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Error Control Policy for Initial Value Problems with Discontinuities and Delays

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Abstract. Runge-Kutta-Nyström (RKN) methods provide a popular way to solve the initial value problem (IVP) for a system of ordinary differential equations (ODEs). Users of software are typically asked to specify a tolerance δ, that indicates in somewhat vague sense, the level of accuracy required. It is clearly important to understand the precise effect of changing δ, and to derive the strongest possible results about the behaviour of the global error that will not have regular behaviour unless an appropriate stepsize selection formula and standard error control policy are used. Faced with this situation sufficient conditions on an algorithm that guarantee such behaviour for the global error to be asympotatically linear in δ as $\delta \to 0$, that were first derived by Stetter. Here we extend the analysis to cover a certain class of ODEs with low-order derivative discontinuities, and the class of ODEs with constant delays. We show that standard error control techniques will be successful if discontinuities are handled correctly and delay terms are calculated with sufficient accurate interpolants. It is perhaps surprising that several delay ODE algorithms that have been proposed do not use sufficiently accurate interpolants to guarantee asymptotic proportionality. Our theoretical results are illustrated numerically.

1. Introduction

Typically an error tolerance δ, that is supplied by the users to control the accuracy of the numerical solution, determines dynamically the meshpoints and the discrete approximations at these points. The software automatically chosses the stepsizes based on δ. The best that we can ask in this situation is that if a fixed problem is solved repeatedly over a resonable range of tolerance values, then the global error should decrease linearly with δ, such a relationship is reffered to as tolerance proportionality (TP) that was first addressed for first order ODEs of IVPs by Stetter [33], [35]. The DETEST package uses a linear least squares fit of error versus tolerance as one criterion for evaluating the performance of an initial value solver see [14], for example. Further analysis directed at explicit Runge-Kutta-Nyström

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methods with continuous extensions was given in [1]. This work is a sequel to [1] and its aim is to extend the existing analysis to allow for ODEs with low-order derivative discontinuities and ODEs with constant delays. In the rest of this section, we very briefly outline the results that will be used later.

We consider the solution of the nonstiff second order ODEs of IVPs

$$y''(t) = f(t, y), \; y(t_0) = y_0, \; y'(t_0) = y'_0 \in \Re^m, \; t_0 \leq t \leq t_{end} \tag{1}$$

It is well known that Runge-Kutta-Nyström (RKN) methods produce approximations for y and y' only at the end of each step. However, there are important applications, that require a continuous approximation of $y(x)$ and $y'(x)$ on every point of a step. In the last few years there has been a lot of research devoted to providing continuous extensions for RKN methods, see for example, Dormand and Prince [10], Papageorgiou and Tsitouras [27], [28]. Horn [18] and Fine [15]. We assume that discrete numerical approximation of the problem (1) is produced by applying the pth order Runge-Kutta-Nyström method. On a particular step from t_n to t_{n+1}, the pth order Runge-Kutta-Nyström method is used to advance the approximations from $y_n \approx y(tn)$ to $y_{n+1} \approx y(tn+1)$ for the solution over a step of length $h_{n+1} = t_{n+1} - t_n$. The local error for the step is defined as $le_{n+1} := y_{n+1} - z_n(t_{n+1})$, where the local solution, $z_n(t)$, satisfies $z''_n = f(t, z_n(t))$ with $z_n(t_n) = y_n$ and $z'_n(t_n) = y'_n$, we also assume that the problem (1) is sufficiently smooth for the local error expansion of the form

$$le_{n+1} = \hat{\psi}(t_{n,}y_n) \; h_n^{p+1} + O\left(h_n^{p+2}\right) \tag{2}$$

to hold, where the continuous function $\hat{\psi}$ is independent of h_n. We further assume that the error estimate $\| E(t_{n,}y_n, h_n) \|$, is computed in the course of the step where

$$E(t_n, y_n, h_n) = \psi(t_n, y_n) \; h_n^p + O\left(h_n^{p+1}\right) \tag{3}$$

and ψ is continuous and independent of h_n, and $\| \psi(t, y(t)) \| \neq 0$ on $[t_0, t_{end}]$. The step is accepted if the condition $\| E(t_n, y_n, h_n) \| \leq \delta$ must hold, where δ is the local error tolerance specified by the user in order to indicate the level of the accuracy required. If this condition is violated, the step from t_n is re-taken with a smaller stepsize. The standard asymptotically based stepsize selection formula for changing stepsize after a successful step is defined as

$$h_{n+1} = \theta h_n \left(\frac{\delta}{\| E \|} \right)^{1/p}, \tag{4}$$

with the safety factor $\theta \in (0, 1)$ is introduced in an attempt to avoid rejected steps, the value $\theta = 0.9$ is typical, other step reduction strategies may be used in practice after a step rejected , but the details are not important for our analysis. Most of the commonly used error control method fit into the above framework; in particular one of the following error control modes is used extrapolated error-per-step or error-per-unit step with a pth order RKN method. For the former choice mode the local error estimate

$$E = est_n = \max\left\{\|\delta_{n+1}\|_\infty, \left\|\delta'_{n+1}\right\|_\infty\right\}$$

and for the latter mode

$$E = est_n = \max\left\{\frac{\|\delta_{n+1}\|_\infty}{h_n}, \frac{\left\|\delta'_{n+1}\right\|_\infty}{h_n}\right\}$$

where $\delta_{n+1} = y_{n+1} - \hat{y}_{n+1}$ and $\delta'_{n+1} = y'_{n+1} - \hat{y}'_{n+1}$.

We will use $\eta(t)$ to denote any continuous interpolant that passes through the meshpoint data $\{t_n, y_n\}$ and takes the values y_n at t_n and y_{n+1} at t_{n+1} for $n = 0, 1, \cdots$. In particular $\eta_I(t)$ denotes the ideal interpolant from [34], which is defined as

$$\eta_{\dot{I}}(t) := z_n(t) + \left[(t - t_n)^2 - (t - t_n)(h_n - 2)\right]\frac{le_{n+1}}{2h_n}, \; t \in [t_n, t_{n+1}] \tag{5}$$

We point out that $\eta_{\dot{I}}(t)$ is not necessarily computable, since we are only concerned with the meshpoint approximation (in this section), and that $\eta'_{\dot{I}}(t)$ generally has a jump discontinuity at each meshpoint t_n.

