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# Explicit *A-Priori* Error Bounds and Adaptive Error Control for Approximation of Nonlinear Initial Value Differential Systems

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**Abstract**—This paper develops and demonstrates a guaranteed *a-priori* error bound for the Taylor polynomial approximation of any degree to the solution of initial value ordinary differential equations. The error bound is explicit and does not require upper bounds on the potentially complicated and intrinsically unknown right-hand side nor on any of its higher-order derivatives as with existing bounds, and thus it provides a valuable tool for the numerous applications in which initial value ode problems arise and for which approximate solutions must be sought. 

**Keywords**—Differential equations, Taylor approximations, *A-priori* error bounds, Initial value problems, Power series.

## 1. INTRODUCTION

The purpose of this paper is to develop and demonstrate an *explicit, a-priori error bound* for the $k^{\text{th}}$ degree Taylor polynomial approximation to the solution of a system of ordinary differential equations of the form

$$\mathbf{x}'(t) = \mathbf{f}(\mathbf{x}(t), t), \qquad \mathbf{x}(a) = \mathbf{x}_0, \tag{1}$$

where $\mathbf{f}$ is real-analytic in each component, $a \in \mathbb{R}$, and $\mathbf{x}_0 \in \mathbb{R}^n$. We also show that our bound is exact for a particular case of (1) and thus a comprehensively tighter bound is not possible. Since systems of the form (1) can always be translated to the origin with a change of independent variable $t \to t + a$, we concentrate on equations of the form

$$\mathbf{x}'(t) = \mathbf{f}(\mathbf{x}(t), t), \qquad \mathbf{x}(0) = \mathbf{x}_0, \tag{2}$$

and the Maclaurin polynomial approximation to the solution.

Many algorithms for approximating solutions of differential systems generate the Maclaurin approximation to the solution to a given degree at each step. Traditional error bounds for

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such approximations, however, generally involve bounds on potentially complicated higher-order derivatives of the right-hand side which most often depend precariously on the unknown solution $\mathbf{x}$ itself. For example, a standard Taylor series method error bound (about $t = 0$) for the system (2) is

$$\left\| \mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j \right\|_{|t| \in [0,T]} \leq \frac{\mathrm{N}_k \, |t|^{k+1}}{(k+1)!}, \tag{3}$$

where each component of $\sum_{j=0}^{k} \mathbf{x}_j t^j$ is the $k^{\text{th}}$ degree Maclaurin polynomial for the corresponding component of $\mathbf{x}(t)$, and the constant $\mathrm{N}_k$ is an upper bound on the norm of the $k^{\text{th}}$ derivative of $\mathbf{f}$, i.e.,

$$\mathrm{N}_k \geq \left\| \mathbf{f}^{(k)} \left( \mathbf{x} \left( t \right), t \right) \right\|_{|t| \in [0,T]}. \tag{4}$$

The inequality (4) can be quite burdensome. For example, to bound the error in the $7^{\text{th}}$ degree Maclaurin series approximation to $x(t)$ for the following problem with relatively modest right-hand side

$$x'(t) = f(x(t), t) = \sin\left( x(t) e^{t^2} \right) t^{-1/2}, \tag{5}$$

the standard error bound requires analysis of $f^{(7)}$ which contains 135 distinct terms, each of which depends on $x(t)$. To illustrate,

$$\begin{aligned} f^{(7)}\left(x(t), t\right) = \; & 3936 \sin\left( x(t) e^{t^2} \right)^5 e^{t^8} t^{-1/2} + \frac{10395}{64} \sin\left( x(t) e^{t^2} \right) t^{-13/2} \\ & + \cdots - 179 \sin\left( x(t) e^{t^2} \right)^3 \cos\left( x(t) e^{t^2} \right)^4 e^{t^{12}} t^{-7/2}; \end{aligned}$$

whereas for the $12^{\text{th}}$ degree Taylor error estimate, $f^{(12)}$ involves over 1000 terms. It is worth noting that an accurate numerical algorithm for computing *any*-order Maclaurin polynomial approximation to the solution of a system of differential equations was developed in [1,2], and has been further explored for a variety of problems (see, e.g., [3,4]).

The above underscores two salient features of a more attractive, useful, and versatile error bound. Such a bound would ideally be

(i) independent of derivatives of the right-hand side of the differential equation and
(ii) easy to recalculate for higher-order approximations.

This paper will develop such an error bound.

Of course, estimates on error and step size can be made with next term extrapolation in the course of a numerical computation, however these estimates are neither *a-priori* nor guaranteed, which is the purpose here. Error bounds for differential systems of the form (2) have been investigated by various authors, and as models of physical systems continue to become more and more complex, the role of guaranteed analytical and computational results cannot be overstated. Previous work includes a-posteriori estimates developed in [5], where it is remarked that a satisfactory theory of adaptive error control does not exist in part due to insufficient knowledge on the critical relationship between error and step size, a characterization widely considered impossible for broadly general nonlinear systems. We remark here that a simple and explicit relationship of this sort is one consequence of our error bound (see the discussion following our proof of Theorem 3). Interval analysis is employed in [6] to develop *a-priori* error bounds for initial value ode systems. Also, Chebyshev polynomials were employed in a series of papers [7–9] to determine *a-priori* error bounds for solutions of nonlinear initial value differential equations of the form $x' = f(t, x)$ where the right-hand side is a real-valued function of the two variables that is not required to be analytic. While here we will assume analyticity, our results are not restricted to $n = 2$ nor do they rely on bounds involving unknown functions or derivatives. Our interest is thus to develop the tightest bound possible under the constraints (i) and (ii) above for *all* systems of

the form (2) (and thus (1)) for general $n$. With the framework to be established here, special classes of initial value ode problems can then lead to tighter bounds holding on larger intervals, and thus to increasing the step-size for which desired accuracy is guaranteed (and so decreasing the computational effort required to march across an interval at guaranteed error controls).

Before proceding to the development of our error bound, we discuss and illustrate the following simple but critical idea: recasting a system of the form (2) as an equivalent autonomous ode system with polynomial right-hand side (*polynomial projection*).

### 1.1. Polynomial Projections of (2)

As any system of the form (2) can be written as an autonomous system by introducing the additional "unknown" $w$, say, so that $w(t) = t$, replacing $t$ everywhere with $w$, and augmenting (2) with the equation $w'(t) = 1$ and initial condition $w(0) = 0$, we need only consider autonomous systems

$$\mathbf{x}' = \mathbf{f}(\mathbf{x}) \tag{6}$$

with initial conditions as in (2). In addition, [1] and [2] establish that, by a suitable introduction of new dependent variables, a large class of differential equations and systems can be recast as first-order systems such that the right-hand side of each component equation contains terms involving only nonnegative integer powers and products of the new dependent variables. Thus, many systems of differential equations (for example, those encountered in classical mechanics) can be rewritten as an equivalent system of equations with a polynomial right-hand side by an appropriate change of variables (polynomial projection, in the terminology of [1,2]). In [3], properties of solutions of (6) for $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ such that each component of $\mathbf{f}$ is a polynomial functional on $\mathbb{R}^n$ are explored, and numerical results for several differential equations recast as polynomial systems are given. Another recent paper [4] exploits this idea for the $N$-body problem of classical physics by projecting the (nonpolynomial) system of differential equations modeling the motion of $N$ particles as a polynomial system. A change of variables sufficient to project an ODE to polynomial form is generally evident from the form of the equation itself, as illustrated with our examples. For the ODE (5),

$$\begin{aligned} &x_1(t) = x(t), && x_2(t) = \sin(x(t)e^{t^2}), && x_3(t) = \cos(x(t)e^{t^2}), \\ &x_4(t) = e^{t^2}, && x_5(t) = t, && x_6(t) = t^{-(1/2)}, \end{aligned} \tag{7}$$

is one possible projection which produces the autonomous polynomial system

$$\begin{aligned} &x_1' = x_2x_6, && x_2' = x_3x_4(2x_1x_5 + x_2x_6), && x_3' = -x_2x_4(2x_1x_5 + x_2x_6), \\ &x_4' = 2x_4x_5, && x_5' = 1, && x_6' = -\frac{1}{2}x_6^3, \end{aligned} \tag{8}$$

with proper initial conditions. The solution component $x_1$ of the system (8) is equivalent to the solution of (5). Other projections are also possible.

