Peer methods with improved embedded sensitivities for parameter-dependent ODEs

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Abstract

Recently, an extension of peer two-step methods to parameter-dependent IVPs has been proposed by the author and E. Kostina where additional embedded stages allow cheap computation of solution derivatives (sensitivities) with respect to problem parameters. For each parameter only one additional 'satellite' stage was used which provides a high-order approximation to a neighboring solution. However, the accuracy of the sensitivities was only first order in the time steps size $h$. In the present paper we derive implicit peer methods where the sensitivity accuracy is of second order with the same number of stages. Approximate implementations yield efficient linearly-implicit methods for stiff problems and explicit predictor-corrector-type versions for nonstiff problems. Tests confirm improved and more robust convergence of inexact Newton iterations in shooting for different applications with nonstiff and stiff IVPs.

Key words. Peer two-step methods, sensitivity analysis for ordinary differential equations, shooting methods.

AMS subject classifications. 65L05, 34C25, 65L07

1 Introduction

Ordinary differential equations are often used for modeling time-dependent real-life systems. These models usually depend on many constants which are parameters of the model and it is often required to estimate the sensitivity of the model to changes of certain parameters, i.e. to approximate the derivative of the solution with respect to these parameters. Such a parameter-dependent ordinary initial value problem may be written in the form

$$y'(t,p) = f(y(t,p),p), \ t \in [t_0,t_{\text{end}}], \ y(t_0,p) = u(p), \quad (1)$$

where $f : \mathbb{R}^n \times \mathbb{R}^q \to \mathbb{R}^n$ is some smooth right-hand side and $u : \mathbb{R}^q \to \mathbb{R}^n$ defines the initial values which also may depend smoothly on the $q$ parameters $p \in \mathbb{R}^q$. The prime denotes the derivative of the solution $y(t,p)$ with respect to

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time, \( y'(t, p) = \frac{\partial y(t, p)}{\partial t} \). In numerical applications like shooting for boundary value problems the number of parameters may be as large as the dimension of the system, \( q \approx n \).

With classical numerical integration schemes like one-step and multistep methods the computation of sensitivities is usually performed by solving one additional neighboring or variational ODE for each parameter, \([12]\), requiring roughly the \((q + 1)th\)-fold effort of the solution of the initial value problem (1) itself. Recently, in \([7]\) an alternative approach was suggested where sensitivities are approximated more cheaply by embedding one additional stage for each neighboring solution in two-step peer methods. Two-step peer methods are time stepping schemes introduced in \([8]\) employing \( s \) neighboring solution in two-step peer methods. Two-step peer methods are approximated more cheaply by embedding one additional stage for each parameter off-steps \((r_1, \ldots, r_s) =: R \subseteq \mathbb{R}^{q \times s} \) span \( R^T = \text{Range}(R) \). In addition to variable time stepsizes \( h_m > 0 \) a small constant stepsize \( \rho \) is used in the parameter space. With these notations, the peer two-step method is again given by \((i = 1, \ldots, s)\)

\[
Y_{mi} - h_m \sum_{j=1}^{i} \gamma_{ij} f(Y_{mj}, \rho_{r_j}) = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(Y_{m-1,j}, \rho_{r_j}), \tag{2}
\]

where \( a_{ij}, b_{ij}, \gamma_{ij}, i, j = 1, \ldots, s \) are coefficients of the method which are elements of square matrices \( A_m = (a_{ij}), B_m = (b_{ij}), \Gamma_m := (\gamma_{ij}) \subseteq \mathbb{R}^{s \times s} \). The index \( m \) indicates that these matrices may change between steps. By introducing matrices \( Y^T_m = (Y_{m1}, \ldots, Y_{ms}) \subseteq \mathbb{R}^{s \times n}, F^T_m = (f(Y_{mi}, \rho_{r_i}))_{i=1}^{s} \) of stage vectors and function evaluations there is also a compact representation of the method (2) by

\[
Y_m - h_m \Gamma_m F_m = B_m Y_{m-1} + h_m A_m F_{m-1}. \tag{3}
\]

The structure of the matrix \( \Gamma_m \) determines the numerical effort in the implementation of the method. In explicit methods it is missing, i.e. \( \Gamma_m = 0, [13] \). For implicit methods a lower triangular structure of \( \Gamma_m \) allows the efficient computation of the approximations \( Y_{mi} \) in (2) on a stage-by-stage basis, see, e.g. [1]. For implicit parallel methods a diagonal form of \( \Gamma_m = \text{diag}(\gamma_{ii}) [11] \) or even \( \Gamma_m = \gamma I \) \([8]\) is usually assumed in the ODE context.

In \([7]\) a rather efficient ‘satellite’ configuration has been identified using only \( q \) additional satellite stages which are embedded in a high-order peer method approximating the central solution trajectory \( y(t, 0) \) where \( \hat{p} = 0 \) is the evaluation point of the sought parameter derivatives. In this satellite configuration
off-steps of the $s > q$ stages are restricted by the choice
\[ c_1 = \ldots = c_q = c_s = 1, \quad r_{q+1} = \ldots = r_s = 0, \quad (4) \]
and $r_1, \ldots, r_q$ comprise a basis of the parameter space $\mathbb{R}^q$. This means that the first stages $Y_{m1}, \ldots, Y_{mq}$ approximate neighboring solutions $y(t_{m+1}, pr_i)$ at the end point $t_{m+1}$ of the current time step and may be used to approximate parameter derivatives with the aid of the reference solution $Y_{ms} \approx y(t_{m+1}, 0)$ by
\[ \frac{\partial y}{\partial p_i}(t_{m+1}, 0) \approx \frac{1}{\rho} (Y_{mi} - Y_{ms}), \quad i = 1, \ldots, q. \quad (5) \]
There is also a restriction on the coefficient matrices which have block triangular structure,
\[ B_m = \begin{pmatrix} I_q & 0 \\ 0 & \hat{B}_m \end{pmatrix}, \quad A_m = \begin{pmatrix} \hat{A}_m & \hat{A}_m \\ 0 & \hat{A}_m \end{pmatrix}, \quad \Gamma_m = \begin{pmatrix} \hat{\Gamma}_m & \hat{\Gamma}_m \\ 0 & \hat{\Gamma}_m \end{pmatrix} \quad (6) \]
with diagonal leading blocks $\hat{B}_m = I_q$, the identity matrix, and $\hat{A}_m, \hat{\Gamma}_m$. Obviously, the stages $Y_{m, q+1}, \ldots, Y_{ms}$ which approximate the central trajectory $y(t, 0)$ due to (4) are decoupled and the blocks $(\hat{A}_m, \hat{B}_m, \hat{\Gamma}_m)$ may define any higher-order standard peer method from literature. A high-order correction from these central stages is fed through $\hat{A}_m, \hat{\Gamma}_m$ to the external stages $Y_{m1}, \ldots, Y_{mq}$ which are mutually independent. Hence, these external stages are satellites to the central stages in a sense. Although the basic satellite step of the methods constructed in [7] is a low-order Euler scheme only, the correction term from the center improved the global error of all stages to the estimate
\[ Y_{mi} - y(t_{mi}, 0) = O(H^k + H\rho), \quad i = 1, \ldots, s, \]
where $k$ is the order of the central peer method and $H = \max\{h_m : t_0 \leq t_m < t_e\}$. Indeed, the methods in [7] used only $s = k + q$ stages instead of the $k(q+1)$ stages corresponding to the usual approach with other methods. Still, the accuracy of the sensitivities (5) was only first order accurate, $O(H + \rho + \ldots)$. It is the aim of the current paper to improve sensitivity approximation to second order accuracy $O(H^2 + \rho + \ldots)$ without increasing the number of stages.