In the following theorem, which is taken from [1, Theorem 3.2.1], we use the convention that "sectionally continuous" means continuous except possibly at the meshpoint t_n, and "sectionally C^2" means continuous with the first and second derivatives which are continuous except possibly at the meshpoints t_n, where the first and second derivatives have jump discontinuities with finite right and left hand limits.

Theorem 1. *Given the initial value problem* (1) *suppose $\eta(t)$ is sectionally C^2 and satisfies $\eta(t_0) = y_0$ and $\eta'(t_0) = y'_0$. Let $\varepsilon(t) := \eta(t) - y(t)$ denote the global error in $\eta(t)$. Define condition* (I) *to be* :

$$\varepsilon(t) = v(t)\delta + r(t), \; t_0 \le t \le t_{end}$$

where $v(t)$ is C^2 and independent of δ and $r(t)$ is sectionally C^2 with zeroth, first and second derivatives of $o(\delta)$. Also, define condition (II) *to be* :

$$\eta''(t) - f(t, \eta(t)) = \gamma(t)\delta + s(t), \; t_0 \le t \le t_{end},$$

where $\gamma(t)$ is continuous and independent of δ and $s(t)$ is sectionally continuous and $o(\delta)$. Then condition (I) *is equivalent to condition* (II).

Condition (I) is a formalization of the concept of tolerance proportionality. For any fixed point $t_0 \le t \le t_{end}$, it ensures that the global error is asymptotically linear in δ. The condition is strong in the sense that it also requires the global error in $\eta'(t)$ and $\eta''(t)$ to be asymptotically linear in δ. The equivalent condition (II) provides a more useful characterization from the point of view of analysis.

We will make the following assumptions regarding the numerical solutions

1. The stepsizes satisfy $\max_n \{h_n\} = o(1)$ as $\delta \longrightarrow 0$,
2. The function $\|\psi(t, y(t))\|$ from (3) is non-vanishing,
3. The initial stepsize is chosen so that

$$\|E(t_0, y_0, h_1)\| = \theta^{-p}\delta + o(\delta), \tag{6}$$

Note that assumption (1) implies convergence of the Runge-Kutta-Nyström solution; that is, $\varepsilon(t) \longrightarrow 0$ as $\delta \longrightarrow 0$ (see, for example, [17, Theorem 3.4]). Also, from assumption (2) the error control criterion $\|E(t_n, y_n, h_n)\| \le \delta$ implies that a function that is $O(h_n^p)$ is also $O(\delta)$. Under assumptions (1), (2), and (3) the ideal interpolant satisfies condition (I), and hence the algorithm exhibits tolerance proportionality, see [1].

The discrete RKN approximation with a continuous extension usually satisfy the condition $q(t_n) = y_n$ and $q(t_{n+1}) = y_{n+1}$ for the solution approximation and $q'(t_n) = y'_n$ and $q'(t_{n+1}) = y'_{n+1}$ for the derivative approximation and hence reffered to as interpolants. Modern interpolants also fit the derivative data at the meshpoints; that is, $q''(t_n) = f(t_n, y_n)$ and $q''(t_{n+1}) = f(t_{n+1}, y_{n+1})$ in which case the corresponding global approximation is a C^2 function. Among the applications for continuous extensions are handling of discontinuities, singularities, delay differential equations, and the need for the numerical solution at a dense set of output points (graphical representation of the solution), see for example, [7], [10], [12], [21]. Such interpolants will not satisfy condition (I) of Theorem 1, although they may satisfy a weaker condition, see [1]. To be more specific, the RKN interpolants that have been proposed in the literature can be split into two groups; if l is the largest integer such that, for any fixed $\sigma \in [0, 1]$,

$$q(t_n + \sigma h_n) - z_n(t_n + \sigma h_n) = O\left(h_n^l\right).$$

In the case of $l = p + 1$ we get a so-called higher-order interpolant but if $l = p$ we get a so-called lower-order interpolant. Higher-order interpolants satisfy

$$q(t) - y(t) = v(t)\,\delta + o(\delta), \ t_0 \le t \le t_{end}, \tag{7}$$

where $v(t)$ is C^2 and independent of δ, but not $q'(t) - y'(t) = v'(t)\ \delta + o(\delta)$.

Hence, higher-order interpolants preserve the TP in the solution approximation, but not in the first derivative approximation. For lower-order interpolants we have $q(t) - y(t) = O(\delta)$, but the leading term in the global error does not in general depend linearly upon δ. This difference in behaviour between the two classes of interpolants plays a key role in our analysis for delay ODEs.

In the next section we look at the effect of overriding the usual stepsize selection mechanism in order to hit an output point exactly or to integrate across a discontinuity. The results of Section 2 are used in Section 3 where error control methods for constant delay ODE systems are analysed. Finally we test our predictions numerically in both sections and give conclusions in Section 4.

2. Output points and discontinuities

Suppose that the RKN method described above reaches the point t_n and uses (4) to compute the stepsize h_{n+1} and to continue the integration.There are certain circumstances under which a method will restrict the stepsize to $h^* < h_{n+1}$ in order to hit the point $t^* := t_n + h^*$ exactly. This may happen, for example, if t^* has been specified as an output point, or if a low-order derivative of the solution is known to have a discontinuity at t^*. In this case, we have

$$z_n(t_n) - y(t_n) = v(t_n)\,\delta + o(\delta).$$

A standard differential inequality [17, Theorem 10.2] then gives

$$z_n(t) - y(t) = O(\delta),\ t_n \le t \le t^*.$$

Assuming that f is Lipschitzian, it follows that

$$z_n'(t) - y'(t) = O(\delta),\ t_n \le t \le t^*,$$

and hence

$$z_n(\bar{t}) - y(\bar{t}) = z_n(t_n) - y(t_n) + O(h^*\delta) = v(t_n)\,\delta + o(\delta).$$