In light of the above discussion, Section 2 (Theorem 3) develops an explicit, general, *a-priori* error bound for the $k^{\text{th}}$ degree Maclaurin polynomial approximation to the solution of (6), where $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ is such that each component of $\mathbf{f}$ is a polynomial functional on $\mathbb{R}^n$. We also show that this bound is exact for at least one such system (Theorem 3), and thus any improvement on this error bound necessarily requires consideration of special cases. In Section 3, we demonstrate our error bound with three example problems.

## 2. ERROR BOUND: POLYNOMIAL SYSTEMS

Given the discussion in Section 1.1, we need only consider systems for which the right-hand side is a polynomial in the dependent variables. We begin a theorem that facilitates the proof of our main result (Theorem 3).

THEOREM 1. *Let $r, s, n \in \mathbb{N}$ with $s \geq r$. Let $\{z_i\}_{i=1}^{s}$ and $\{u_i\}_{i=1}^{r}$ be analytic functions such that, for $t$ in the interval of convergence, $z_i(t) = \sum_{j=0}^{\infty} z_{ij} t^j$, $i = 1, \ldots, s$ and $u_i(t) = \sum_{j=0}^{\infty} u_{ij} t^j$, $i = 1, \ldots, r$. Also, for $q_s \equiv \prod_{i=1}^{s} z_i$ and $p_r \equiv \prod_{i=1}^{r} u_i$, let $q_{sk}$ and $p_{rk}$ denote the $k^{\text{th}}$ degree coefficients in the series expansions of $q_s$ and $p_r$, respectively. If $z_{ij} \geq 0$ and $z_{i0} = 1 \; \forall \; j \in \mathbb{N}$ and $i = 1, \ldots, s$, and if*

$$z_{ij} \geq |u_{ij}|, \qquad \text{for } i = 1, \ldots, r \text{ and } j = 0, \ldots, n, \tag{9}$$

*then*

$$q_{sk} \geq |p_{rk}|, \qquad \text{for } k = 0, \ldots, n. \tag{10}$$

PROOF.

CASE 0 $s = r = 1$. By definition, we have only two analytic functions $z_1$, $u_1$ with Maclaurin coefficients $z_{1j}$, $u_{1j}$, respectively, ($j \in \mathbb{N}$), and thus, $q_1 = z_1$, $p_1 = u_1$ and (10) is exactly (9).

CASE 1 $s = r = 2$. Using Cauchy products to form the coefficients of a series resulting from the product of two series, we have that for $k \in \{0, 1, \ldots, n\}$,

$$|p_{2k}| = \left| \sum_{j=0}^{k} u_{1j} u_{2k-j} \right| \leq \sum_{j=0}^{k} |u_{1j}| \, |u_{2k-j}| \leq \sum_{j=0}^{k} z_{1j} z_{2k-j} = q_{2k}.$$

CASE 2 $s = r > 2$. We proceed by induction. By definition and Case 1, $q_2 = z_1 z_2$ and $p_2 = u_1 u_2$ are analytic functions such that $q_{2k} \geq |p_{2k}|$ for $k = 0, \ldots, n$. The analytic functions $q_i, p_i$ for $i \in \{3, \ldots, r\}$ are defined recursively as

$$q_i = q_{i-1} z_i \qquad \text{and} \qquad p_i = p_{i-1} u_i,$$

so that on assuming $q_{i-1k} \geq |p_{i-1k}|$ for $k = 0, \ldots, n$, the hypothesis (9) and the Case 1 result for two functions give

$$q_{ik} \geq |p_{ik}| \qquad \text{for } k = 0, \ldots, n,$$

validating the induction. Thus,

$$q_{r\,k} \geq |p_{r\,k}|, \qquad \text{for } k = 0, \ldots, n. \tag{11}$$

CASE 3 $s > r$. Using the recursive definitions of $q_i$ and $p_i$, we have that $q_s = q_r \prod_{i=r+1}^{s} z_i$ where (11) holds since $r < s$. Also, the coefficients $q_{sk}$ for each $k \in \{0, \ldots, n\}$ contain a term following from the product of the $k^{\text{th}}$ degree coefficient of $q_r$ with the remaining constant coefficients, that is, of the form

$$q_{rk} \prod_{i=r+1}^{s} z_{i0} = q_{rk},$$

where the equality follows from the hypotheses of Theorem 1. In addition, as all remaining terms contributing to $q_{sk}$ are positive, it follows that

$$q_{sk} \geq q_{rk} \geq |p_{rk}|, \qquad \text{for } k = 0, \ldots, n. \qquad \blacksquare$$

With Theorem 1 in hand, we next exploit the simple idea of rescaling an IVODE system to further facilitate our error bound (Theorem 3). Let $n, N \in \mathbb{N}$ and consider the constant coefficient first-order autonomous polynomial system

$$\mathbf{x}' = \mathbf{h}(\mathbf{x}), \qquad \mathbf{x}(0) = \mathbf{a}, \tag{12}$$

where $\mathbf{x}, \mathbf{a} \in \mathbb{R}^n$ and $\mathbf{h}$ is a polynomial functional. Then (12) has the form

$$x_i' = \sum_{j_1=0}^{N} \sum_{j_2=0}^{N} \cdots \sum_{j_n=0}^{N} A_{i,j_1,j_2,\ldots,j_n} x_1^{j_1}, x_2^{j_2}, \ldots, x_n^{j_n}, \qquad x_i(0) = a_i, \quad i = 1, \ldots, n. \tag{13}$$

The change of dependent variables

$$x_i = c_i y_i \text{ where } c_i = \begin{cases} a_i, & \text{if } |a_i| > 1, \\ 1, & \text{if } |a_i| \leq 1, \end{cases} \tag{14}$$

for $i = 1, \ldots, n$ leads to the equivalent (scaled) system

$$y_i' = \sum_{j_1=0}^{N} \sum_{j_2=0}^{N} \cdots \sum_{j_n=0}^{N} B_{i,j_1,j_2,\ldots,j_n} y_1^{j_1}, y_2^{j_2}, \ldots, y_n^{j_n}, \qquad y_i(0) = b_i, \tag{15}$$

where

$$B_{i,j_1,j_2,\ldots,j_n} = \frac{A_{i,j_1,j_2,\ldots,j_n} c_1^{j_1}, c_2^{j_2}, \ldots, c_n^{j_n}}{c_i}, \qquad b_i = \begin{cases} 1, & \text{if } |a_i| > 1, \\ a_i, & \text{if } |a_i| \leq 1. \end{cases} \tag{16}$$

We denote the nonlinear transformation $\mathbf{B}_N : \mathbb{R}^n \to \mathbb{R}^n$, by

$$\mathbf{B}_N [\mathbf{y}] = \mathbf{f}, \tag{17}$$

where with (15),

$$y_i' = f_i(y_1, y_2, \ldots, y_n), \tag{18}$$

and each $f_i$ is clearly a polynomial function of its arguments. Then the $L_\infty$ subordinate norm for the transformation defined by

$$\|\mathbf{B}_N\| = \sup \{\|\mathbf{B}_N [\mathbf{u}]\| : \mathbf{u} \in \mathbb{R}^n \text{ where } \|\mathbf{u}\| = 1\} \tag{19}$$

is equivalent to

$$\|\mathbf{B}_N\| = \max_{1 \leq i \leq n} \left\{ \sum_{j_1=0}^{N} \sum_{j_2=0}^{N} \cdots \sum_{j_n=0}^{N} |B_{i,j_1,j_2,\ldots,j_n}| \right\}, \tag{20}$$

that is, $\|\mathbf{B}_N\|$ is the largest row sum of the absolute value of the coefficients of the transformation.