We will discuss and apply satellite embedding for three well-known classes of parallel peer methods, namely the singly-implicit methods from [8], the multi-implicit methods from [11], and the explicit methods from [10]. Singly-implicit methods have the advantage that a LU-decomposition need be computed only once per time step and may be re-used in every stage (center and satellites). Since LU decompositions do not parallelize well, however, iterative methods like Krylov methods are an alternative for the stage equations. In this case the diagonals $\gamma_{ii}$ of $\Gamma_m$ may be different and such multi-implicit methods have better stiff stability properties, see [11]. In this paper, however, we will not use parallelization or Krylov approximations in order to avoid additional difficulties and errors.
In Section 2 we reconsider order conditions for parameter-dependent ODEs and present those required for second-order accuracy of sensitivities. The main result here is that the satellite steps are based on the trapezoidal rule. In Section 3 the global error is considered shortly and the attunement of time and parameter stepsizes is addressed. Section 4 is devoted to cheap approximations of the implicit trapezoidal rule for the satellites in the context of explicit and linearly-implicit peer methods for the central trajectory. The main focus here is on accurate predictors available from the highly accurate central solution. To this end we shortly review and reformulate the three classes of peer methods used in the applications. In Section 5 these methods are applied again to some problem types from [7] in order to demonstrate improvements. One of these problems was the computation of time-periodic solutions of the 1D-diffusion-reaction Brusselator from [4] by shooting. With difference discretization on the original small space grid of 31 points this problem is only mildly stiff and tractable with explicit integration methods. Now, with implicit peer methods at hand the number of space grid points may be increased leading to stiff problems. In fact, convergence of Newton’s method is not affected by stiffness and the computed time periods indeed show second order convergence in the space grid size.

2 Order conditions

The accuracy of the peer method (3) can be determined by inspection of the residual of the exact solution \( y(t, p) \), i.e.

\[
h_m \Delta_{m,i} = y(t_{m,i}, \rho r_i) - h_m \sum_{j=1}^{i} \gamma_{ij} y'(t_{m,j}, \rho r_j) - \sum_{j=1}^{s} \left( b_{ij} y(t_{m-1,j}, \rho r_j) + h_m a_{ij} y'(t_{m-1,j}, \rho r_j) \right).
\]

(7)

Taylor expansion is applied now with respect to both stepsizes \( h_{m-1} \) and \( \rho \). The stepsize \( h_m \) is written with the aid of the stepsize ratio \( \sigma_m = h_m / h_{m-1} \). Since the variables \( t \) and \( p = (p_1, \ldots, p_q) \) of \( y \) have a different meaning we separate the notation for the derivatives with respect to \( t \) and \( q \) by

\[
y^{(t,\alpha)} := \frac{\partial^{|\alpha|}}{\partial t^{|\alpha|}} y(t_{m-1}, 0)
\]

with a multi-index \( \alpha = (\alpha_1, \ldots, \alpha_q) \). The usual multi-index notation is used with \( |\alpha| = \alpha_1 + \ldots + \alpha_q \) and \( r^\alpha_j = r_1^{\alpha_1} \cdots r_q^{\alpha_q} \). Now, Taylor expansion of (7) at
the point \((t_{m-1},0)\) gives

\[
\begin{align*}
    h_m \Delta_m &= \sum_{\ell \geq 0} \sum_{\alpha \geq 0} \frac{1}{\ell! \alpha!} \rho^{\alpha} ( (1 + \sigma_m c_i)^{\ell} r_i^\alpha - \sum_{j=1}^{s} b_{ij} c_j^\ell r_j^\alpha ) h_m^{\ell} y^{(\ell,\alpha)} \\
    &- \sigma_m \sum_{j=1}^{s} (\gamma_{ij}(1 + \sigma_m c_j)^{\ell} r_j^\alpha + a_{ij} c_j^\ell r_j^\alpha) h_m^{\ell+1} y^{(\ell+1,\alpha)} \\
    &= (1 - \sum_{j=1}^{s} b_{ij}) y^{(0,0)} + \sum_{\ell \geq 1} \sum_{\alpha \geq 0} \frac{1}{\ell! \alpha!} \rho^{\alpha} ( (1 + \sigma_m c_i)^{\ell} r_i^\alpha \\
    &- \sum_{j=1}^{s} (b_{ij} c_j^\ell r_j^\alpha + \sigma_m \ell \gamma_{ij}(1 + \sigma_m c_j)^{\ell-1} r_j^\alpha + \sigma_m \ell a_{ij} c_j^{\ell-1} r_j^\alpha) ) y^{(\ell,\alpha)}.
\end{align*}
\]

For convenience the order conditions will be labeled with the stepsize factors \(h^a \rho^b\) \((a,b \in \mathbb{N})\). They are written down with the aid of the diagonal node matrix \(C := \text{diag}(c_i)\) and the vector of ones \(\mathbf{1} = (1,\ldots,1)^T\). So, the usual order conditions \(h^0 \rho^0\) with respect to the time stepsize are ([7])

\[
\begin{align*}
    h^0 \rho^0: & \quad B_m \mathbf{1} = \mathbf{1} \\
    h^0 \rho^0: & \quad (I + \sigma_m C)^{\ell} \mathbf{1} = \sigma_m \ell \Gamma_m (I + \sigma_m C)^{\ell-1} \mathbf{1} + B_m C^\ell \mathbf{1} + \sigma_m \ell A_m C^{\ell-1} \mathbf{1}, \quad \ell \geq 1.
\end{align*}
\]

Obviously, the order conditions with \(\ell > 0\) depend on the current stepsize ratio \(\sigma_m\). Hence, not all of the coefficient matrices may be constant over different steps and that’s why we indicated this dependence by the index: \(A_m, B_m, \Gamma_m\).