Since $v(t)$ is C^2, and independent of δ, we have

$$z_n(t^*) - y(t^*) = v(t^*)\,\delta + o(\delta). \tag{8}$$

Now the numerical approximation $y^* \approx y(t^*)$ satisfies $y^* - z_n(t^*) = O(h^{*\ p+1})$, and hence $y^* - z_n(t^*) = o(\delta)$, so that, from (8), we have

$$y^* - y(t^*) = v(t^*)\,\delta + o(\delta), \tag{9}$$

showing that TP in the solution is maintained at t^*. To examine the first derivative approximation and the second derivative approximation $\eta_I'(t)$ and $\eta_I''(t)$ we note from (5) that

$$\eta_I'(t^*) - y'(t^*) = z_n'(t^*) + [2(t^* - t_n) - (h^* - 2)]\,\frac{le^*}{2h^*} - y'(t^*)$$
$$\eta_I''(t^*) - y''(t^*) = z_n''(t^*) + \frac{le^*}{h^*} - y''(t^*)$$

where le^* denote the local error over the last step, $le^* := y^* - z_n(t^*)$. Hence

$$(10)\quad \begin{aligned} \eta_I''(t^*) - y''(t^*) &= f(t^*, z_n(t^*)) - f(t^*, y(t^*)) + \frac{le^*}{h^*} \\ &= f_y(t^*, y(t^*))(z_n(t^*) - y(t^*)) + O([z_n(t^*) - y(t^*)]^2) \\ &= f_y(t^*, y(t^*))\, v(t^*)\,\delta + \frac{le^*}{h^*} + o(\delta), \end{aligned}$$

using (8). Now the quantity le^*/h^* behaves like $O(h^{*\,p})$ as $h^* \longrightarrow 0$, and hence will not necessarily be negligible compared with the first term in (10). The key point to note is that, as $\delta \longrightarrow 0$, h^* will follow a decaying sawtooth pattern, changing discontinuously each time a meshpoint coincides with t^*. Hence le^*/h^* will not behave like a linear function of δ, and it follows that TP in $\eta_I'(t^*)$ and $\eta_I''(t^*)$ can not be guaranteed. However, the continuous interpolant, $q(t)$ for which $q'(t^*) = y^{*\prime}$ and $q''(t^*) = f(t^*, y^*)$, satisfy

$$(11)\quad \begin{aligned} q''(t^*) - y''(t^*) &= f(t^*, y^*) - f(t^*, y(t^*)) \\ &= f_y(t^*, y(t^*))\ v(t^*)\ \delta + o(\delta), \end{aligned}$$

using (9). The function $f_y(t, y(t))\, v(t)$ is independent of δ, and hence we have a proportionality result for $q''(t^*)$. In the case where the final stepsize is reduced to hit t^* exactly, we can conclude for $t_0 \le t \le t^*$ that

1. $\eta_I'(t)$ and $\eta_I''(t)$ give TP at all t except $t = t^*$,
2. $q''(t)$ gives TP at no t except $t = t^*$.

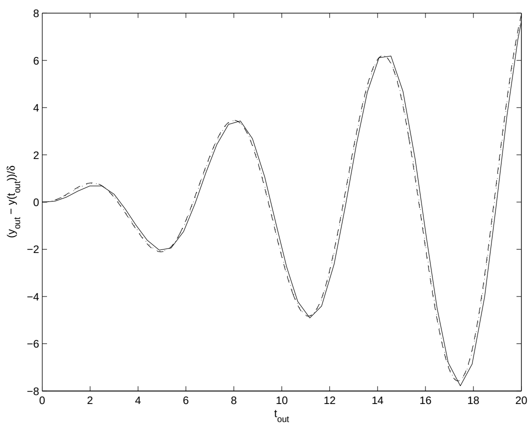

Figure 1: Harmonic oscillator equation.

We illustrate these phenomena using the harmonic oscillator equation

$$(12)\qquad y''(t) = -y(t), \quad y(0) = 1, \quad y'(0) = 0,$$

which has solution $y(t) = \cos(t)$. We implemented the third and fourth order pair RKN4(3)4FM that appears in ([11], 1987) in extrapolated error-per-step mode; that is, with the fourth-order formula advancing the solution and the difference between the third and fourth order values giving the error estimate. Mixed relative-absolute weights were used in the error measure. The code was made to reduce the final stepsize, if necessary, so as to hit the output point $t^* = t_{out}$ exactly. The problem was solved repeatedly using 100 equally spaced values of t^* in $[0, 20]$, and after each integration we recorded the global error in y^*, $f(t^*, y^*)$, and $\eta_I^{''}(t^*)$. Since $\eta_I^{''}(t^*)$ is not computable in general, we used the approximation $f(t^*, \bar{w}(t^*)) + l\bar{e}^* / h^*$. Here $\bar{w}(t^*)$ is the result of a step from $\{t_n, y_n\}$ of length h^* using an eighth-order RKN formula, and $l\bar{e}^* = y^* - \bar{w}(t^*)$. The test were performed for error tolerances of $\delta = 10^{-i}$, $i = 4, 6, 8$. The results are plotted in Figures $1 - 3$. In these and all subsequent figures, discrete values are joined by straight lines for clarity, and the line type changes from solid to dotted to dashed/dotted as the tolerance decreases.

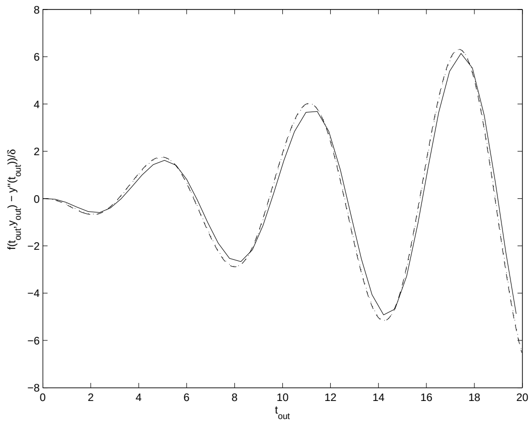

Figure 2: Harmonic oscillator equation.

We see from Figure 1 that the global error to tolerance ratio for y^* appears to be converging to a discernible limit function as δ decreases. The TP behaviour of $f(t^*, y^*)$, given in Figure 2, is also reasonably good. For $\eta_I^{''}(t^*)$, however, the ratio does not settle down to a limit.

Comparing Figures 2 and 3 we see that the $\eta_I^{''}(t^*)$ ratios seem to correspond to those for $f(t^*, y^*)$. This is what we would expect from equation (10) and (11); the nonsmooth term le^* / h^* in (10) is clearly making its presence felt.

Next, we must consider what happens when the integration is re-started from the point t^*. This is essentially the same as applying the method to a new initial value problem, except that the initial value y^* is not exact, but satisfies (9). It can be shown that Theorem 1 extends to the case where the initial value has an error that is asymptotically linear in δ.

