambda \in \mathbb{C}, \quad |\lambda| >> 1. \tag{12}$$

If $\mathrm{Re}(\lambda) << 0$ then the solution of (12) can be divided into two phases, the fast transient and a slow manifold to which the solution is attracted. As pointed out in the introduction, the local error depends strongly on whether the initial values are on the slow manifold or not.

So, rather than using the series (11) to represent the exact and numerical solutions, we search for expansions of the form

$$\begin{aligned} y(t_0+h) &= \sum_{v\in V} \varphi(v)(z)\, h^{\rho(v)}\, F(v)(Q_0), \\ y_1 &= \sum_{v\in V} \psi(v)(z)\, h^{\rho(v)}\, F(v)(Q_0), \end{aligned} \tag{13}$$

where $z = \lambda h$, V is an index set (but different from the previous), $\varphi(v)$ and $\psi(v)$ are functions of z, $\rho(v)$ is again the order, and $F(v)$ is the elementary differential evaluated at some point Q_0. As long as we are interested in the transient behaviour, the choice $Q_0 = (t_0, y_0)$ is natural, when studying the slow solution some point near the slow manifold is more convenient. In any case, these expansions should be chosen such that $F(v)$ *is independent on the stiffness parameter* λ. There are several advantages with such a representation. First of all, if $\varphi(v)$ and $\psi(v)$ are bounded, then the expansions can be used to represent the solutions for quite large values of h. Further, if

$$\varphi(v) = \psi(v), \qquad \forall v \in V, \quad \rho(v) \le p,$$

then the local error is of order $p+1$ independent of λ. But, as we will see, it is also useful to study the difference $\varphi(v) - \psi(v)$ for different values of z.

The idea is fully explored in [10]. In the present paper we restrict ourself to demonstrate the idea and some of its interpretations on the linear problem

$$y' = \lambda y + f(t), \qquad y(t_0) = y_0, \qquad \lambda \in \mathbb{C}^-, \quad |\lambda| >> 1. \tag{14}$$

The exact solution is given by

$$y(t_0+h) = \mathrm{e}^{\lambda h} y_0 + \mathrm{e}^{\lambda h} \int_0^h \mathrm{e}^{-\lambda \tau} f(t_0+\tau) d\tau.$$

Taking the Taylor expansion of $f(t_0+\tau)$ around $\tau = 0$ and integrating each term separately gives

$$y(t_0+h) = \mathrm{e}^{z} y_0 + \sum_{q=1}^{\infty} \phi_q(z) h^q f^{(q-1)}(t_0). \tag{15}$$

The initial value y_0 is on the smooth manifold if

$$y_0 = -\sum_{q=1}^{\infty} \frac{f^{(q-1)}(t_0)}{\lambda^q}. \tag{16}$$

Table 3. Weight functions for the linear problem

q	$\phi_q(z)$	$\psi_q(z)$		
		IMEX3	CM3	HO3C
0	e^z	$\frac{8(z^3-6z+6)}{3(z-2)^4)}$	e^z	e^z
1	$\frac{\mathrm{e}^z-1}{z}$	$\frac{-3z^3+32z^2-72z+48}{3(z-2)^4}$	$\frac{\mathrm{e}^z-1}{z}$	$\frac{\mathrm{e}^z-1}{z}$
2	$\frac{\mathrm{e}^z-1-z}{z^2}$	$\frac{-25z^2+84z-72}{18(z-2)^3}$	$\frac{\mathrm{e}^z-1-z}{z^2}$	$\frac{\mathrm{e}^z-1-z}{z^2}$
3	$\frac{\mathrm{e}^z-1-z-\frac{z^2}{2}}{z^3}$	$\frac{-27z^2+100z-96}{72(z-2)^3}$	$\frac{\mathrm{e}^z-1-z-\frac{z^2}{2}}{z^3}$	$\frac{\mathrm{e}^z-1-z}{3z^2}$
4	$\frac{\mathrm{e}^z-1-z-\frac{z^2}{2}-\frac{z^3}{6}}{z^4}$	$\frac{-89z^2+364z-384}{1296(z-2)^3}$	$\frac{(6-z)\mathrm{e}^z-6-5z-2z^2}{12z^3}$	$\frac{2(\mathrm{e}^z-1-z)}{27z^2}$