Let $m$ represent the largest degree of any single term in $\mathbf{f}$ with nonzero coefficient. Both $\mathbf{f}$ and its partials are bounded on the convex set $\|\mathbf{y} - \mathbf{b}\| < L$, with $\mathbf{b}$ defined in (16), where

$$\|\mathbf{f}\| \leq \|\mathbf{B}_N\| (L+1)^m \qquad \text{and} \qquad \left\| \frac{\partial \mathbf{f}}{\partial y_k} \right\| \leq m \|\mathbf{B}_N\| (L+1)^m ; \tag{21}$$

thus a unique solution of (15) for $t \in (-L/(\|\mathbf{B}_N\|(L+1)^m), L/(\|\mathbf{B}_N\|(L+1)^m))$ exists by standard analysis. The interval length is maximized for $m \geq 2$ at $L = 1(m-1)$ yielding,

$$t \in \left( -\frac{1}{M} \left( \frac{m-1}{m} \right)^m, \frac{1}{M} \left( \frac{m-1}{m} \right)^m \right), \tag{22}$$

where

$$M = (m-1) \|\mathbf{B}_N\| . \tag{23}$$

In addition, the sequence of Picard iterates converges uniformly to the unique solution of (15) on the interval in (22). Further, since $\mathbf{f}$ is polynomial these iterates also produce the power series representation of the solution about $t = 0$ (see [1,2]), implying that the solution $\mathbf{y}$ to (15) is analytic about $t = 0$ with an interval of convergence at least that given by (22). Since

$$\mathbf{y}' = \mathbf{B_N}[\mathbf{y}], \qquad \mathbf{y}(0) = \mathbf{b}, \tag{24}$$

has analytic solution $\mathbf{y}$, a series expansion of the form

$$\mathbf{y} = \sum_{j=0}^{\infty} \mathbf{y}_j t^j \tag{25}$$

exists and then $\mathbf{f}$ has a similar expansion

$$\mathbf{f} = \sum_{j=0}^{\infty} \mathbf{f}_j t^j, \tag{26}$$

where for consistency and ease of notation here and subsequently, we denote the constant coefficients of the above series by $\mathbf{y}_j$ and $\mathbf{f}_j$. Since the transformation $\mathbf{B}_N$ is polynomial, for a given $k \in \mathbb{N}$ the coefficient $\mathbf{f}_k$ only depends on the coefficients $\{\mathbf{y}_j\}_{j=0}^{k}$. This makes it possible to generate $\{\mathbf{y}_j\}_{j=0}^{\infty}$ recursively using (24) by the recursion

$$\begin{aligned} \mathbf{y}_0 = \mathbf{b}, \qquad \mathbf{f}_0 = \mathbf{f}(\mathbf{y}_0), \\ \mathbf{y}_{k+1} = \frac{\mathbf{f}_k}{k+1}, \end{aligned} \tag{27}$$

and (27) indicates that

$$\|\mathbf{y}_{k+1}\| = \frac{\|\mathbf{f}_k\|}{k+1}. \tag{28}$$

Examine the real positive sequence $\{z_j\}_{j=0}^{\infty}$ defined by the coefficients from

$$z = \sum_{j=0}^{\infty} z_j \, t^j, \tag{29}$$

where $z$ is the unique (analytic) solution to the IVP

$$z' = \|\mathbf{B}_N\| \, z^m, \qquad z(0) = 1. \tag{30}$$

The positive coefficients $\{z_j\}_{j=0}^{\infty}$ can also be determined recursively using (30). On defining $g = z^m$,

$$\begin{aligned} z_0 &= 1 \\ z_{k+1} &= g_k \|\mathbf{B}_N\|/(k+1), \end{aligned} \tag{31}$$

where $g_k$ is the coefficient of the $k^{\text{th}}$ degree term in the series expansion of $g$. Again since $g$ is polynomial $g_k$ only depends on the coefficients $\{z_j\}_{j=0}^{k}$.

We are now in a position to state and prove the second theorem. Theorem 2 will set up the framework to prove our error bound (Theorem 3) which is the primary result of this paper, while Theorem 5 establishes that there is no *universally* finer error bound than that of Theorem 3.

THEOREM 2. *The $\mathbf{y}_j$ as defined through (27) and the $z_j$ as defined through (31) are such that $\|\mathbf{y}_j\| \leq z_j$, $\forall\, j \in \mathbb{N}$.*

PROOF. The proof for $j = 0$ is immediate from (15),(16) and (31) as

$$\|\mathbf{y}_0\| = \|\mathbf{b}\| \leq 1 = z_0. \tag{32}$$

Thus, we need only show that

$$\|\mathbf{y}_j\| \leq z_j, \quad j = 0, \ldots, k \qquad \Rightarrow \qquad \|\mathbf{y}_j\| \leq z_j, \quad j = 0, \ldots, k+1. \tag{33}$$

From (28),

$$\|\mathbf{y}_{k+1}\| = \frac{\|\mathbf{f}_k\|}{k+1} \tag{34}$$

and by the induction hypothesis

$$|y_{ij}| \leq \|\mathbf{y}_j\| \leq z_j, \qquad \text{for } j = 0, \ldots, k \text{ and } i = 1, \ldots, n, \tag{35}$$

where $y_{ij}$ represents the $j^{\text{th}}$ degree coefficient of the series of $y_i$. Since $z_0 = 1$, Theorem 1 and the knowledge that the highest degree term with nonzero coefficient for any $i = 1, \ldots, n$ in $f_i$ is $m$, gives that for each term in $\mathbf{f}$, the $k^{\text{th}}$ degree coefficient of the product series is such that

$$\left| \left[ y_1^{j_1} y_2^{j_2} \ldots y_n^{j_n} \right]_k \right| \leq g_k, \tag{36}$$

where again $g = z^m$. Using (15), (20), and (36),

$$|f_{i\,k}| \leq \sum_{j_1=0}^{N} \sum_{j_2=0}^{N} \cdots \sum_{j_n=0}^{N} |B_{i,j_1,j_2,\ldots,j_n}|\, g_k \leq \|\mathbf{B}_N\| g_k, \tag{37}$$

for $i = 1, \ldots, n$, which implies

$$\|\mathbf{f}_k\| \leq \|\mathbf{B}_N\|\, g_k. \tag{38}$$

Finally, (27) and (31) imply that

$$\|\mathbf{y}_{k+1}\| \leq \frac{\|\mathbf{B}_N\|\, g_k}{k+1} = z_{k+1}, \tag{39}$$

which establishes (33) and thus completes the induction. ∎

On solving (30),

$$z(t) = \begin{cases} e^{\|\mathbf{B}_N\| t}, & \text{for } m = 1, \\ \dfrac{1}{(1 - Mt)^{1/(m-1)}}, & \text{for } m \geq 2, \end{cases} \tag{40}$$

where $M$ is given by (23). Theorem 2 along with (14), (25), (29), and (40) thus establish our main result.