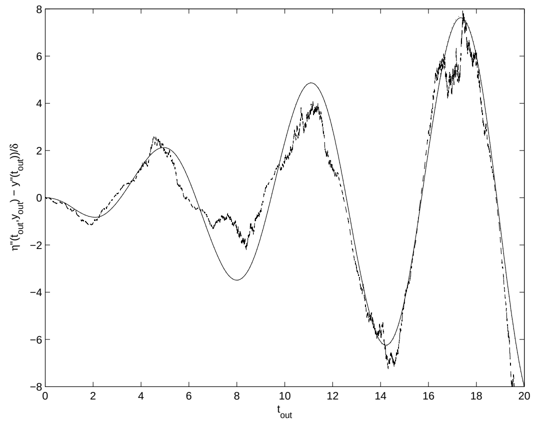

Figure 3: Harmonic oscillator equation.

A more general version of this result is proved in the next section. It follows that TP is maintained after crossing t^*, and by induction, when a finite number of discontinuities are encountered.

We illustrate this behaviour using the following problem,

$$y''(t) = -y(t) - 3\sin(2t) - sign(y), \quad y(0) = 0, \quad y'(0) = 3,$$

that is also used in [31] and involves a discontinuities function

$$sign(y) = \begin{cases} +1 & if \;\; y \geq 0 \\ -1 & if \;\; y < 0 \end{cases},$$

that causes the second derivative of $y(t)$ changes sign. This is a simplified model of a system with a relay. It has been used (Shampine et al. (1976)) to test how well codes cope with a lack of smoothness, see [31].

Generally a proper treatment of such a problem would require integrating until y changes sign locating carefully where this happend, and restarting there with the new equation corresponding to y of the new sign.

The problem was solved with the RKN algorithm described earlier, and the range of integration was $0 \leq t \leq 6\pi$ except that the stepsize selection was altered so that rather than including the points of discontinuity in the mesh, we crossed them with stepsizes of $o(\delta)$.

This was done in attempt to model the more realistic situation where the discontinuities are not known exactly [13], [16]. Figure 4 records the global error to tolerance ratios at the meshpoints for $\delta = 10^{-i}, \; i = 4, 6, 8$.

In Figure 5 we present the corresponding picture when the standard stepsize selection strategy was not changed. In the former case the ratios appear to be

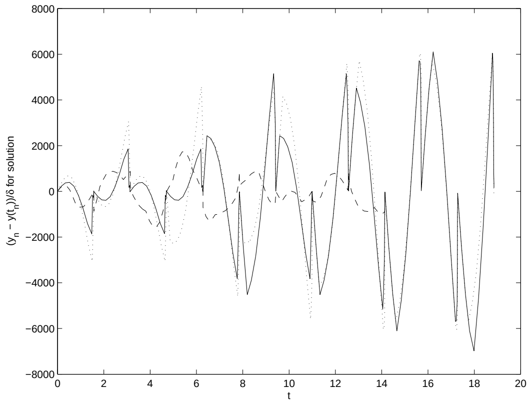

Figure 4: Model of a system with a relay.

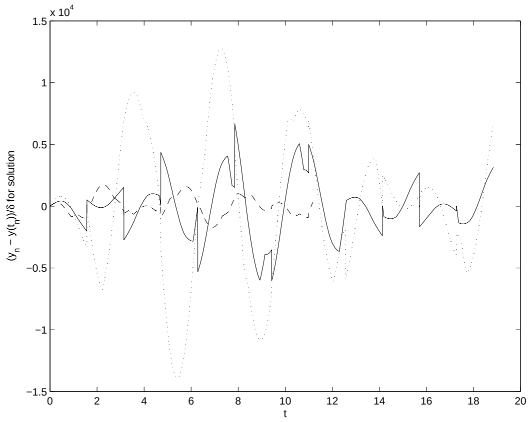

Figure 5: Model of a system with a relay.

approching a limit, whereas in the latter case the errors are much larger and do not settle down.

3. ODEs with constant delays

One of the simplest examples of a delay differential equation is given by

$$\begin{aligned} y''(t) &= -y\,(t-1)\,,\ t \geq 0, \\ y\,(t) &= 1,\ \ y'\,(t) = 0,\ t \in [-1, 0]\,. \end{aligned} \tag{13}$$

One easily realizes that, in general, at the point $t = t_0$ the solution does not join smoothly the initial function $y(t) = \phi(t)$, and therefore jump discontinuities in y' and $y''\,(t)$ can occure at any point $t^* \in (t_0, t_{end})$. This means that this discontinuity is propagated in such a way that $y^{(i)}(t)$ is discontinuous at $t = i-1$, and the solution on the interval $[i, i+1]$ is a polynomial of degree $i+1$ and this is a discontinuity of order $i+1$ at $t = i$.

The general problem considered here is a system of ODEs with k constant delays, which we write as

$$\begin{aligned} y''(t) &= F\left(t, y(t), y(t-\sigma_1), \cdots, y(t-\sigma_k)\right) \in \Re^m, 0 \le t \le t_{end}, \\ y(t) &= \phi(t), \quad y'(t) = \phi'(t), \quad t \in [-\sigma_k, 0]. \end{aligned} \tag{14}$$

We assume that the delays are ordered so that $0 < \sigma_1 < \sigma_2 < \ldots < \sigma_k$, and that the initial function, $\phi(t)$, has $p+1$ continuous derivatives . As we noted in the example (13), if $\phi(t)$ does not match $y(t)$ smoothly at $t = 0$, then derivative discontinuities will be propagated throughout the solution. It can be shown that $y'(t)$ and $y''(t)$ are generally discontinuous at $t = 0$ and that a discontinuity in $y^{(k)}(t)$ at $t = t^*$ leads to a possible discontinuity in $y^{(k+1)}(t)$ at $t = t^* + \sigma_j$, for $j = 1, 2, \cdots, k$. For an analysis of the location and order of discontinuities in more general classes of delay ODEs, see [4], [5], [8], [23], [36], [37].