A series similar to (15) can be derived for the numerical solution. Applying (10) on (14) and replacing f by its Taylor expansion gives

$$y_1 = r(z)y_0 + h\sum_{i=1}^{s}\beta_i(z)f(t_0+c_ih) = r(z)y_0 + \sum_{q=1}^{\infty}\psi_q(z)h^q f^{(q-1)}(t_0), \quad (17)$$

where

$$\psi_q(z) = \frac{1}{(q-1)!}\sum_{i=1}^{s}\beta_i(z)c_i^{q-1}.$$

For convenience we will use the notation $\phi_0(z) = \mathrm{e}^z$ and $\psi_0(z) = r(z)$. Table 3 lists the functions ϕ_q as well as ψ_q for the methods given in Table 1 and 2. The local truncation error is given by

$$y(t_0+h) - y_1 = \mathcal{E}_0 y_0 + \sum_{q=1}^{\infty}\mathcal{E}_q(z)h^q f^{(q-1)}(t_0), \quad (18)$$

where the error functions $\mathcal{E}_q$ are given by

$$\mathcal{E}_q(z) = \phi_q(z) - \psi_q(z).$$

Obviously, the error is of order $p+1$ independent of the stiffness parameter λ if

$$\mathcal{E}_q(z) = 0, \qquad q = 1, 2, \cdots p,$$

and for the three methods under consideration

$$p^{\mathrm{IMEX3}} = 0, \qquad p^{\mathrm{CM3}} = 3 \quad \text{and} \qquad p^{\mathrm{HO3C}} = 2.$$

Only the IMEX method has a local error depending on the initial value y_0. IMEX methods approximate the exponential e^z by a rational function $r(z)$, thus $\mathcal{E}_0 \sim \lambda^{\rho+1}h^{\rho+1}$ for some ρ. This term usually dominates the error when λ is large. However, if the initial value is on the slow manifold (16), then

$$y(t_0+h)-y_1=\sum_{q=1}^{\infty}\tilde{\mathcal{E}}_q(z)h^q f^{(q-1)}(t_0),$$

with $\tilde{\mathcal{E}}_q=\mathcal{E}_q-\mathcal{E}_0/z^q$. For IMEX3 these terms are

$$\tilde{\mathcal{E}}_1=0,\quad \tilde{\mathcal{E}}_2=\frac{7z^3-8z^2}{18(z-2)^4},\quad \tilde{\mathcal{E}}_3=\frac{-9z^3+62z^2-64z}{72(z-2)^2},\quad \cdots$$

giving $\tilde{p}^{\mathrm{IMEX3}}=2$. In the following, we will use the term IMEX3(s) to denote the situation when the initial value is on the slow manifold.

Examination of the error functions in the extreme cases, like the nonstiff, the strongly damped and the highly oscillatory case, gives further insight into the behaviour of the local error.

The nonstiff case

This situation is characterised by $|z|$ small and the error functions can be studied in terms of their series expansions. For the methods in question, the dominant terms of $\mathcal{E}_q$ are given by

q	IMEX3	IMEX3(s)	CM3	HO3C
0	$\frac{1}{48}z^4+\mathcal{O}(z^5)$	0	0	0
1	$\frac{1}{48}z^3+\mathcal{O}(z^4)$	0	0	0
2	$-\frac{1}{144}z^2+\mathcal{O}(z^3)$	$-\frac{1}{36}z^2+\mathcal{O}(z^3)$	0	0
3	$-\frac{5}{144}z+\mathcal{O}(z^2)$	$-\frac{1}{18}z+\mathcal{O}(z^2)$	0	$-\frac{1}{72}z+\mathcal{O}(z^2)$
4	$\frac{1}{216}+\mathcal{O}(z)$	$-\frac{7}{432}+\mathcal{O}(z)$	$\frac{1}{720}+\mathcal{O}(z)$	$\frac{1}{216}z+\mathcal{O}(z^2)$