For \(q \gg 1\) the overall number of order conditions increases dramatically with each order condition in \(\rho\). Hence, in [7] only conditions of the form \(h^0 \rho^1\) have been considered and we will do this here, too. The first two conditions are

\[
\begin{align*}
    h^1 \rho^0: & \quad B_m R^T = R^T, \\
    h^1 \rho^0: & \quad (I - \sigma_m C - B_m C - \sigma_m (A_m + \Gamma_m)) R^T = 0.
\end{align*}
\]

It is easily seen that each such condition requires roughly \(q\) additional stages for the peer method, in general, to provide enough degrees of freedom. In the configuration (4) the first \(q\) satellite stages are located off the central trajectory and at the end of the time interval, \(r_j \neq 0, c_j = 1, 1 \leq j \leq q\). Using also a unit basis for the corresponding parameter off-steps \((r_j)\) leads to the conditions

\[
R = E_q^T := (I_q,0), \quad C R^T = C E_q = E_q
\]

and the order conditions \(h^0 \rho\) and \(h^1 \rho\) simplify to

\[
B_m E_q = E_q, \quad (A_m + \Gamma_m) E_q = E_q.
\]

This means that the first \(q\) columns of both \(B_m\) and \(A_m + \Gamma_m\) are the first \(q\) unit vectors. Requiring in addition small norm of the matrix \(B_m\) also the condition \(E_q^T B_m = E_q^T\) was used in [7] leading to the block diagonal form (6).
With only two order conditions \( h^0 \rho, h^1 \rho \) the embedded parameter derivatives are only first order accurate in \( h \), \([7]\). Although this was sufficient for several applications we now intend to improve this accuracy without the use of additional stages and discuss the next order condition, \([5]\).

**Lemma 1** The condition \( h^2 \rho \) for the peer method (2) is given by

\[
(I + \sigma_m C)^2 - 2\sigma_m \Gamma_m (I + \sigma_m C) - B_m C^2 - 2\sigma_m A_m C) R^T = 0.
\]

Under the assumptions \( 9 \) it simplifies to

\[
(A_m - \Gamma_m) E_q = 0.
\]

**Proof** The multi-indices satisfying \( |\alpha| = 1 \) are simply the unit vectors in \( q \)-space. This means that matrices in the order conditions \( h^2 \rho \) are multiplied by the different rows of \( R^T \) instead of the vector \( \mathbb{1} \). This gives the first assertion. Now, with \( 9 \) the condition simplifies again by

\[
0 = ((I + \sigma_m C)^2 - 2\sigma_m \Gamma_m (I + \sigma_m C) - B_m C^2 - 2\sigma_m A_m C) E_q
\]

\[
= \sigma_m ((2 + \sigma_m) E_q - 2(1 + \sigma) \Gamma_m E_q) - \frac{A_m E_q}{2}
\]

\[
= \sigma_m (2 + \sigma_m)(A_m + \Gamma_m) E_q - \frac{2(1 + \sigma_m) \Gamma_m E_q - 2AE_q}{2}
\]

\[
= \sigma^2 (A_m - \Gamma_m) E_q.
\]

□

There is a simple consequence of Lemma 1: for satellite configurations satisfying the order conditions \( \rho, h^2 \rho \) holds

\[
A_m E_q = \Gamma_m E_q, \quad (A_m + \Gamma_m) E_q = E_q \Rightarrow \quad \Gamma_m E_q = A_m E_q = \frac{1}{2} E_q.
\]

Hence, each leading \( q \times q \)-block of the matrices \( A_m, \Gamma_m \) and \( B_m \) is a fixed multiple of the identity matrix. In fact, the time step for the satellite stages, \( i = 1, \ldots, q \), reads

\[
Y_{m,i} - \frac{h_m}{2} F_{m,i} = Y_{m-1,i} + \frac{h_m}{2} F_{m-1,i} + h_m \sum_{j>q} (\gamma_{ij} F_{m,j} + a_{ij} F_{m-1,j}).
\]

Obviously, these are decoupled steps of the implicit trapezoidal rule with a higher order correction computed from the central stages \( Y_{m-1,j}, Y_{m,j}, \ j = q+1, \ldots, s \).

These results mean that the block structure of the coefficient matrices is even more restricted and (6) is now replaced by

\[
B_m = \begin{pmatrix} I_q & 0 \\ 0 & \hat{B}_m \end{pmatrix}, \quad A = \begin{pmatrix} \frac{1}{2} I_q & \hat{A}_m \\ 0 & \hat{A}_m \end{pmatrix}, \quad G = \begin{pmatrix} \frac{1}{2} I_q & \hat{G}_m \\ 0 & \hat{G}_m \end{pmatrix}.
\]

The lower diagonal blocks \( \hat{B}_m, \hat{A}_m, \hat{G}_m \) define the peer method for the central trajectory at \( p = 0 \) and may be chosen as any known peer method from literature, see \S 4.1. The off-diagonals \( \hat{A}, \hat{G} \in \mathbb{R}^{q \times (s-q)} \) describe the information
transferred from the central solution to the satellites. In addition to the identities (10), (12) the structure (14) also means \( E_q^T B = E_q, \ E_q^T A = (\frac{1}{2} I, \hat{A}) \) and \( E_q^T G = (\frac{1}{2} I, \hat{G}) \) which allows to simplify the ordinary order conditions \( h^\ell \rho^0 \) in the satellite stages \( Y_{m,i}, 1 \leq i \leq q \). The next lemma makes use of the Kronecker symbol \( \delta_{ij} \).

**Lemma 2** For a peer method satisfying (4) and (14) the \( h^\ell \rho^0 \) order condition for the satellite stages \( Y_{mi} \) with \( 1 \leq i \leq q \) is given by

\[
\sum_{j=q+1}^{s} (\gamma_{ij}(1 + \sigma_m c_j)^{\ell-1} + a_{ij} c_j^{-1}) = \frac{(1 + \sigma_m)^{\ell} - 1}{\sigma_m \ell} - \frac{(1 + \sigma_m)^{\ell-1} + 1}{2}. \tag{15}
\]

With the choice \( a_{ij} = 0 \) for \( i \leq j, \ j > q \), these conditions for \( 1 \leq \ell \leq k \) are equivalent with

\[
\sum_{j=q+1}^{s} \gamma_{ij} c_j^{\ell-1} = \frac{1}{\ell} - \frac{1}{2} - \frac{1}{2} \delta_{1\ell}, \ 1 \leq \ell \leq k. \tag{16}
\]