We assume that F in (14) is a smooth function of each of its arguments, and in particular that if $s(t)$ is a given function with $p+1$ continuous derivatives, then the standard initial value problem (IVP)

$$\begin{aligned} y''(t) &= F\left(t, y(t), s(t-\sigma_1), \cdots, s(t-\sigma_k)\right), \\ y(0) &= y_0, \quad y'(0) = y_0', \end{aligned}$$

is sufficiently smooth for the expansions (2) and (3) to hold for any initial values y_0 and y_0'. Now due to the discontinuity propagation in (14), it follows that there exist a finite number of points $\{\hat{t}_i\}_{i=1}^{m}$ such that $0 < \hat{t}_1 < \hat{t}_2 < \cdots < \hat{t}_m$ and $y(t)$ has $p+1$ continuous derivatives over each subinterval $(\hat{t}_i, \hat{t}_{i+1})$, and also over $(\hat{t}_m, \infty)$.

Moreover, the discontinuity points $\hat{t}_i$ can be computed a priori. The most natural approach for solving (14) numerically is to use an interpolation procedure to approximate the retarded values, $y(t-\sigma_i)$, and then to apply a standard ODE method to the resulting IVP, see [2], [17], [22], [24] ,[25 − 29] for examples. Here, we assume that an explicit RKN method is used, with error control and stepsize selection as described in Section 1, and with a corresponding interpolant. In other words, we apply the RKN method to the ODE

$$\begin{aligned} y^{q\,\prime\prime}(t) &= F\left(t, y^q(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right), 0 \le t \le t_{end}, \\ y^q(0) &= \phi(0), \; y^{q\,\prime}(0) = \phi'(0), \end{aligned} \tag{15}$$

where $q(t) := \phi(t)$ for $t \in [-\sigma_k, 0]$, and for $t > 0$, $q(t)$ denotes either a higher or lower-order interpolant to the discrete approximation, as described in Section 1. The superscript q emphasises that y^q depends upon q, and therefore upon the error tolerance δ. Note that since we are concerned with an $h_n \longrightarrow 0$ analysis, we may assume that on a general step from t_n to t_{n+1}, the retarded values needed by the

RKN scheme lie to the left of t_n, and hence interpolation rather than extrapolation can be used . We will suppose that the discontinuity points $\hat{t}_i$ are located a priori and incorporated into the mesh. Our aim is to examine what conditions on the interpolation process are necessary / sufficient to guarantee tolerance proportionality.

We note immediately that the first smooth subinterval will be $(0, \sigma_1)$ and that on this subinterval we are, in effect, solving the standard IVP

$$\begin{aligned} y''(t) &= F(t, y(t), \phi(t-\sigma_1), \cdots, \phi(t-\sigma_k)), \\ y(0) &= \phi(0), \quad y'(0) = \phi'(0). \end{aligned} \tag{16}$$

Since this ODE does not depend upon δ, the results mentioned in Section 1 apply directly, and in particular we conclude that higher-order interpolants will satisfy (7) over $\left(0, \hat{t}_1\right)$ while lower-order interpolants give $q(t) - y(t) = O(\delta)$, but do not give (7) in general. Now suppose that we re-start at $\hat{t}_1 = \sigma_1$. To proceed with the analysis we define the local solution over a general step from t_n to t_{n+1} by

$$\begin{aligned} z_n^{q\,\prime\prime}(t) &= F(t, z_n^q(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)), \\ z_n^q(t_n) &= y_n, \quad z_n^{q\,\prime}(t_n) = y_n', \end{aligned} \tag{17}$$

and the local error at t_{n+1} by

$$le_{n+1}^q = y_{n+1} - z_n^q(t_{n+1}).$$

The corresponding ideal interpolant can then be defined by

$$\eta_I^q(t) := z_n^q(t) + \left[(t-t_n)^2 - (t-t_n)(h_n - 2)\right] \frac{le_{n+1}^q}{2h_n}, \; t \in [t_n, t_{n+1}].$$

Our approach is to examine the global error $\eta_I^q(t) - y(t)$ over $\left(\hat{t}_1, \hat{t}_2\right)$ by splitting it into two components, $y^q(t) - y(t)$ and $\eta_I^q(t) - y^q(t)$. First we look at $y^q(t) - y(t)$, and show that with higher-order interpolation if we regard $y^q(t)$ as an approximation to $y(t)$ then condition (II) of Theorem 1, and hence also condition (I) , is satisfied.

Using $f^y(t, s(t))$ to denote $F(t, s(t),\ y(t-\sigma_1), \cdots, y(t-\sigma_k))$, for a given function $s(t)$, we have

$$\begin{aligned} y^{q\,\prime\prime}(t) - f^y(t, y^q(t)) &= F(t, y^q(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)) \\ &\quad - F(t, y^q(t), y(t-\sigma_1), \cdots, y(t-\sigma_k)). \end{aligned} \tag{18}$$

Hence

$$y^{q\,\prime\prime}(t) - f^y(t, y^q(t)) = O(\max_i \|q(t-\sigma_i) - y(t-\sigma_i)\|).$$

Since we solved a standard IVP (16) over the first subinterval, and know that $O(\max_i \|q(t-\sigma_i) - y(t-\sigma_i)\|) = O(\delta)$ for either higher or lower-order interpolants. Using this in (18) it follows from a standard differential inequality, see, for example, [17,Theorem 10.2], that $\|y^q(t) - y(t)\| = O(\delta)$. Further, writing $y^q(t) = y(t) + (y^q(t) - y(t))$ and $q(t - \sigma_i) = y(t - \sigma_i) + [q(t - \sigma_i) - y(t - \sigma_i)]$ in (18) and expanding , we find that

$$
\begin{aligned}
& y^{q\,\prime\prime}(t) - f^y(t, y^q(t)) \\
= \; & \sum_{i=1}^{k} \frac{\partial F}{\partial z_i}(t, y(t), y(t - \sigma_1), \cdots, y(t - \sigma_k))(q(t - \sigma_i) - y(t - \sigma_i)) \\
& + O(\max_i \|q(t - \sigma_i) - y(t - \sigma_i)\|^2) \\
& + O(\|y(t) - y^q(t)\| \max_i \|q(t - \sigma_i) - y(t - \sigma_i)\|) \\
& + O(\|y(t) - y^q(t)\|^2),
\end{aligned}
$$

where $\partial F / \partial z_i$ denotes the partial derivative of $F(t, y, z_1, z_2, \cdots, z_k)$ with respect to z_i. It follows that

$$
\begin{aligned}
& y^{q\,\prime\prime}(t) - f^y(t, y^q(t)) \\
= \; & \sum_{i=1}^{k} \frac{\partial F}{\partial z_i}(t, y(t), y(t - \sigma_1), \cdots, y(t - \sigma_k))(q(t - \sigma_i) - y(t - \sigma_i)) \\
& + O(\delta^2).
\end{aligned} \tag{19}
$$