By inserting this into (18), keeping in mind that $z=\lambda h$, we obtain the following expressions for the local error:

$$y(x_0+h)-y_1$$
$$=\begin{cases}\left(\frac{\lambda^4}{48}y_0+\frac{\lambda^3}{48}f-\frac{\lambda^2}{144}f'-\frac{5\lambda}{144}f''+\frac{1}{216}f'''\right)h^4+\mathcal{O}(h^5) & \text{for IMEX3}\\ \left(-\frac{\lambda^2}{36}f'-\frac{\lambda}{18}f''-\frac{7}{432}f'''\right)h^4+\mathcal{O}(h^5)) & \text{for IMEX3(s)}\\ \left(\frac{\lambda}{720}f'''-\frac{1}{2880}f^{(4)}(t_0)\right)h^5+\mathcal{O}(h^6) & \text{for CM3}\\ \left(-\frac{\lambda}{72}f''+\frac{1}{216}f'''\right)h^4+\mathcal{O}(h^5) & \text{for HO3C}\end{cases}.$$

The error terms all depend on some power of λ. Since $|\lambda|>>1$ by assumption, we will prefer this power to be as small as possible. In this sense the exponential integrators outperform the IMEX method in the transient case. The situation improves significantly in the slow case, but still the error is $\sim\lambda^2$ for the IMEX method while it is $\sim\lambda$ for the exponential methods. The order of the local error of CM3 is one more than expected, and the error constants are about 1/10 of those for HO3C. However, the higher order only occurs in the linear case, for a nonlinear problem the order reduces to 4.

Rapid decay

In this case we assume $\mathrm{Re}(z) << 0$, such that all transients represented by exponential functions are completely damped. In this case it makes sense to write the error functions as inverse power series of z. The dominant terms of $\mathcal{E}_q$ are given by

q	IMEX3	IMEX3 (s)	CM3	HO3C
0	$-\frac{8}{3z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	0	0	0
1	$-\frac{8}{3z^2}+\mathcal{O}\big(\frac{1}{z^3}\big)$	0	0	0
2	$\frac{7}{18z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	$\frac{7}{18z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	0	0
3	$-\frac{1}{8z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	$-\frac{1}{8z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	0	$-\frac{1}{6z}+\mathcal{O}\big(\frac{1}{z^2}\big)$
4	$-\frac{127}{1296z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	$-\frac{127}{1296z}+\mathcal{O}\big(\frac{1}{z^2}\big)$	$-\frac{1}{12z^2}+\mathcal{O}\big(\frac{1}{z^3}\big)$	$-\frac{5}{54z}+\mathcal{O}\big(\frac{1}{z^2}\big)$

The local truncation error behaves as

$$y(t_0+h)-y_1=\begin{cases}\big(-\frac{8}{3\lambda}y_0-\frac{8}{3\lambda^2}f\big)\frac{1}{h}+\mathcal{O}\big(\frac{1}{\lambda^2h^2}+\frac{h}{\lambda}\big) & \text{for IMEX3}\\ \frac{7}{8\lambda}hf'+\mathcal{O}\big(\frac{1}{\lambda^2}+\frac{h^2}{\lambda}\big) & \text{for IMEX3 (s)}\\ -\frac{1}{12\lambda^2}h^2f'''+\mathcal{O}\big(\frac{h}{\lambda^3}+\frac{h^3}{\lambda^2}\big) & \text{for CM3}\\ -\frac{1}{6\lambda}h^2f''+\mathcal{O}\big(\frac{h^3}{\lambda}+\frac{h}{\lambda^2}\big) & \text{for HO3C}\end{cases}.$$

In the transient case the error of IMEX3 goes as $\sim 1/h$. The error increases as the stepsize decreases! This phenomenon is known from the literature as "the hump". The situation is improved in the slow case, but still the IMEX method has a local error of one order less than the two exponential RK-methods. For very stiff problem, the $1/\lambda^2$ behaviour of CM3 is an advantage.

Rapid oscillations

In this situation, we assume $|z|$ large and λ purely imaginary. The IMEX3 method is not constructed for solving oscillatory problems, so its behaviour is not considered here. For the two exponential RK-methods, the exponentials will represent rapid oscillations in the error functions which are dominated by the terms:

q	CM3	HO3C
3	0	$-\frac{1}{6z}+\mathcal{O}\big(\frac{1}{z^2}\big)$
4	$\frac{\mathrm{e}^z-1}{12z^2}+\mathcal{O}\big(\frac{1}{z^3}\big)$	$-\frac{5}{54z}+\mathcal{O}\big(\frac{1}{z^2}\big)$

The absolute value of the local truncation error is

$$|y(t_0+h)-y_1|=\begin{cases}\frac{1}{12|\lambda|^2}Mh^2f'''(t_0)+\mathcal{O}\big(\frac{h^3}{|\lambda|^2}+\frac{h}{|\lambda|^3}\big),\ M\in[0,2] & \text{for CM3}\\ \frac{1}{6|\lambda|}h^2f''(t_0)+\mathcal{O}\big(\frac{h^3}{|\lambda|}+\frac{h}{|\lambda|^2}\big) & \text{for HO3C}\end{cases}.$$

Both methods have local errors of order 2. But again, the $1/\lambda^2$ term for the CM3 method results in very small errors for stiff systems.