**Proof** The satellite stages may be selected by multiplication with \( E_q^T \) from the left. The first \( q \) diagonals of the node matrix \( C \) are one due to (4), yielding \( E_q^T C = E_q^T \), and the \((n-q) \times (n-q)\) diagonal matrix of the central method will be denoted by \( \hat{C} \). Then, with coefficient matrices of the form (14) the satellite part of the condition for \( h^\ell \rho^0 \) becomes

\[
0 = E_q^T \left( (I + \sigma_m C)^{\ell} - B_m C^{\ell} - \sigma_m \ell \Gamma^m_m(I + \sigma_m C)^{\ell-1} - \sigma_m \ell A_m C^{\ell-1} \right) \mathbb{I}
\]

\[
= ((1 + \sigma_m)^{\ell} - 1) \mathbb{I} - \sigma_m \ell \left( \frac{1}{2} I, \hat{\Gamma}^m_m \right)(I + \sigma_m C)^{\ell-1} \mathbb{I} - \sigma_m \ell \left( \frac{1}{2} I, \hat{A}^m_m \right) C^{\ell-1} \mathbb{I}
\]

\[
= \left( ((1 + \sigma_m)^{\ell} - 1 - \sigma_m \ell \frac{1}{2} (1 + \sigma_m)^{\ell-1} + 1) \right) \mathbb{I}
\]

\[
- \sigma \ell \left( \hat{\Gamma}_m(I + \sigma_m \hat{C})^{\ell-1} \mathbb{I} + \hat{A}_m(C^{\ell-1}) \right) \mathbb{I}
\]

which is written out as the first assertion (15). Choosing \( \hat{A}_m = 0 \) it becomes

\[
\sum_{j=1}^{\ell} \sum_{\nu=q+1}^{s} \gamma_{ij} c_{\nu}^{\ell-1} c_{j-1}^{\ell-1} \left( \frac{\ell - 1}{\ell} \right) = \frac{(1 + \sigma_m)^{\ell} - 1}{\sigma_m \ell} - \frac{1}{2} ((1 + \sigma_m)^{\ell-1} + 1)
\]

\[
= \sum_{j=1}^{\ell} \sigma_{m}^{j-1} \left( \frac{\ell}{\ell} \left( \frac{\ell}{j-1} \right) - \frac{1}{2} \left( \frac{\ell - 1}{j-1} \right) \right) - \frac{1}{2}
\]

\[
= \sum_{j=1}^{\ell} \left( \frac{1}{j} - \frac{1}{2} \right) \sigma_{m}^{j-1} \left( \frac{\ell - 1}{j-1} \right) - \frac{1}{2}
\]

In a collection of these conditions with \( 1 \leq \ell \leq k \) both sides are multiplied by the triangular matrix with entries \( \sigma_{m}^{j-1} \left( \frac{\ell - 1}{j-1} \right) \) from the right. Removing this matrix factor we arrive at (16) which may be written shortly as
Figure 1: Dependencies between central and satellite stages.

\[
e^T_{i} \hat{\Gamma}_m V_{s-q} = u^T := (0, 0, -\frac{1}{6}, -\frac{1}{4}, -\frac{3}{10}, \ldots) = (\frac{1}{7}, -\frac{1}{2}, -\frac{1}{2}, \delta t_k)_{k=1}, \quad \text{where } V_{s-q} \text{ is the Vandermonde matrix with the nodes of the center stages and } e_i \text{ the } i\text{-th unit vector. This removal of the triangular factor is equivalent with using a Taylor expansion at } t_m \text{ which would have been more convenient in the special case } A_m = 0. \square
\]

\textbf{Remark} Obviously, the right-hand sides in the conditions of Lemma 2 are independent of the satellite index \(i\). Hence these conditions may be satisfied with coefficients where \(A_m, \hat{\Gamma}_m\) have constant rows, which means rank one. This yields a decisive practical advantage in the implementation since the correction term to the trapezoidal rule in (13) is the same for all \(q\) satellites. Hence, it will be computed only once in practice and simply added to all satellites. Choosing also \(A_m = 0\) its coefficients \(\hat{\Gamma}_m \equiv \hat{\Gamma} = \mathbb{I}(u^T V_{s-q}^{-1})\) are step-independent. Obviously these coefficients do not depend on the choice of the central peer method, only on its nodes \(c_i\).

Especially if the number of parameters \(q\) is large (e.g. \(q \approx n\) in shooting with initial values) the amount of work for the satellite stages may be dominating. Hence, in practical implementations it is convenient to compute the satellites \(Y_{m1}, \ldots, Y_{mq}\) only after a time step for the central solution is accepted. In this case, however, the central stages \(Y_{m,s-q+1}, \ldots, Y_{ms}\) are known and this most recent information should be used, most conveniently by choosing \(A_m = 0\). Hence, the final form for the satellite stages is given by

\[
Y_{m,i} - \frac{h_m}{2} F_{m,i} = Y_{m-1,i} + \frac{h_m}{2} F_{m-1,i} + h_m \sum_{j>q} \gamma_{1j} F_{m,j}, \quad i = 1, \ldots, q \quad (17)
\]

with the step-independent coefficients \((\gamma_{1j}) = u^T V_{s-q}^{-1}\) from (16). Figure 1 [7] depicts this process.

\section{The global error}

The essential requirement for the convergence of peer two-step methods is zero-stability. For the trivial ODE \(y' = 0\) the method (3) reduces to the recursion \(Y_m = B_m Y_{m-1}\) and boundedness of solutions requires the boundedness of the
matrix family \( \{B_m\}_{m \geq 1} \). This means that a constant \( K \) exists such that for all \( m \geq 1 \) uniformly holds

\[
\|B_mB_{m-1} \cdots B_{m-i}\| \leq K, \quad 1 \leq i \leq m,
\]  

(18)

see, e.g. [8], [7]. Due to the block diagonal form (6) of these matrices, condition (18) is equivalent with the same condition on the family of lower diagonal blocks \( \{\hat{B}_m\}_{m \geq 1} \) from (6) which represent the \( B \)-coefficients of the center method.

Stability discussions of peer methods for stiff nonlinear systems are rather difficult. Results on algebraic stability, for instance, are known for low-order methods, only, [6]. However, convergence in the non-stiff setting follows from zero-stability (18) similar to multistep methods, see [3] and [7]. Relying on these results we summarize the conditions and results for the trapezoidal satellite peer method in the following theorem.

**Theorem 3** Consider a peer two-step method (3) with off-steps (4). Let the method for the center stages \( Y_{m,q+1}, \ldots, Y_{ms} \), given by the matrices \( \hat{B}_m, \hat{A}_m, \hat{\Gamma}_m \) in (6), have order \( k \in \mathbb{N} \). If \( \Delta_{m} = \mathcal{O}(h_{m}^{k} + h_{m}^{2} \rho) \), \( 1 \leq i \leq q \), then the local error in these stages is

\[
Y_{mi} - y(t_{mi}) = \mathcal{O}(H^{k} + H^{2} \rho), \quad i = 1, \ldots, s, \quad t_{m} \leq t_{\text{end}}.
\]  

(19)

Due to the satellite structure this error does not contain a \( \rho^{2} \) contribution, cf. [7]. The error of the one-sided difference quotient is \( \mathcal{O}(\rho) \) with exact solution values. Adding the errors (19) for the satellites the sensitivities (5) satisfy

\[
-\frac{1}{\rho} (Y_{mi} - Y_{ms}) - \frac{\partial y}{\partial p_{i}} (t_{m+1}, 0) = \mathcal{O}(H^{2} + \rho + \frac{H^{k}}{\rho}), \quad i = 1, \ldots, q.
\]  

(20)

With this estimate we may consider a proper coupling of the two stepsizes. Adapting \( \rho \) to the time stepsize the error (20) is minimized for \( \rho \sim \frac{H}{2} \) yielding a minimal value of \( \mathcal{O}(H^{2} + H^{k/2}) \). Hence, the better satellite approximation pays off only for methods having order four, at least. Due to this requirement as basic methods for the central stages we will consider only peer methods of order four from the families derived in [8], [11] and [10]. In a variable-stepsizes implementation with tolerance \( \text{tol} \sim H^{k} \) the optimal choice for the parameter stepsizes translates to \( \rho \sim \sqrt{\text{tol}} \) which corresponds to the rule obtained in [7], Section 4, by different arguments.