THEOREM 3. *The series expansion* $\sum_{j=0}^{\infty} \mathbf{x}_j\, t^j$ *of the solution* $\mathbf{x}(t)$ *to the initial value system (12), or equivalently (12), is such that*

$$\left\| \mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j \right\| \leq \begin{cases} \|\mathbf{c}\| \left( e^{\|\mathbf{B}_N\| |t|} - \sum_{j=0}^{k} z_j\, |t|^j \right), & \text{for } m = 1, \\ \|\mathbf{c}\| \left( \dfrac{1}{(1 - M\,|t|)^{1/(m-1)}} - \sum_{j=0}^{k} z_j\, |t|^j \right), & \text{for } m \geq 2, \end{cases} \tag{41}$$

*for any* $k \in \mathbb{N}$, *where* $\mathbf{c} = [c_1, \ldots, c_n]$ *is defined in (14) and* $t$ *is such that* $|t| < 1/M$.

PROOF. We remark first that it is straightforward to demonstrate explicitly that the power series for $\mathbf{x}(t)$ converges and satisfies the IVODE system (13). Using Theorem 2,

$$\left| y_i(t) - \sum_{j=0}^{k} y_{ij}\, t^j \right| \leq \begin{cases} e^{\|\mathbf{B}_N\| |t|} - \sum_{j=0}^{k} z_j\, |t|^j, & \text{for } m = 1, \\ \frac{1}{(1 - M|t|)^{1/(m-1)}} - \sum_{j=0}^{k} z_j\, |t|^j, & \text{for } m \geq 2. \end{cases} \tag{42}$$

Multiplying both sides of (42) by $|c_i|$, using (14), and noting that

$$x_i(t) = c_i y_i(t) = \sum_{j=0}^{\infty} c_i y_{ij} t^j, \qquad \text{where } x_{ij} = c_i y_{ij}, \tag{43}$$

establishes the result (41). ∎

COROLLARY 4. *A simpler but slightly less tight bound than that given in Theorem 3 is the following:*

$$\left\| \mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j t^j \right\| \leq \frac{\|\mathbf{c}\| \, |Mt|^{k+1}}{1 - |Mt|}, \qquad \text{for } m \geq 2, \tag{44}$$

*for any value of* $k \in \mathbb{N}$, *with* $|t| < 1/M$. *A component form of (44) is*

$$\left| x_i(t) - \sum_{j=0}^{k} x_{ij} t^j \right| \leq \frac{|c_i| \, |Mt|^{k+1}}{1 - |Mt|}, \qquad \text{for } m \geq 2. \tag{45}$$

PROOF. A standard series technique easily generates the coefficients $\{z_j\}_{j=0}^{\infty}$ by the linear recursion,

$$z_{k+1} = \left( \frac{(m-1)k+1}{k+1} \right) \frac{M}{m-1} z_k, \qquad z_0 = 1. \tag{46}$$

Thus, while the coefficients $z_j$ in (41) may at first glance appear computationally expensive to generate, (46) shows that this is not the case. Also, since

$$\frac{(m-1)k+1}{k+1} \leq m-1, \tag{47}$$

for $k \in \mathbb{N}$ and $m \geq 2$, the positive sequence defined by the recursion

$$u_{k+1} = M u_k, \qquad u_0 = \|\mathbf{c}\|, \tag{48}$$

is such that $z_k \leq u_k$ for all $k \in \mathbb{N}$. The series expansion of the function $u(t) = \|\mathbf{c}\|/(1 - Mt)$ has coefficients $u_k$ generated by (48), and thus is a geometric series. As such, the well-known closed form formula for the tail of the series allows for the corollary's alternative to (41). ∎

Computing the bound of Corollary 4 is immediate upon setting up the scaled polynomial system as opposed to the tighter Theorem 3 bound, however it is worth remarking that even the error bound (41) is far more computationally friendly than error bounds currently in the literature. We also remark that the interval of convergence developed in the proof of Theorem 3 is larger than that in (22) as the bound employed there for $\|\mathbf{f}(\mathbf{y})\|$, while sufficient for our purposes, is not the least upper bound.

The error bound of Theorem 3 for the Maclaurin approximation to the solution of (12), or equivalently, (13), is noteworthy as it *depends strictly on the known coefficients and given initial conditions* of the system and not on potentially complicated higher-order derivatives of the right-hand side, as with traditional error bounds. Nor does it depend on any bounds of any sort on the unknown(s). Also, to achieve a bound on higher-degree Taylor approximations of the solution, recomputing the error bound of Theorem 3 simply requires a change in the parameter $k$. As illustrated in the Introduction, to accomplish this with (3),(4) or similar traditional error bounds, analysis of higher-order right-hand side derivatives which often grow exponentially in number of terms per differentiation can be tedious if not prohibitive.

As mentioned in section 1, many numerical algorithms used for approximating solutions of differential systems generate the Maclaurin approximation to the solution to a given degree at each step. Thus the error bound here is a powerful computational tool, allowing the numerical analyst potentially for the first time to explicitly calculate a step size for the given degree, so that with the exception of round-off error, the accuracy in the approximation is *guaranteed a-priori* to be less than a desired tolerance at a given step. Once a step is taken the error bound is recomputed based on the updated initial conditions to choose a subsequent step-size. This error bound is particularly useful for the Algebraic Maclaurin Method discussed in [3], which generates the Maclaurin approximation to the solution at each step and allows the user to choose

independently an arbitrary step-size and *degree* in the Maclaurin approximation at each step. Having step-by-step direct control over the step-size is typical, but having step-by-step ability to choose an arbitrary degree (order of accuracy) is much less common and has tremendous benefits. In addition, the error bound of Theorem 3 has enormous potential to provide analogous results for the multitude of numerical algorithms used for approximating solutions of differential systems which, at each step, are derived to be theoretically equivalent to the desired degree to the Maclaurin approximation to the solution. Runge-Kutta algorithms are one such example. To conclude this section, we establish the following theorem.

THEOREM 5. *There is no error bound that is universally finer than that of Theorem 3 for all systems of the form (12).*

PROOF. Consider the IVODE problem whose solution is easily computed to be $x_1(t) = 1/(1-t)$

$$x_1' = x_1^2, \qquad x_1(0) = 1. \tag{49}$$

From (13)–(20), $n = 1$, $m = 2$, $N = 2$, $\|\mathbf{B}_1\| = 1$, and so from (23), $M = 1$. The error bound of Theorem 3 for (49) is then

$$\left| x_1(t) - \sum_{j=0}^{k} x_{1j} t^j \right| \leq \frac{|t|^{k+1}}{1-|t|} \qquad \text{for } |t| < 1, \tag{50}$$

where the $x_{1j}$ are coefficients of the Maclaurin series of $x_1(t) = 1/(1-t)$, a well-known series with all coefficients identically equal to 1. This however implies that strict equality holds in (50), and so for the special case (49) of (12), the error bound (41) is exact and cannot be improved upon. Thus, a *universally* finer general error bound applicable to *all* systems of the form (12) is not possible. ∎

Table 1. Comparison of error bounds for $1/(1-t)$.