Now, with a higher-order interpolant we have

$$q(t - \sigma_i) - y(t - \sigma_i) = v_i(t)\,\delta + o(\delta),$$

where $v_i(t) := v(t - \sigma_i)$ is continuous and independent of δ, and hence from (19)

$$y^{q\,\prime\prime}(t) - f^{\,y}(t, y^q(t)) = \Gamma(t)\,\delta + o(\delta),$$

where $\Gamma(t)$ is continuous and independent of δ, and the $o(\delta)$ remainder is clearly continuous. We may thus apply the equivalence result of Theorem 1 to deduce that

$$y^q(t) - y(t) = V(t)\,\delta + R(t), \tag{20}$$

where $V(t)$ is C^2 and independent of δ, and $R(t)$ is sectionally C^2 with zeroth, first and second derivative of $o(\delta)$. For the lower-order interpolant, however, we know that, in general, $q(t - \sigma_i) - y(t - \sigma_i)$ does not behave linearly (asymptotically) as a function of δ, and hence (20) does not hold in general. Next we show that the error control method causes the ideal interpolant $\eta_I^q(t)$ to give TP relative to the approximate true solution $y^q(t)$. To do this we generalise Theorem 1 to allow for the fact that $y^q(t)$ depends upon δ.

Theorem 2. *Recall that $y(t)$ is the solution to* (14)*, and let $y^q(t)$ be the solution to* (15)*. Suppose $\eta(t)$ is sectionally C^2 approximation to $y^q(t)$ and let $\varepsilon(t) := \eta(t) - y^q(t)$ denote the corresponding error. Suppose that*

$$\varepsilon(\hat{t}_1) = K\delta + o(\delta), \tag{21}$$

where k is a constant vector. Then the following conditions are equivalent

$$(\mathrm{I}) \ : \quad \varepsilon(t) = v(t)\,\delta + r(t)\,, \ \ t \in \left(\hat{t}_1, \hat{t}_2\right),$$

where $v(t)$ is C^2 and independent of δ,and $r(t)$ is sectionally C^2 with zeroth, first and second derivatives of $o(\delta)$.

$$\begin{aligned}(\mathrm{II}) \quad : \quad & \eta''(t) - F\left(t, \eta(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right) \\ = \quad & \gamma(t)\,\delta + s(t)\,, \quad t \in \left(\hat{t}_1, \hat{t}_2\right),\end{aligned}$$

where $\gamma(t)$ is continuous and independent of δ and $s(t)$ is sectionally continuous and $o(\delta)$.

Proof. The proof is based on the proof of [1,Theorem 3.2.1]. We introduce a third condition, (III), and then prove that (I) $\Longrightarrow$ (II), (II) $\Longrightarrow$(III), and (III) $\Longrightarrow$ (I).

$$(\mathrm{III}) \ : \ \in''(t) - F_y\left(t, y^q(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right)\ \epsilon(t) = \gamma(t)\,\delta + u(t)\,,$$

where $\gamma(t)$ is the function appearing in condition (II), and $u(t)$ is sectionally continuous and $o(\delta) + O(\epsilon(t)^2)$. Here $F_y(t, y, z_1, z_2, \cdots, z_k)$ denotes the partial derivative of $F(t, y, z_1, z_2, \cdots, z_k)$ with respect to y.

(I) $\Longrightarrow$ (II) : writing $\eta(t) = y^q(t) + \epsilon(t)$ we have

$$\begin{aligned}& \eta''(t) - F\left(t, \eta(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right) \\ = \quad & \in''(t) - F_y\left(t, y^q(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right)\ \epsilon(t) + \hat{w}(t)\,,\end{aligned}$$

where $\hat{w}(t) = O(\epsilon(t)^2)$. Hence, since $q(t-\sigma_i) - y(t-\sigma_i) = O(\delta)$ and $y^q(t) - y(t) = O(\delta)$,

$$\begin{aligned}& \eta''(t) - F\left(t, \eta(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right) \\ = \quad & \in''(t) - F_y\left(t, y(t), y(t-\sigma_1), \cdots, y(t-\sigma_k)\right)\ \epsilon(t) + w(t)\,,\end{aligned}$$

where $w(t) = O(\epsilon(t)\ \delta + \epsilon(t)^2)$. Finally, using (I),

$$\begin{aligned}& \eta''(t) - F\left(t, \eta(t), q(t-\sigma_1), \cdots, q(t-\sigma_k)\right) \\ = \quad & \delta\left[\ v''(t) - F_y\left(t, y(t), y(t-\sigma_1), \cdots, y(t-\sigma_k)\right) v(t)\right] \\ & + r''(t) - F_y\left(t, y(t), y(t-\sigma_1), \cdots, y(t-\sigma_k)\right)\ r(t) + w(t)\,,\end{aligned}$$

which has the required form.

(II) $\Longrightarrow$(III) : This follows as in the proof of [1, Theorem 3.2.1].

(III) $\Longrightarrow$(I) : Let $v(t)$ denote the unique solution to the linear initial value problem

$$v''(t) - F_y\left(t, y(t), y(t-\sigma_1), \cdots, y(t-\sigma_k)\right) v(t) = \gamma(t)\,, \tag{22}$$

where $v\left(\hat{t}_1\right) = K, \ \ v'\left(\hat{t}_1\right) = K$.

From (III), we have

$$\in'' (t) - F_y (t, y (t), y (t - \sigma_1), \cdots, y (t - \sigma_k)) \ \epsilon (t) = \gamma (t) \ \delta + \bar{u} (t), \tag{23}$$

where $\bar{u} (t)$ is sectionally continuous and $o (\delta) + O(\epsilon (t)^2)$. From (22) and (23), $\epsilon (t) - \delta v (t)$ satisfies

$$\begin{aligned} & (\epsilon (t) - \delta v (t))'' - F_y (t, y (t), y (t - \sigma_1), \cdots, y (t - \sigma_k)) (\epsilon (t) - \delta v (t)) \\ = \ & \bar{u} (t), \end{aligned} \tag{24}$$

where $\epsilon \left(\hat{t}_1\right) - \delta v \left(\hat{t}_1\right) = K$, and $\epsilon' \left(\hat{t}_1\right) - \delta v' \left(\hat{t}_1\right) = K$. If we put $W (t) = \epsilon (t) - \delta$ $v (t)$ in (24) we get

$$W''(t) - F_y (t, y (t), y (t - \sigma_1), \cdots, y (t - \sigma_k)) W (t) = \bar{u} (t), \tag{25}$$

where $W \left(\hat{t}_1\right) = K$, $W'(\hat{t}_1) = K$.