### 4 Explicit and linearly-implicit time steps

For convenience, the peer methods have been discussed in implicit form (2) where each stage systems is nonlinear. Numerical tests indicate that implementations with several Newton steps have an advantage for rather crude accuracies
only, [1]. For sharper tolerances, however, linearly-implicit versions performing only one Newton step are often more efficient due to their smaller overhead since accurate predictors are available for peer methods due to their high stage order. Also, for nonstiff problems a predictor-corrector approximation for the trapezoidal satellite steps (13) will be considered. In §4.1 and §4.2 we discuss the choice of peer methods for the center stages. Since these stages are decoupled from the satellites by (6) we discuss them in the setting of standard ODEs without distinguishing between $B_m, A_m, \Gamma$ and $B_m, A_m, \Gamma_m$.

4.1 Implicit parallel peer methods

For stiff problems the satellite stages will be embedded in two families of peer methods which have been introduced as linearly-implicit W-methods in the literature. The first family of singly-implicit methods comes from the original paper [8] while multi-implicit methods have been discussed in [11]. In the latter paper, an alternative formulation of peer W-methods was given consisting of one Newton step for implicit methods. This will be used in our implementation since an easy transition to full Newton iteration is possible and the satellite stages will be implemented in this way, too. For both methods additional auxiliary variables $\tilde{Y}_m, K_m \in \mathbb{R}^{s \times n}$ are used temporarily in form of a predictor and corrector step,

$$\tilde{Y}_m := \Theta_m Y_{m-1}, \quad Y_m := \tilde{Y}_m + K_m.$$  \hfill (21)

The predictor $\Theta_m Y_{m-1}$ simply corresponds to polynomial extrapolation, [8]. For the singly-implicit methods from [8] the stage increments are computed by

$$K_m (I - h_m \gamma T)^T := (\gamma I + \hat{\beta}_m) (h_m F(\tilde{Y}_m) - E \tilde{Y}_m),$$  \hfill (22)

with an approximation $T \approx f_y(Y_{m-1,s},0)$ of the Jacobian and for the multi-implicit methods from [11] by

$$K_m - h_m \Gamma_m K_m T^T := \Gamma_m (h_m F(\tilde{Y}_m) - E \tilde{Y}_m).$$  \hfill (23)

We note that for increments $K$ stored in stacked vector form the system matrix in (23) has the well-known direct product form $I - h_m \Gamma_m \otimes T$. For the discussion following now the precise definitions of the coefficient matrices in these steps is needed. They are based on the Vandermonde matrix $V = (c_{i+1}^{j-1})_{i,j=1}^s$, the Pascal matrix $P = (\binom{i+1}{j-1})_{i,j=1}^s$, the diagonal matrices $S_m := \text{diag}(1, \sigma_m, \ldots, \sigma_m^{s-1})$, $D = \text{diag}(1, 2, \ldots, s)$ and the shift matrix $F_0 := (\delta_{i,j+1})$. The extrapolation matrix is $\Theta_m = VS_m PV^{-1}$ and $E = VDF_0^T V^{-1}$ corresponds to differentiation. In (22) the additional matrix $\hat{\beta}_m := \beta_m \Theta_m^{-1}$ is required with $\beta_m := VF_0 D^{-1} S_m V^{-1}$ from [8]. It provides stiff stability, see Lemma 4. We shortly verify the essential stability properties of both methods.
Lemma 4 For the transformed stability matrix $\tilde{M}_m$ of the singly-implicit method (21), (22) holds
\[ \tilde{M}_m(0) = (e_1 e_1^T - \gamma DF_0^T)S_mP, \quad M_m(\infty) = -\frac{1}{\gamma} F_0 D^{-1} S_m. \] (24)

The stability matrix of the multi-implicit method (21), (23) satisfies
\[ M_m(0) = (I - \Gamma_m E) \Theta_m, \quad M_m(\infty) = 0. \] (25)

Proof With $F_m = 0$, $T = 0$ we get $K_m = - (\gamma I + \hat{\beta}_m) E Y_m$ in (22) and $Y_m = (\Theta_m - (\gamma I + \hat{\beta}_m) E \Theta_m) Y_{m-1}$. Since $E \Theta_m = \sigma_m \Theta_m E$ by [8] it follows that
\[ \tilde{M}_m(0) = S_m P - (\gamma I + F_0 D^{-1}) D F_0^T S_m P = (I - \gamma D F_0^T - F_0 F_0^T) S_m P \]
which gives the desired result since $F_0 F_0^T = I - e_1 e_1^T$. For the method (23) the matrix $\beta_m$ is missing, we simply have $K_m = - \Gamma_m E Y_m$ and $M(0) = (I - \Gamma_m E) \Theta_m$.

For the test equation with $f(y) = \lambda y$, $T = \lambda$ and $\lambda \to \infty$ (22) gives $K_m = - (I + \frac{1}{\gamma} \hat{\beta}_m) Y_m$ and $Y_m = - \frac{1}{\gamma} \hat{\beta}_m \Theta_m = - \frac{1}{\gamma} \beta_m$ which is equivalent with the assertion. Again, the multi-implicit case is simpler with $K_m = - Y_m$ and $Y_m = 0$.

Lemma 4 shows the main differences in the stability properties of the two classes. The singly-implicit methods are optimally zero-stable with a two-point spectrum \{0, 1\} of $M_m(0)$. However, in the stiff limit only $\varrho(M_m(\infty)) = 0$ holds in (24). On the other hand the multi-implicit methods provide optimal stiff damping by $M_m(\infty) = 0$ but the eigenvalues of $M_m(0)$ are quite evenly distributed in the interval \{-1, 1\} for stepsizes ratios $0 < \sigma_m < 1$.

The design of these simply-implicit and multi-implicit methods in [8] and [11] was based on the structure of transformed matrices like $V^{-1} B_m V$, i.e. on a Nordsieck-type representation. Hence, basic accuracy and stability properties of these methods do not depend on the choice of the nodes $c_i$ and we will exploit this freedom to improve the efficiency of the overall methods with embedded satellites.