| | $k = 10$ | | $k = 100$ | |
|---|---|---|---|---|
| t | Taylor | Theorem 3 | Taylor | Theorem 3 |
| 0.1 | 0.35407E − 10 | 0.11111E − 10 | 0.46480E − 96 | 0.11111E − 100 |
| 0.5 | 2.0 | 0.000978 | 1.99999 | 0.78886E − 30 |
| 0.9 | 0.31381E + 12 | 3.13811 | 0.23905E + 98 | 0.00239 |
| 0.95 | 0.23298E + 16 | 11.3760 | 0.28520E + 131 | 0.11249 |

The proof of Theorem 5 also brings to light another potential asset of the error bound established in this paper. While the standard Taylor series error bound for the $k^{\text{th}}$ degree Maclaurin polynomial approximation to $x_1(t) = 1/(1-t)$ is easily calculated to be $|x_1(t) - \sum_{j=0}^{k} x_{1j}\, t^j| \leq |t|^{k+1}/(1-|t|)^{k+2}$, it is also well-known to grow rapidly for $t$ away from zero within the interval of convergence $(-1, 1)$ and thus is not particularly useful. Table 1 demonstrates this, comparing this standard Taylor Series error bound with our Theorem 3 error bound in (50) for several values of $t$. As noted above, here the bound of Theorem 3 gives the exact absolute error in the approximation.

A similar comparison can be made for the two error bounds in the Maclaurin polynomial approximation for any functions built from the elementary functions. For another simple example, consider $f \circ g$ where $f(t) = \ln t$, $g(t) = t + 1$. On letting $x_1 = \ln(t+1)$ and $x_2 = 1/(t+1)$, the corresponding polynomial IVODE system with $\ln(t+1)$ as its first solution component is

$$x_1' = x_2, \quad x_1(0) = 0, \qquad x_2' = -x_2^2, \quad x_2(0) = 1. \tag{51}$$

It follows from (13)–(20) that $n = 2, m = 2, N = 2, \|\mathbf{B}_2\| = 1$, and so here again (23) gives $M = 1$. The error bound of Theorem 3 for the first component of (51) is then

$$\left| x_1(t) - \sum_{j=0}^{k} x_{1j}\, t^j \right| \leq \frac{|t|^{k+1}}{1 - |t|}, \tag{52}$$

where the $x_{1j}$ are the coefficients of the Maclaurin series of $\ln(t+1)$. The standard Taylor series error bound for the $k^{\text{th}}$ degree Maclaurin polynomial approximation to the function $x_1(t) = \ln(t+1)$ is easily calculated to be

$$\left| x_1(t) - \sum_{j=0}^{k} x_{1j}\, t^j \right| \leq \frac{1}{(n+1)} \frac{|\,t|^{k+1}}{(1 - |\,t|)^{k+1}}, \tag{53}$$

and is also well-known to grow rapidly for $t$ away from zero within the interval of convergence $(-1, 1]$. Table 2 demonstrates this, comparing the standard Taylor Series error bound in (53), our Theorem 3 error bound in (52), and the exact error in the $k^{\text{th}}$ degree Maclaurin polynomial approximation to $\ln(t+1)$ for several values of $t$. While this dramatic improvement over the Taylor bound is clearly not realized for all functions (for example, $e^t$), the potential impact of Theorem 3 in the approximation of a function by its Taylor series is evident.

Table 2. Comparison of error bounds and exact error for $\ln(t+1)$.

| | $k = 10$ | | | $k = 100$ | | |
|---|---|---|---|---|---|---|
| $t$ | Taylor | Theorem 3 | Exact | Taylor | Theorem 3 | Exact |
| 0.1 | 0.29E − 11 | 0.111E − 10 | 0.833E − 12 | 0.414E − 98 | 0.111E − 100 | 0.901E − 103 |
| 0.5 | 0.09091 | 0.00098 | 0.00003 | 0.00990 | 0.789E − 30 | 0.261E − 32 |
| 0.9 | 0.285E+10 | 3.1381 | 0.0157 | 0.237E + 95 | 0.0024 | 0.125E − 6 |
| 0.95 | 0.106E + 14 | 11.376 | 0.0277 | 0.141E + 128 | 0.1125 | 0.00003 |

## 3. ERROR BOUND EXAMPLES

We conclude with three illustrative examples: a representative test problem from the literature, a return to the example (5) from the Introduction, and a problem with known exact solution from nonlinear solid mechanics.

EXAMPLE 1. A test problem considered by a number of authors (see e.g., [5,10–12]) is given by

$$\begin{aligned} x_1' &= \frac{1}{2}\frac{x_1}{t+1} - 2t x_2, \qquad x_1(0) = 1, \\ x_2' &= \frac{1}{2}\frac{x_2}{t+1} + 2t x_1, \qquad x_2(0) = 0, \end{aligned} \tag{54}$$

and has explicit solution

$$x_1(t) = \sqrt{t+1}\cos(t^2), \qquad x_2(t) = \sqrt{t+1}\sin(t^2). \tag{55}$$

It is remarked in [10] that this problem becomes increasingly difficult to solve as $t$ increases due to the increasing frequency of oscillation inherent in the solution components, and that a fairly difficult example demonstrating the use of the error estimates based on extrapolation in [10] is to numerically solve (54) on the interval $[0, 10]$. (The interval $[0, 3]$ was employed in [5,11,12]).

On letting $x_3 = t$ and $x_4 = 1/(t+1)$, the solutions $x_1, x_2$ of the nonautonomous, non-polynomial system (54) are equivalent to the solutions $x_1, x_2$ of the autonomous polynomial system

$$\begin{aligned} x_1' &= \frac{1}{2}x_1x_4 - 2x_3x_2, \quad x_1(0) = 1; \qquad x_3' = 1, \qquad x_3(0) = 0; \\ x_2' &= \frac{1}{2}x_2x_4 + 2x_3x_1, \quad x_2(0) = 0; \qquad x_4' = -x_4^2, \quad x_4(0) = 1. \end{aligned} \tag{56}$$

To apply Theorem 3, (13)–(23) give $n = 4$, $m = 2$, $N = 2$, $c_i = 1$, $1 \le i \le 4$, and $\|\mathbf{B}_2\| = M = 5/2$. On assuming $x_i(t) = \sum_{j=0}^{\infty} x_{ij}t^j$ is the Maclaurin expansion of each solution component $x_i$ and taking $t \in (-2/5, 2/5)$, (45) gives the following bounds on the absolute errors in the $k^{\text{th}}$ degree Maclaurin polynomial approximations to the solutions of (54) for $t$ in this interval:

$$|x_i(t) - \sum_{j=0}^{k} x_{ij}\, t^j| \le \frac{|(5/2)\, t|^{k+1}}{1 - |(5/2)\, t|}, \qquad i = 1, 2. \tag{57}$$

The bounds in (57) are useful in a variety of ways. First, pick $T$ in the interval $(0, 2/5)$. It is then a simple exercise to determine the degree $k$ of the Taylor polynomial that is *guaranteed* to approximate the solution on $(-T, T)$ to *any* desired accuracy, with the numerical computation restricted only by machine epsilon and machine round-off error. As remarked earlier, the *Algebraic Maclaurin Method* rapidly computes this polynomial for very large $k$; programming this example in double precision Fortran 90 with a 32 bit processor and machine epsilon $\epsilon = 2^{-52}$, we obtain the following results (Table 3) which demonstrate extraordinary accuracy for the representative step size and degree pairs shown.