To solve equation (25) we reduce it to a system of two first order equations by putting

$$\begin{aligned} W' (t) &= Z (t) \\ Z' (t) &= F_y (t, y (t), y (t - \sigma_1), \cdots, y (t - \sigma_k)) W (t) + \bar{u} (t) \end{aligned}$$

where $W \left(\hat{t}_1\right) = K$, and $Z \left(\hat{t}_1\right) = K$. This gives $x' (t) = A (t) \ x (t) + H (t)$ and $x \left(\hat{t}_1\right) = [W \left(\hat{t}_1\right), Z \left(\hat{t}_1\right)]^T$, where

$$x (t) = [W (t), Z (t)]^T, \ A (t) = \begin{bmatrix} 0 & 1 \\ F_y (t, y (t), y (t - \sigma_1), \cdots, y (t - \sigma_k)) & 0 \end{bmatrix}$$

and $H (t) = [0, \bar{u} (t)]^T$.

This initial value problem has a particular solution of the form ([3], 1988)

$$x (t) = [W (t), Z (t)]^T = X (t) \left[\epsilon \left(\hat{t}_1\right) - \delta \ v \left(\hat{t}_1\right) + \int_{\hat{t}_1}^{t} X^{-1} (\rho) \ H (\rho) \ d\rho\right],$$

where the fundamental solution matrix $X (t)$ is defined by

$$X (t) = A (t) \ X (t), \ X \left(\hat{t}_1\right) = I.$$

Note that $X (t)$ is independent of δ, and that $\epsilon \left(\hat{t}_1\right) - \delta v \left(\hat{t}_1\right) = \epsilon \left(\hat{t}_1\right) - \delta K = o (\delta)$. It follows that $\epsilon (t) - \delta v (t) = r (t)$, where $r (t)$ is $o (\delta) + O(\epsilon (t)^2)$ and continuous, and $r' (t)$ is $o (\delta) + O(\epsilon (t)^2)$ and sectionally continuous and $r'' (t)$ is $o (\delta) + O(\epsilon (t)^2)$ and sectionally continuous leading to the desired result. □

Now the approximate problem

$$y^{q\,\prime\prime} (t) = F(t, y^q (t), q (t - \sigma_1), \cdots, q (t - \sigma_k)),$$

is the one that the RKN method is actually being asked to solve. We would like to apply the standard ODE analysis in [1] in order to conclude that the error control causes codition (II) to hold. There is, however, one complication that the higher or lower-order interpolant $q(t)$ is typically only a C^2 function, and hence the approximate problem is not smooth enough for (2) and (3) to hold. We can sidestep this difficulty by noting that the RKN process samples F at a discrete set of points. For each δ, we could replace $q(t)$ by a smoother function that interpolates $q(t)$ at these discrete points and the numerical solution would remain unchanged. Hence we may pretend that $q(t)$ is globally C^{p+1}. It follows that condition (II) in Theorem 2 is satisfied, allowing us to deduce the desired result.

Corollary 3. *Suppose that we solve* (14) *over* $\left[\hat{t}_1, \hat{t}_2\right]$ *in the manner described above, using either a higher or lower-order interpolant. Then, provided that given* $y(t)$ *for* $t \leq \hat{t}_1$, $\|\psi(t, y(t))\| \neq 0$ *over* $\left[\hat{t}_1, \hat{t}_2\right]$ *in* (3), *the ideal interpolant satisfies*

$$\eta_I^q(t) - y^q(t) = \hat{V}(t)\,\delta + \hat{R}(t)\,, \tag{26}$$

where $\hat{V}(t)$ *is continuous and independent of* δ, $\hat{V}(t) \in C^2\left(\hat{t}_1, \hat{t}_2\right)$, *and* $\hat{R}(t)$ *is sectionally* C^2 *with zeroth, first and second derivatives of* $o(\delta)$. *When a higher-order interpolant is used we may thus combine* (20) *and* (25) *to give*

$$\eta_I^q(t) - y(t) = \bar{V}(t)\ \delta + \bar{R}(t)\,, \tag{27}$$

where $\bar{V}(t)$ *is continuous and independent of* δ, $\bar{V}(t) \in C^2\left(\hat{t}_1, \hat{t}_2\right)$, *and* $\bar{R}(t)$ *is sectionally* C^2 *with zeroth, first and second derivatives of* $o(\delta)$. *On the other hand, with a lower-order interpolant we see that since* (20) *does not hold, in general the leading term in* $\eta_I^q(t) - y(t)$ *will not be linear. Now on a general step from* t_n *to* t_{n+1} *in the integration over* $\left[\hat{t}_1, \hat{t}_2\right]$ *we have* $\eta_I^q(t) - z_n^q(t) = O\left(h_n^{p+1}\right)$ *and, for a higher-order interpolant,* $q(t) - z_n^q(t) = O\left(h_n^{p+1}\right)$. *Hence* $q(t) - \eta_I^q(t) = O\left(h_n^{p+1}\right)$, *so that* $q(t) - \eta_I^q(t) = o(\delta)$ *and, using* (26),

$$q(t) - y(t) = \bar{V}(t)\,\delta + o(\delta)\,. \tag{28}$$

This shows that a higher-order interpolant maintains TP in the $y(t)$ *approximation across* $\left[\hat{t}_1, \hat{t}_2\right]$. *By induction,* (26) *and* (27) *remain true when a finite number of smooth subintervals are crossed. The induction is valid provided that the tail of backvalues never crosses into the current subinterval; that is,* $\hat{t}_{i+1} - \hat{t}_i \leq \sigma_1$. *There are two cases where this condition does not hold. First, if the coupling in* (14) *is weak, we may be able to take smooth subintervals with width bigger than* σ_1. *Second, the integration may proceed into the final smooth region* $\left(\hat{t}_m, \infty\right)$. *We will show how to deal with the second case. The first case can be handled similarly. Given any fixed point* $t > \hat{t}_m$, *let* t_{N_1} *be the furthermost meshpoint such that* $t_{N_1} - \hat{t}_m \leq \sigma_1$, *and in general let* t_{N_r} *be the furthermost meshpoint such that* $t_{N_r} - \hat{t}_{N_{r}-1} \leq \sigma_1$. *In this manner the range* $\left[\hat{t}_m, t\right]$ *can be divided into a finite number of subintervals of width* $(\leq \sigma_1)$. *Now we can inductively obtain* (26) *and* (27) *over each subinterval,* *so that eventually*

$$q(t) - y(t) = \bar{V}(t)\,\delta + o(\delta)\,, \tag{29}$$

at the given point t.