Methods of order four fit best with the trapezoidal satellites according to the discussion at the end of §3. Hence, we used only the five-stage methods from both classes. Since the satellite steps (17) require a LU-decomposition with $\gamma_i \equiv \frac{1}{2}$ it is mandatory to choose also $\gamma = \frac{1}{2}$ for the singly-implicit center method (22) losing the superconvergence property from [8]. Also, nonnegative nodes $e \equiv (0,0,4,1,6,2,1)$ were chosen. This singly-implicit method for the center has order 4.

For the multi-implicit method (23) from [11] an essential requisite for zero-stability was the linear relation between the diagonal elements $\gamma_{ii} = g_0 + g_1 c_i$, $i = 1, \ldots, s$ and the nodes $c_i$. However, zero stability only depends on the parameter $g_1$. Hence, we choose $g_0 = 0$ here in order to exploit the FSAL property in conjunction with the special first node $c_0 = 0$, [9]. This choice gives
\( \gamma_{11} = c_1 = 0 \) and the computation of the first stage is saved since \( Y_{m1} = Y_{m-1,s} \).

One drawback of the multi-implicit methods with direct solvers for the stage systems is that several LU-decompositions per time step have to be computed, namely 4 for the 5-stage FSAL method. In order to save at least one decomposition we chose the node \( c_2 \) with \( \gamma_{22} = g_1 c_2 = \frac{1}{2} \) such that the corresponding LU-decomposition can be re-used in the satellite step. Since zero-stability restricts the choice of \( g_1 \), cf. Remark 1.2 in [11], we chose \( g_1 = 0.3125 \) for a maximal stepsize ratio \( \sigma = 1.4 \) and \( c_2 = 1.6 \). The remaining free positive nodes \( c_3, c_4 \) were adapted to yield a small norm of the matrix \( \Theta \) in the predictor step (21) for \( \sigma = 1 \). Here again, the superconvergence condition (4.7) in [11] was not satisfied. With these choices, \( g_1 = 0.3125 \), \( \gamma_{ii} = g_1 c_i \geq 0 \) and \( c^T = (0, 1.6, 0.26, 2.2, 1) \) the multi-implicit center method also has order 4.

### 4.2 Explicit parallel peer methods

Efficient explicit parallel peer methods (\( \Gamma = 0 \)) have been derived in [10]. In this class the matrix \( B_m = B \) is constant and optimally zero-stable with a two point spectrum \( \{0, 1\} \). We will use the 4-stage method \texttt{epp4y} having order 4 from this class with nodes \( c_1, \ldots, c_4 \in [1, 1.9] \) (these nodes will be \( c_{q+1}, \ldots, c_{q+4} \) for parameter ODEs). The method is absolutely stable for real \( z \in [-0.741, 0] \) and has global order 5 for fixed stepsizes. Full details of this method can be found in the EPPEER package at \texttt{www.mathematik.uni-marburg.de/~schmitt/peer/} and \texttt{numerik.mathematik.uni-halle.de/forschung/software/}.

### 4.3 Trapezoidal steps for satellite stages

The linearly-implicit implementation of the peer method for the center stages was possible in §4.1 since the high-order predictor (21) exists. In order to get an approximate solution for the trapezoidal step (13) within the error level \( h_m \Delta_m = \mathcal{O}(h_m^{11} + h_m^3 \rho) \) of its solution with only one corrector step a sufficiently accurate predictor with error \( \mathcal{O}(h_m^{11} + h_m^3 \rho) \) is required.

Since the center correction in (17) is identical for all satellite stages it is computed only once after the peer step for the central stages \( Y_{m,q+1}, \ldots, Y_{ms} \) has been completed including a successful stepsize selection. In this case accurate approximations for the solutions \( y(t_m, 0), \, y(t_m, \rho r_i) \) and derivatives \( y'(t_m, 0), \, y'(t_m, \rho r_i) \) at the start of the time interval and one solution \( y(t_m + h_m, 0) \) at its end are known. These data are located at three corners of the rectangle \( [t_m, t_{m+1}] \times [0, \rho] \) and may be used to predict the solution at the fourth corner \( Y_{m,i} \approx y(t_{m+1}, \rho r_i) \). Looking at the Taylor expansion it is seen that an \( \mathcal{O}(h^2 \rho) \) predictor requires an approximation of the mixed derivative \( y^{(1,1)} = \partial^2 y / \partial t \partial r_i y(t_m, 0) \) which is available by \( \rho y^{(1,1)} \approx y'(t_m, \rho r_i) - y'(t_m, 0) \approx F_{m-1,i} - F_{m-1,s} \) without additional evaluations of the right-hand side \( f \). Using these values the following predictor is obtained

\[
\hat{Y}_{mi} := Y_{ms} - (Y_{m-1,s} + h_m F_{m-1,s}) + (Y_{m-1,i} + h_m F_{m-1,i}). \tag{26}
\]
For later use we note that it approximates the ideal predictor
\begin{equation}
\rho_{mi} := y(t_m + h_m, 0) + y(t_m, \rho_{ri}) - y(t_m, 0) + h_m (y'(t_m, \rho_{ri}) - y'(t_m, 0)).
\end{equation}

The arrangement of terms here stresses the interpretation that \(y(t_m + h_m, 0)\) is modified by an explicit Euler step for the difference function \(y(t, \rho_{ri}) - y(t, 0)\). Since explicit steps are not appropriate for stiff problems we consider nonstiff and stiff problems separately.

- For nonstiff problems a simple predictor-corrector implementation of the trapezoidal satellite step (13) with (26) reads \((1 \leq i \leq q)\)

\begin{equation}
\begin{aligned}
\tilde{Y}_{mi} &:= Y_{m-1,i} + Y_{ms} - Y_{m-1,s} + h(F_{m-1,i} - F_{m-1,s}), \\
F_{mi} &:= f(\tilde{Y}_{mi}, \rho_{ri}) \\
Y_{mi} &:= Y_{m-1,i} + \frac{h_m}{2} (F_{m-1,i} + F_{mi}) + h_m (\tilde{\Gamma} F_{m})_1.
\end{aligned}
\end{equation}

Here, the constant central correction is abbreviated by \((\tilde{\Gamma} F_{m})_1 \equiv (\tilde{\Gamma} F_{m})_1 := \sum_{j>q} \gamma_{ij} F_{mj}, 1 \leq i \leq q\). The amount of work for this step is still only one \(f\)-evaluation per stage as for the first-order satellites from [7]. However, memory for \(qn\) additional numbers is required now for saving the function values \(F_{m-1}\).