Table 3. Errors in approximating the solution $x_1$ of Example 1.

| $t$ | Degree $k =$ | Relative Error | Absolute Error |
|---|---|---|---|
| 0.0025 | 5 | $< \epsilon$ | $< \epsilon$ |
| 0.25 | 60 | $< \epsilon$ | $< \epsilon$ |
| 0.375 | 471 | $< \epsilon$ | $< \epsilon$ |
| 0.399 | 13432 | $< \epsilon$ | $< \epsilon$ |

We also graphically illustrate the error bound for several values of $k$ for this example. Figures 1 –4 plot the log of the absolute error in the Maclaurin approximation of $x_1(t)$ (the left-hand side of $(57)_1$) against the log of the error bound (the right-hand side of $(57)_1$) over the interval $t \in [0, 2/5)$ with a maximum allowed error of $10^{-6}$.

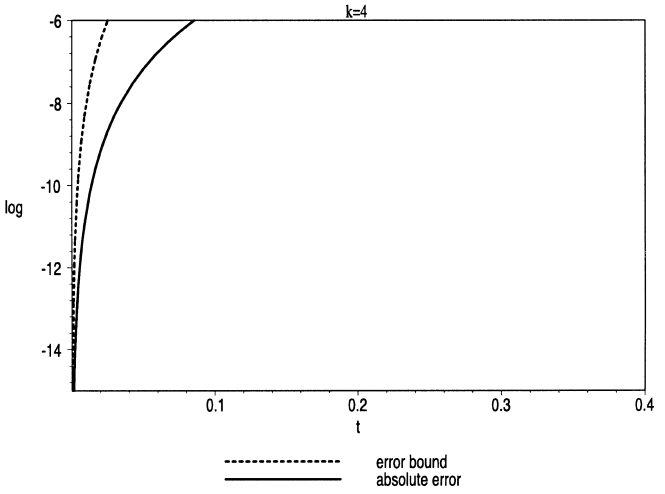


Figure 1.

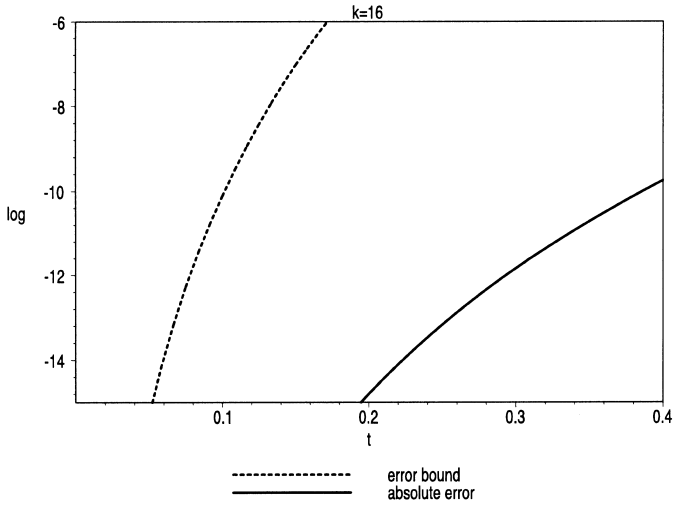


Figure 2.

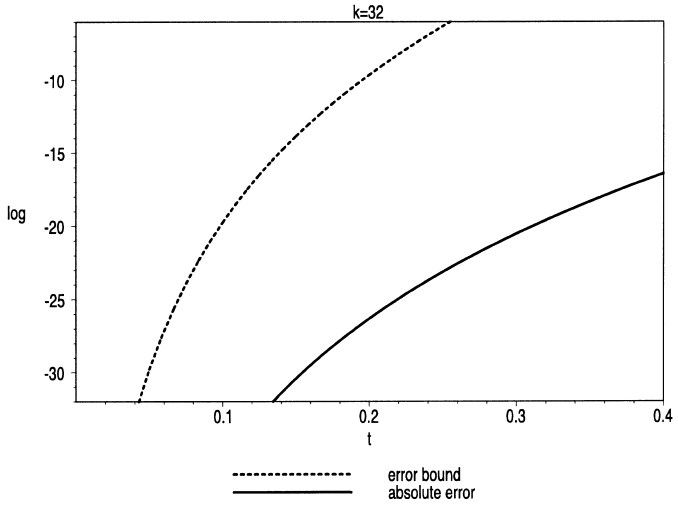


Figure 3.

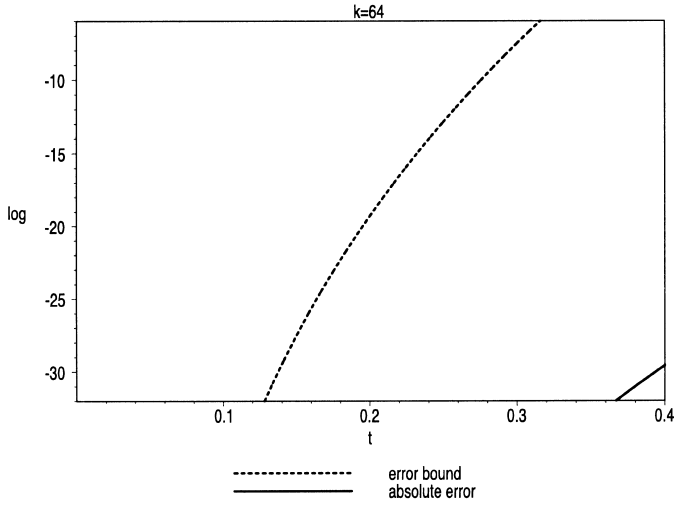


Figure 4.

Note that in each plot, the error bound (dotted curves) lies clearly above the actual absolute error curves for each value of $k$. Also note that as $k$ increases, for a chosen error tolerance, the stepsize computed from the error bound increases toward its limiting value of $1/M$. Figures 3 and 4 also show that even an error tolerance of $10^{-32}$ is achievable for the range of stepsizes below where the dotted curve intersects the $t$ axis. Thus, this also indicates the potential for remarkable accuracy with the error bound if a high enough degree $k$ for the Maclaurin polynomial approximation is chosen, despite the intrinsic singularity in the error bound at $\pm 1/M$.

The step size $t$ computed from the error bound which guarantees the desired accuracy also increases dramatically with the degree to which one computes the Maclaurin polynomial approximation to the solution $x_1$. From Figures 1–4 for example, an error of less than $10^{-6}$ is guaranteed by the error bound for step sizes of $\approx 0.025, 0.17, 0.26$, and $0.32$ for $k = 4, 16, 32$,and 64, respectively. When $k = 64$, Figure 4 shows that a stepsize of $\approx 0.13$ produces accuracy to within approximately $10^{-30}$. The numerics corresponding to Figures 3 and 4 were computed with MAPLE 9.5, as the necessary precision for this example exceeded that available with double precision FORTRAN 90 on a 32-bit machine. As $k$ increases, Figures 1–4 also show that the step size $t$ computed from the error bound of Theorem 3 for a particular desired accuracy can be significantly smaller than the actual step one could take. Similar results hold for the Maclaurin series and error bound for $x_2(t)$. Of course, the ability to compute higher degree Maclaurin polynomial approximations to solutions of differential equations is crucial to fully exploit the power of our error bound. The beauty of the Algebraic Maclaurin Method [3] is the algorithmic ease at which such increased-order approximations can be achieved (a simple parameter that can be altered *on-the-fly* controls the order of the method), especially in comparison with other schemes such as Taylor Series methods or Runge-Kutta where a fixed order (e.g., $4^{\text{th}}$ or $5^{\text{th}}$) is standard, and computing higher-order algorithms is formidable, if not prohibitively cumbersome.