To verify the analysis, we implemented a four-stage RKN formula-pair, RKN(3,4), consisting of a third and a fourth-order formula [11] in extrapolated error -per-step mode, so that $p = 4$. Two alternatives were used for the interpolant $q(t)$. First, we used the 3rd and 4th order RKN formulas as well interpolation by degenerate cubic splines to construct a locally fourth-order interpolant. In this case the local order of $q(t)$ is $l = 4 = p$, and the interpolant is of lower-order. The resulting method will be denoted $P4L4$. Second, we used the 3rd and 4th order RKN formulas with interpolation of fourth degree to construct a locally fifth-order interpolant [19], [20], [30]. In this case the local order of $q(t)$ is $l = 5 = p + 1$, and the interpolant is of higher-order. This method will be denoted $P4L5$. we also implemented a $p = 5,\ l = 6$ method, which refer to as $P5L6$, consisting of the fourth-and fifth-order RKN pair from [32], in extrapolated error-per-step mode, along with the quintic Hermite interpolant. We mention that the $p = 5,\ l = 6$ combination has proved to be a popular choice [22], [24].

The algorithms were tested on the delayed harmonic oscillator equation

$$\begin{aligned} y''(t) &= -y(t-1), \quad t \geq 0, \\ y(t) &= 1,\ y'(t) = 0,\ t \in [-1, 0]. \end{aligned}$$

The global error to tolerance behaviour of the three methods for $\delta = 10^{-i},\ i = 4, 6, 8$ is plotted in Figures $6 - 8$.

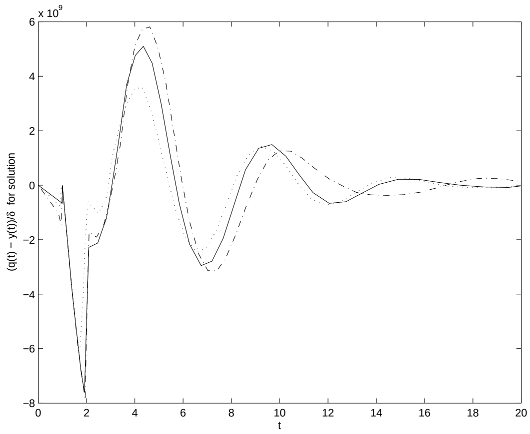

Figure 6: Delay harmonic oscillator equation P4L4 method

Here the global error in $q(t)$ was computed at 101 equally spaced points in the range $[0, 20]$. The numerical solution with $\delta = 10^{-10}$ was taken to be the true solution in each case. For $P4L4$ method, in Figure 6, the global error ratios do not seem to converge to a limit. We see in Figure 7 that the global error ratios for the $P4L5$ method behave smoothly and appear to approach a limit function. This illustrates the potential difference in behaviour between higher and lower-order interpolants that our analysis predicted.

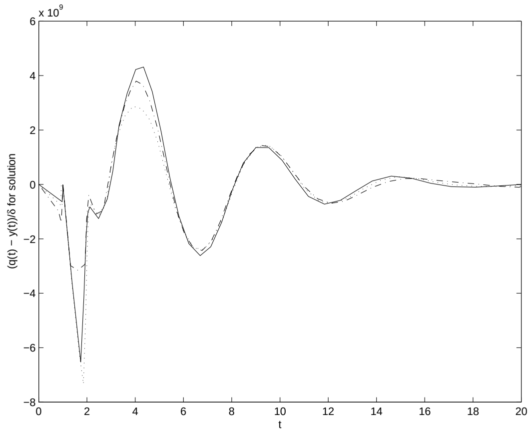

Figure 7: Delay harmonic oscillator equation P4L5 method

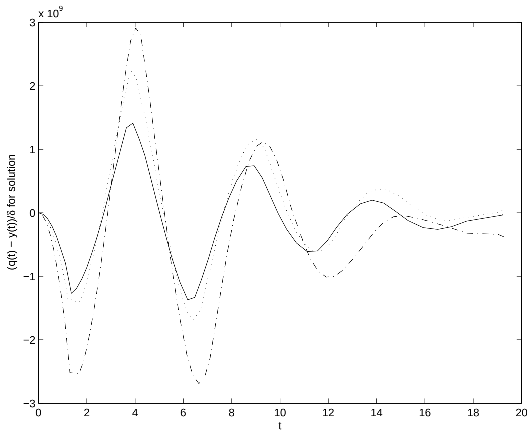

Figure 8: Delay harmonic oscillator equation P5L6 method

The $P5L6$ method in Figure 8 also exhibits nonlinear variation of global error ratios. Here, all the three methods displayed good tolerance proportionality. Some authors in [6] investigated higher and lower-order interpolation in a slightly different context and also found that higher-order interpolants give significant advantages.

4. Conclusion

The global error will not have regular behaviour unless an appropriate stepsize selection formula and standard error control policy are used. Under these circumstances a linear relationship of TP may exist between the global error and the local error tolerance, δ. The main conclusion of this work is that when a pth-order RKN formula is used to solve a constant delay system of ODEs, higher-order (locally $O\left(h_n^{p+1}\right)$) interpolation is necessary and sufficient to guarantee asymptotic TP. It is perhaps surprising therefore, that several of the algorithms that have been put forward in the literature use lower-order (locally $O\left(h_n^P\right)$) interpolants (see, for example, [19], [22], [24]).With a fixed stepsize and lower-order interpolant, Oppelstrup [26] and Roth [29] state that the global error behaves like $O\left(h^p\right)$, that is, of course, the best order that can be achieved. For the variable stepsize case analysed here, this corresponds to the fact that lower-order interpolants allow the global error to be bounded linearly with δ. To convert the bound into an equality, higher-order interpolation must be performed.

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