We conclude this section with a numerical example.

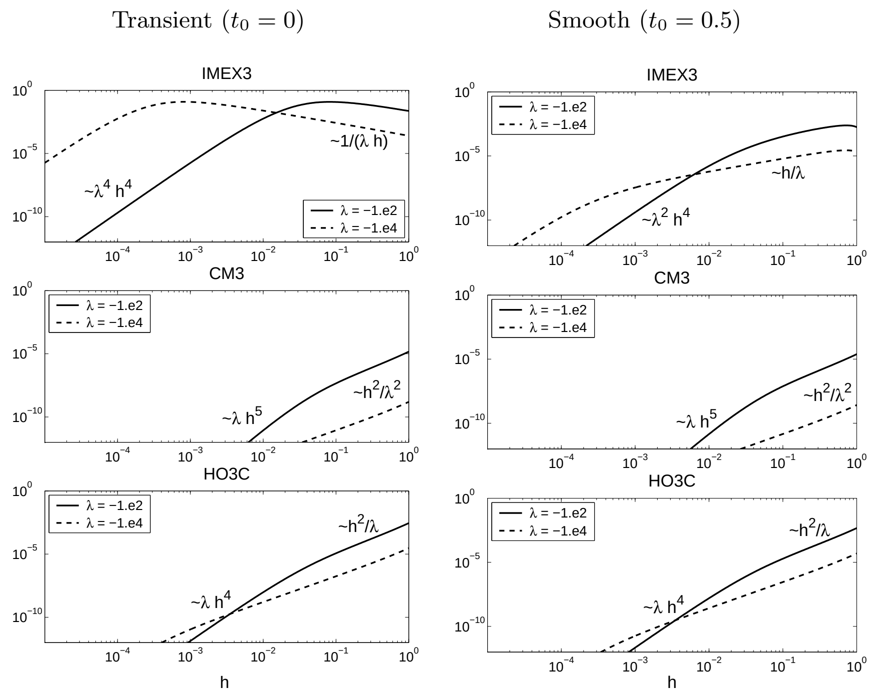

Fig. 2. Local error in the rapid decay case.

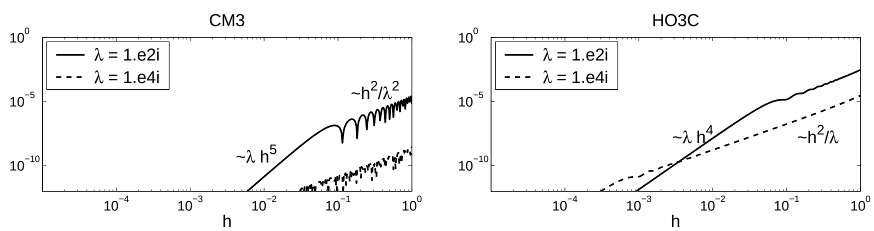

Fig. 3. Local error in the rapid oscillation case.

Example 1. Consider the equation

$$y' = \lambda y + \mathrm{e}^t, \qquad y(0) = y_0,$$

with exact solution

$$y(t) = \mathrm{e}^{\lambda t} y_0 + \frac{\mathrm{e}^{\lambda t} - \mathrm{e}^t}{\lambda - 1}.$$

Figure 2 shows the local error in the rapid decay case, both in the transient and the slow case. Figure 3 shows the local error in the highly oscillatory case. Both verify the theoretical results.

3.1 Remarks

As demonstrated in the introduction of this paper, even exponential integrators might behave different when applied to problems with a nonstiff term depending on y. An explanation for this behaviour is given in [10].

The investigation of a single Fourier mode, linear or nonlinear, will certainly not necessarily give a representative solution of more complex equations. But it is a quite straightforward tool to reveal certain characteristic properties of a method, as we have seen. Further research will hopefully result in a similar theory for systems of equations.

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