Further, it is straightforward to obtain an accurate numerical solution on an interval $[0, T]$ with $T \geq 2/5$ by stepping out to $T$, where a $k^{\text{th}}$ degree Taylor polynomial of the solution at the current step is used to approximate the solution at the next step. The calculated solutions at the step value then serve as initial conditions for generating the Taylor polynomial of the next step, and the value of $M$ is recalculated. For example, if a step size of $1/(2M)$ is taken, solving $(45) < \epsilon$ for $k$ shows that any degree $k$ Maclaurin polynomial approximation with

$$k > \frac{-\ln(\epsilon/|c_1|)}{\ln(2)} \tag{58}$$

provides an absolute error at that step which is less than $\epsilon$, with the exception of machine round-off error. There is still of course propagation error of $O(\epsilon)$ per step resulting from using initial conditions that are calculated approximations at each step, but the step error from solving the differential system at the machine numbers for the system coeffiecients and initial conditions at the given step is guaranteed *a-priori* to be less than $\epsilon$. Table 4 demonstrates our results on using this procedure to approximate the solution to Example 1.

Table 4. Errors in approximating the solution $x_1$ of Example 1.

| $t$ | Steps | Average Degree $k$ | Relative Error | Absolute Error |
|---|---|---|---|---|
| 5 | 93 | 53 | 0.9145E − 15 | 0.222E − 14 |
| 10 | 421 | 53 | 0.5885E − 13 | 0.1683E − 12 |
| 100 | 67542 | 54 | 0.6939E − 11 | 0.664E − 10 |
| 300.1 | 730001 | 55 | 0.5383E − 10 | 0.9338E − 9 |

We first remark that previous studies in the literature for this problem were restricted to $t \in [0, 3]$, or more recently $t \in [0, 10]$, due to computational difficulties arising for large $t$. Thus, Table 4 demonstrates that large intervals for $t$ are not problematic here. It is also interesting to note that the value $t = 300.1$ was chosen to emphasize that even the FORTRAN 90 compiler does not

evaluate the function $x_1(t) = \sqrt{t+1}\cos(t^2)$ at $t = 300.1$ to within double precision machine epsilon $\epsilon$, but has relative error of $0.25\text{E}-12$ and absolute error of $0.433\text{E}-11$ due to problems inherent in evaluating library functions at large argument values. (The FORTRAN 90 compiler more accurately handles large integer values of $t$). In this light as well, our stepping algorithm based on the error bound of Theorem 3 to solve this intial value differential system on $[0, T]$ for large $T$ shows remarkable accuracy.

Since the Algebraic Maclaurin Algorithm relies solely on the four basic machine arithmetic operations $+, -, *, /$ and none of the compiler's intrinsic numerical functions, including exponentiation, it is not difficult to accurately determine the algortihm's computational cost or to analyze round-off error. The computational cost amounts to the total number of long operations (*ops*) required to approximate the solution given the degree $k$ at each step. For the system in (56), this is $(5/2)(k^2 + 5k)(ops)$. The largest cost comes from *ops* involving machine multiplication specifically related to the Cauchy products involved in generating the Maclaurin coefficents of the nonlinear terms in the system.

Given a fixed-order $k$ and a known $\epsilon$ we could also solve (57) for a step size $t^*$. Assuming that $t^* < 1/(2M)$ and choosing

$$t^* < \frac{1}{M}\left(\frac{\epsilon}{2|c_i|}\right)^{1/(k+1)} \tag{59}$$

provides an *a-priori* step error less than $\epsilon$. This use of the bound would be more attractive in fixed-order algorithms such as traditional Taylor series methods, and requires no analysis of higher-order derivatives of the system. Further, there is potential to determine both an ideal step size and order so that processing time is minimized and the desired accuracy is achieved. This of course would depend on the structure of the numerical algorithm implemented to create the Taylor approximation and the given problem. If a high degree of guaranteed accuracy is the ultimate goal, it is difficult to conceive of a stepping algorithm where *a-priori* bounds at each step are not useful.

EXAMPLE 2. We reconsider our sample equation (5) augmented by the initial condition $x(1) = 1$ for another demonstration of salient features of the error bound developed in this paper, that is,

(i) its independence of bounds on the intrinsically unknown right-hand side of the differential equation and its derivatives
(ii) its ease of recalculation for higher-order approximations.

The projection introduced in (7) produces the autonomous polynomial IVODE system

$$\begin{aligned} &x_1' = x_2x_6, && x_2' = 2x_1x_3x_4x_5 + x_2x_3x_4x_6, && x_3' = -2x_1x_2x_4x_5 - x_2^2x_4x_6, \\ &x_4' = 2x_4x_5, && x_5' = 1, && x_6' = -\frac{1}{2}x_6^3, \end{aligned} \tag{60}$$

with initial conditions that follow as $x_1(1) = 1$, $x_2(1) = \sin(e)$, $x_3(1) = \cos(e)$, $x_4(1) = 1$, $x_5(1) = 1$, $x_6(1) = 1$. In applying Theorem 3, it follows from (13)–(20) that $n = 6$, $m = 4$, $N = 3$, $c_i = 1$, $1 \le i \le 6$, $\|\mathbf{B}_3\| = 3$, and thus by (23), $M = 9$. On translating for the initial conditions, we write the Taylor expansion of each solution component $x_i$ as $x_i(t) = \sum_{j=0}^{\infty} x_{ij}(t-1)^j$ where $|t-1| < 1/M$ and so $t \in (8/9, 10/9)$. Then (41) gives the following bounds on the absolute errors in the $k^{\text{th}}$ degree Taylor polynomial approximations to the solutions of (60) for $t$ in the above interval

$$\left\| \mathbf{x}(t) - \sum_{j=0}^{k} \mathbf{x}_j\,(t-1)^j \right\| \le \left| \frac{1}{(1 - 9\,|(t-1)|)^{\frac{1}{3}}} - \sum_{j=0}^{k} z_j\,|t-1|^j \right| \tag{61}$$

where, via (46), the coefficients $\{z_j\}_{j=0}^{k}$ are easily generated by the simple recursion

$$z_{k+1} = \left(\frac{3k+1}{k+1}\right) 3z_k, \qquad z_0 = 1. \tag{62}$$

From the above it is easy exploit the equivalent polynomial system (60) and subsequent initial conditions to determine that the $7^{\text{th}}$ degree Taylor polynomial approximation to the solution of (5) subject to $x(1) = 1$ is guaranteed to have single precision accuracy for a step of approximately 0.026. The error bound also guarantees this accuracy for the $12^{\text{th}}$ degree Taylor polynomial approximation with a step of approximately 0.045. Recalculating the alternative bound (41) for higher-order Taylor polynomial approximations to achieve greater accuracy with larger step sizes is a simple matter; for example, a $500^{\text{th}}$ degree Taylor polynomial approximation delivers guaranteed single precision accuracy with a step of $\approx 0.107$ (near the limiting value of $1/9$).