- For stiff problems all explicit \(F\)-terms in (28) need to be stabilized by linearly-implicit steps using additional back substitutions with the known LU-decomposition of the matrix \(\frac{2}{h} I - T\) where \(T = f_y(t_{m-1}, Y_{m-1,s})\). In a more complicated fashion the trapezoidal satellite step (13) is approximated by the linearly-implicit scheme

\begin{equation}
\begin{aligned}
\left(\frac{2}{h} I - T\right) L_i &:= F_{m-1,i} - F_{m-1,s} \\
\tilde{K}_i &:= Y_{m,s} - Y_{m-1,s} + 2 L_i \\
\tilde{Y}_{mi} &:= Y_{m-1,i} + \tilde{K}_i, \quad F_{mi} := f(\tilde{Y}_{mi}, \rho_{ri}) \\
\left(\frac{2}{h} I - T\right) (K_i - \tilde{K}_i) &:= F_{m-1,i} + F_{mi} - \frac{2}{h} \tilde{K}_i + 2(\tilde{\Gamma} F_{m})_1, \\
Y_{mi} &:= \tilde{Y}_{mi} + (K_i - \tilde{K}_i).
\end{aligned}
\end{equation}

This step again requires only one \(f\)-evaluation (per satellite stage) and two additional substitutions.

We note that (28) and (29) are predictor-corrector implementations of type \(P(EC)\) requiring only one function evaluation at \(\tilde{Y}_{mi}\) which is also used in the following time step. Of course, this evaluation may be repeated by a final step \(F_{mi} := f(Y_{mi}, \rho_{ri})\) to yield a \(P(EC)E\) type scheme. However, due to the use of five solution data the predictors \(\tilde{Y}_{mi}\) appear to be so close to \(Y_{mi}\) that only
negligible differences between both variants have been observed in our numerical tests and the more expensive $P(EC)E$ version is not used.

The accuracy of these predictors is verified in the following lemma. Here, it is helpful to note that the predictor in (29) is an approximation for the ideal linearly-implicit predictor

$$\hat{p}_{mi} := y(t_m + h_m, 0) + y(t_m, \rho r_i) - y(t_m, 0)$$

$$+ h_m(I - \frac{h}{2} T)^{-1} (y(t_m, \rho r_i) - y(t_m, 0)).$$

**Lemma 5** For a sufficiently smooth solution $y$ the ideal predictors (27) and (30), with arbitrary $T$, both satisfy the error estimate

$$\left\{ \begin{array}{c}
y(t_m + h_m, \rho r_i) - p_{mi} \\
y(t_m + h_m, \rho r_i) - \hat{p}_{mi}
\end{array} \right\} = O(h_m^2), \quad \rho, h_m \to 0.
$$

**Proof** a) Considering the directional difference function $v(t) := y(t, \rho r_i) - y(t, 0)$ again the error of the predictor (27) reduces to $y(t_m + h_m, \rho r_i) - p_{mi} = v(h_m) - v(0) - h_m v'(0)$ which is the error of the explicit Euler scheme. Hence, with some $\tau \in (t_m, t_{m+1})$, $\hat{\rho} \in (0, \rho)$ and the multi-index $\alpha = e_i, |\alpha| = 1$, it holds that

$$y(t_m + h_m, \rho r_i) - p_{mi} = \frac{1}{2} h_m^2 \rho y^{(2,\alpha)}(\tau, \hat{\rho} r_i).$$

b) For the linearly-implicit predictor (30) we have

$$y(t_m + h_m, \rho r_i) - \hat{p}_{mi} = y(t_m + h_m, \rho r_i) - p_{mi} - h_m^2 (2I - h_m T)^{-1} T v'(0)$$

For $h_m \to 0$ the matrix factor is bounded and there is an additional error contribution $\frac{1}{2} h_m^2 \rho y^{(1,\alpha)}(0, \hat{\rho} r_i)$ which fits in the assertion. □

**Remark** The explicit and linearly-implicit trapezoidal steps (28), (29) no longer fit exactly in the framework of peer methods. Rather, they are General Linear Methods [2] with internal stages $\tilde{y}_{mi}$. Without giving details we note that they still may be written artificially as peer methods with several vanishing columns in some coefficient matrices.

As a simple test for the accuracy of the computed sensitivities we consider a modification of a well-known differential equation from dynamical systems theory having the unit circle as limit cycle. The two-parameter problem

$$\left( \begin{array}{c}
y'_1 \\
y'_2
\end{array} \right) = \left( \begin{array}{c}
- p_1 y_2 \\
\frac{1}{p_1} y_1
\end{array} \right) + p_2 (1 - y_1^2 - p_1^2 y_2^2) \left( \begin{array}{c}
y_1 \\
y_2
\end{array} \right)$$

(31)

has the ellipse $\{(y_1, y_2) : y_1^2 + p_1 y_2^2 = 1\}$ as limit cycle and the solutions are spirals where $p_2 > 0$ controls the rate of attraction. The solution with initial values $y(0) = (\frac{1}{2}, 0)^T$ is given by

$$y(t, p) = \frac{1}{\sqrt{1 + 3e^{2pt}}} \left( \begin{array}{c}
\cos(t) \\
\sin(t)/p_1
\end{array} \right)$$

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Figure 2: Accuracy of parameter derivatives for spiral ODE with different $\rho$ using fixed stepsizes (left) and stepsize control (right)

and its parameter derivatives at $t = 1$ and $\hat{\rho} = (1, 2)^T$ are

$$
\frac{\partial y}{\partial \rho} = \begin{pmatrix}
0 & 0.02739897001 \\
-0.8192639438 & 0.04267136754
\end{pmatrix}.
$$

In order to demonstrate the improved accuracy of solution derivatives to this non-stiff problem the fourth-order explicit parallel method epp4y from [10] is used with embedded satellites (28). For this combination the error of the sensitivities with constant stepsize $h$ has the form $(\rho + h^2 + h^4/\rho)$ by (20). The left diagram in Figure 2 shows runs with a series of fixed stepsizes $hs$ for different choices of $\rho$. In the curves with fixed $\rho = 10^{-2}, 10^{-4}, 10^{-6}$ those parts behaving like $\rho$ and $h^4/\rho$ are easily identified. Only in the curve for $\rho = 10^{-2}$ (crosses) the $h^2$-behaviour may be discovered. Coupling both stepsizes by $\rho = h^2$ (black dots) shows the expected error behaviour $O(h^2)$ as the almost exact envelope of the other curves. The diagram on the right in Figure 2 presents the same computations with stepsize control in the integration. A nearly optimal choice for the parameter stepsize is given by $\rho = \sqrt{\text{tol}}$ (bullets) and we will use this kind of coupling

$$
\rho = a\sqrt{\text{tol}}
$$

in all computations with different constants $a$.

5 Applications

An important application area for sensitivity approximations are Newton-type iterations in shooting. In this context the embedded sensitivities have been employed in [7] for different problem types, namely in searching parameters and initial values for time-periodic solutions and in parameter identification of observed trajectories. Here, we will compare the new second-order approximation
with the older scheme only for the Brusselator,

\[
\begin{align*}
y_1' &= d_1 \frac{\partial^2 y_1}{\partial x^2} + \alpha - (\beta + 1)y_1 + y_1^2 y_2, \\
y_2' &= d_2 \frac{\partial^2 y_2}{\partial x^2} + \beta y_1 - y_1^2 y_2,
\end{align*}
\]

(33)

\(\alpha, \beta > 0\). With positive diffusion constants \(d_1, d_2 > 0\) it is a parabolic equation and will be used with Dirichlet boundary conditions

\(y_1(t, 0) = y_1(t, 1) = \alpha, \quad y_2(t, 0) = y_2(t, 1) = \beta/\alpha\).

Using a finite difference approximation with only 31 interior grid points the problem of computing time-periodic solutions here was introduced in [4]. Since the resulting MOL system is only mildly stiff with diffusion constants \(d_1 = 0.008, d_2 = 0.004\) the problem was also solved in [7] with explicit embedded peer methods and we will compare the performance with the new satellites (28). The parameters here are the unknown initial values, \(y_0 = p, q = n = 62\). With a finer space discretization, say \(N \in \mathbb{N}\) interior grid points, the problem becomes increasingly stiff and this is a convenient application for the implicit peer methods with satellites (29). Here, band solvers are efficient for the linear stage systems. This yields a demanding test for these methods since the number of parameters increases by \(q = n = 2N\), too. In the end we will see that the convergence of the computed time period \(T\) has indeed second order accuracy with respect to the space stepsize.

However, we will consider (33) as an ODE first, \(y \in \mathbb{R}^2\), with \(d_1 = d_2 = 0\) and search for parameters \(p = (\alpha, \beta) \in \mathbb{R}^2\) belonging to a periodic solution through \(y_0 = (1.8, 1.8)^T\) as in [7]. The only difference to [7] is the use of the fourth-order method \texttt{epp4y} mentioned in Section 4 for the central stages in all computations. Figure 3 shows the residuals over the number of iterations in Newton’s method for a set of tolerances \(tol = 10^{-2j}, j = 1, \ldots, 4\). Good choices for the parameter stepsizes were used with \(\rho = 0.2 \sqrt{tol}\) for the simple satellites from [7] (left diagram) and \(\rho = \sqrt{tol}\) for (28) on the right, see (32). Obviously there is a remarkable improvement with the trapezoidal satellites leading to almost quadratic convergence for sharp tolerances.
Figure 4: Shooting for time-periodic solutions of 1D-Brusselator ($N = 31$) with explicit method **epp4y**, sensitivities of first-order (left) and second-order (right).

For the 1D-Brusselator we also compare the explicit four-stage method **epp4y** with the old and new satellite types and the same parameter stepsizes $\rho$ as before. The parameters of the differential equation are $(\alpha, \beta) = (2, 5.45)$ and the start approximation for the Newton iteration are $y_1(0, x) \equiv 2.5$, $y_2(0, x) \equiv 3.2$ as in [7]. Here, the differences in Figure 4 are only small, the more accurate satellites save one iteration, at best, for $tol \leq 10^{-6}$. This little improvement is probably due to the mild stiffness of the problem, the performance of the implicit methods at the same problem is much better for $tol = 10^{-4}$, see Figure 5.

With finer space discretizations the 1D-Brusselator becomes stiff and implicit methods are needed. In fact we use this problem also for comparing the singly-implicit and multi-implicit 5-stage peer methods from Section 4.1 with stepsize control and the trapezoidal satellites (29). It turns out that good choices for the parameter stepsizes (32) require a much larger constant $a = 400$ than for explicit methods and convergence may sometimes depend critically on this constant. First, we repeat the last test and present the results for Newton’s iteration with grid size $N = 31$ and integration tolerances $tol = 10^{-4}, 10^{-6}, 10^{-8}$ in Figure 5. Open marks indicate the singly-implicit method and filled symbols are for the multi-implicit scheme. Obviously, results for both types are so close that they are nearly indistinguishable. We note that unlike Figure 4 the iteration does not converge with implicit methods if a lower order satellite predictor is used, for instance an $O(h)\rho$-predictor obtained by omitting the linearly-implicit contribution $L_i$ in (29).

Since the Lipschitz constant of $f$ is of order $4d_2(N + 1)^2$ in this example, its value is around 16 for $N = 31$ and increases to $10^8$ for $N = 255$. Still, convergence of Newton’s method with the implicit time integration methods is robust and not affected by stiffness. This can be seen in Figure 6 with the results for grid sizes $N = 127$ and $N = 255$. We remind that the number of satellite stages in these cases is equal to the problem size which is $p = n = 2N = 510$ for the finest grid. Even with so many stages the singly-implicit method still has an advantage and has slightly shorter computing times since the multi-implicit method (23) requires 3 more LU-decompositions per time step for the
Figure 5: Shooting for 1D-Brusselator ($N = 31$) with implicit peer methods.

Figure 6: Shooting for 1D-Brusselator with implicit peer methods, grid size $N = 127$ left and $N = 255$ right.
central stages. For these larger problems some differences between both types of
tools are visible in Figure 6. However, the speed of convergence depends in
a nontrivial way on the constant \(a\) in (32) and may change for different choices.
Finally, we note that results with a costlier \(P(EC)E\)-implementation, see §4.3,
are very close to those presented here.

With computations for different space grids it is also of interest to monitor
the computed time periods \(T\) and discuss its convergence with respect to the
space grid size \(1/(N+1)\) as an independent check for the shooting method. The
computed time periods and the observed orders are given in (34).

\[
\begin{array}{|c|c|c|}
\hline
N+1 & T & \Delta T & \text{order} \\
\hline
32 & 3.434865564 & & \\
64 & 3.434969415 & 0.103851 \cdot 10^{-3} & \\
128 & 3.434995142 & 0.25727 \cdot 10^{-4} & 2.013 \\
256 & 3.435001617 & 0.6475 \cdot 10^{-5} & 1.990 \\
\hline
\end{array}
\]

(34)

Obviously the observed orders are in good agreement with the order two of the
finite-difference space discretization. This shows that the shooting method with
peer time integration is efficient and correct.

In [7] also the identification of the parameters of an observed Brusselator
ODE solution was considered. However, since the results with the trapezoidal
satellite approximation showed hardly an improvement in the speed of conver-
gence these results are not shown, here.

**Conclusion**

The extended order conditions for second-order accurate embedded parameter
sensitivities of peer two-step methods with a satellite configuration can only be
satisfied with implicit methods. However, due to the high stage order of peer
methods sufficiently accurate predictors for linearly-implicit implementations
are available. Even explicit satellite approximations for non-stiff problems are
possible without loss of accuracy using one \(f\)-evaluation per step and parameter.
Applications in shooting methods for time-periodic solutions show improved
convergence of Newton’s iteration compared to the first-order sensitivities from
an earlier paper. In a method-of-lines problem the linearly-implicit methods
perform well for different grid sizes and levels of stiffness. The results are verified
by monitoring the convergence of the time period with respect to the grid size.
For MOL systems the singly-implicit methods are clearly preferable if direct
solution methods are used for the linear systems.

**References**