EXAMPLE 3. As a final example, we consider a second-order IVODE

$$\frac{d^2r}{dR^2} = \frac{3r}{2R^2} - \frac{1}{R}\frac{dr}{dR} - \frac{1}{2r}\left(\frac{dr}{dR}\right)^2, \qquad r(2) = \frac{3}{2}3^{1/3}, \qquad \frac{dr}{dR}(2) = \frac{7}{12}3^{1/3}, \tag{63}$$

which arises in modeling the spherically symmetric deformation resulting in a cavitated sphere (sphere with an internal spheroidal void) in compressible nonlinear elasticity. For the mathematical model (63), the sphere is composed of a homogeneous, isotropic Murphy material (see, e.g., [13] and references cited therein). The independent variable $R \geq 0$ represents the spherical radius at any point in the original (undeformed) configuration of the sphere, while the dependent variable $r = r(R)$, the spherical radius in the deformed configuration, determines the radial deformation of the sphere. The outer surface of the original sphere is defined in (63) by $R = 2$. The IVODE (63) is one of the few equations which arise in compressible nonlinear elasticity for which an explicit solution is available; $r(R) = (1 + R^3)^{2/3}/R$ solves (63). While the ODE in (63) is not a first-order polynomial system, it is straightforward to show that on employing the change of variables

$$x_1 = \frac{1}{R}, \qquad x_2 = r, \qquad x_3 = \frac{dr}{dR}, \qquad x_4 = \frac{1}{r}, \qquad \text{and} \qquad t = R - 2, \tag{64}$$

the solution $r$ of (63) is equivalent to the solution $x_2$ of the autonomous initial value polynomial system

$$\begin{array}{llll} \dfrac{dx_1}{dt} = -x_1^2, & \dfrac{dx_2}{dt} = x_3, & \dfrac{dx_3}{dt} = \dfrac{3}{2}x_2x_1^2 - x_3x_1 - \dfrac{1}{2}x_3^2x_4, & \dfrac{dx_4}{dt} = -x_4^2x_3, \\ x_1(0) = \dfrac{1}{2} \equiv a_1, & x_2(0) = \dfrac{3}{2}3^{1/3} \equiv a_2, & x_3(0) = \dfrac{7}{12}3^{1/3} \equiv a_3, & x_4(0) = \dfrac{2}{3}3^{-1/3} \equiv a_4. \end{array} \tag{65}$$

As mentioned in the Introduction, the simple change of variables (64) is suggested by the form of (63) although other choices are possible. The above system is now in the form (13), where from (13)–(20), $n = 4$, $m = 3$, $N = 2$, $c_1 = c_3 = c_4 = 1$, $c_2 = (3/2)3^{1/3}$. The equivalent system (15) for this example is

$$\begin{array}{llll} \dfrac{dy_1}{dt} = -y_1^2, & \dfrac{dy_2}{dt} = \dfrac{y_3}{\frac{3}{2}3^{1/3}}, & \dfrac{dy_3}{dt} = \dfrac{3}{2}\left(\dfrac{3}{2}3^{1/3}\right)y_2y_1^2 - y_3y_1 - \dfrac{1}{2}y_3^2y_4, & \dfrac{dy_4}{dt} = -y_4^2y_3, \\ y_1(0) = \dfrac{1}{2} \equiv b_1, & y_2(0) = 1 \equiv b_2, & y_3(0) = \dfrac{7}{12}3^{1/3} \equiv b_3, & y_4(0) = \dfrac{2}{3}3^{-1/3} \equiv b_4, \end{array} \tag{66}$$

and so $\|\mathbf{B}_2\| = (3/2)((3/2)3^{1/3}) + 1 + 1/2 < 4.75$. Thus by (23), we take $M = 9.5$ for simplicity.

By Corollary 4 and writing the Taylor expansion of each solution component $x_i$ as $x_i(t) = \sum_{j=0}^{\infty} x_{ij}t^j$ where $|t| < 1/M = 2/19$, (45) gives the following bounds on the absolute errors in the $k^{\text{th}}$ degree Taylor polynomial approximations for the solution component $x_2(R)$, that is, the solution $r(R)$ of the original ivode

$$\left| x_2(R) - \sum_{j=0}^{k} x_{2j}\,(R-2)^j \right| \leq \frac{(3/2)3^{1/3}\,|9.5\,(R-2)|^{k+1}}{1 - |9.5\,(R-2)|}, \tag{67}$$

over the interval $(2-2/19, 2]$, where for this problem, $R > 2$ is outside the physical domain. The Maclaurin coefficients for the solutions of the system (65) were generated numerically in FORTRAN 90 using the Algebraic Maclaurin Method [3] for several values of $k$. Plotting the absolute error in the Maclaurin approximation $|x_2(R) - \sum_{j=0}^{k} x_{2j}(R-2)^j|$ against the error bound (67) for various error tolerances leads to plots similar to those in Example 1. For $k = 16$, the absolute error is smaller than what double precision FORTRAN 90 on a 32-bit machine can capture, and as $k$ increases, the stepsize computed from the bound for a chosen error tolerance increases toward its limiting value. As with the previous examples, the error bound demonstrates the potential for remarkable accuracy for $R \in (0, 2]$ by stepping across the interval and using appropriate degree Maclaurin polynomial approximations at each step.

## 4. CONCLUDING REMARKS

The general error bounds developed here also provide a foundation for building more refined explicit, *a-priori*, error bounds for important special subclasses of ODE systems. Our approach also provides numerical analysts with new tools for making guaranteed predictions about the solutions of IVODE models that otherwise prove analytically intractable.

## REFERENCES

1. G.E. Parker and J.S. Sochacki, Implementing the Picard Iteration, *Neural, Parallel, and Scientific Computation* **4**, 97–112, (1996).
2. G.E. Parker and J.S. Sochacki, A Picard-McLaurin theorem for initial value PDE's, *Abstract and Applied Analysis* **5** (1), 47–63, (2000).
3. D.C. Carothers, G.E. Parker, J.S. Sochacki and P.G. Warne, Some properties of solutions to polynomial systems of differential equations, *Electron. J. Diff. Eqns.* **2005** (40), 1–17, (2005).
4. C.D. Pruett, J.W. Rudmin and J.M. Lacy, An adaptive N-body algorithm of optimal order, *Journal of Computational Physics* **187**, 298–317, (2003).
5. D. Estep, *A posteriori* error bounds and global error control for approximations of ordinary differential equations, *SIAM J. Numer. Anal.* **32**, 1–48, (1995).
6. G.F. Corliss, Guaranteed error bounds for ordinary differential equations, In *Theory and Numerics of Ordinary and Partial Differential Equations, Adv. Numer. Anal, IV*, (Edited by M. Ainsworth, *et. al.*) pp. 1–75, Oxford Univ. Press, New York, (1995).
7. L. Jódar, A.E. Posso and H. Castejón, Constructive polynomial approximations with *a priori* error bounds for nonlinear initial value differential problems, *Computers Math. Applic.* **38** (7/8), 9–19, (1999).
8. B. Chen, R. García-Bolós and L. Jódar, Frobenius-Chebyshev polynomial approximations with *a priori* error bounds for nonlinear initial value differential problems, *Computers Math. Applic.* **41** (3/4), 269–280, (2001).
9. B. Chen, R. García-Bolós, L. Jódar and M.D. Roselló, The truncation error of the two-variable Chebyshev series expansions, *Computers Math. Applic.* **45** (10/11), 1647–1653, (2003).
10. L.F. Shampine and L.S. Baca, Global error estimates for ODEs based on extrapolation methods, *SIAM J. Sci. Comput.* **6**, 1–14, (1985).
11. P. Merluzzi and C. Brosilaw, Runge-Kutta integration algorithms with built-in estimates of the accumulated truncation error, *Computing* **20**, 1–16, (1978).
12. A. Prothero, Estimating the accuracy of numerical solutions to ordinary differential equations, In *Computational Techniques for Ordinary Differential Equations*, (Edited by I. Gladwell and D.K. Sayers), pp. 103–128, Academic Press, New York, (1980).
13. C.O. Horgan, On axisymmetric solutions for compressible nonlinearly elastic solids, *Z. Angew. Math. Phys. (ZAMP)* **46**, S107–S125, (1995).