Guaranteed Error Bounds for a Class of Picard-Lindelöf Iteration Methods

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Abstract We present a new version of the Picard-Lindelöf method for ordinary differential equations (ODEs) supplied with guaranteed and explicitly computable upper bounds of an approximation error. The upper bounds are based on the Ostrowski estimates and the Banach fixed point theorem for contractive operators. The estimates derived in the paper take into account interpolation and integration errors and, therefore, provide objective information on the accuracy of computed approximations.

1 Introduction

In this paper, we discuss a new version of the Picard-Lindelöf method for solving the Cauchy problem

$$\frac{du}{dt} = \varphi(u(t),t), \quad u(t_0) = u_0, \tag{1}$$

where the solution $u(t)$ (which may be a scalar or vector function) must be found on the interval $[t_0, t_K]$.

Existence and uniqueness of the solutions follow from the Picard-Lindelöf theorem and the Picard existence theorem or from the Cauchy–Lipschitz theorem (see [1, pp. 1–15], [3]).

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The problem (1) can be numerically solved by various well-known methods (e.g., the methods of Runge–Kutta and Adams). Typically, the methods are furnished by a priori asymptotic estimates which show theoretical properties of the iteration algorithm. However, these estimates may have mainly a qualitative meaning and do not provide all necessary information about error bounds. This is the goal of a posteriori error estimation methods. We deduce such type of estimates and suggest a version of the Picard-Lindelöf method as a tool for constructing a fully reliable approximation of (1).

The Picard-Lindelöf iteration is one of the efficient known numerical methods for ODEs. Furthermore, it can be used not only for ODEs but for t-dependent algebraic and functional equations (see, e.g., [5, 6]). It was shown that the speed of convergence is quite independent of the step sizes. Numerical methods based on Picard-Lindelöf iterations for dynamical processes (the so-called waveform relaxation in the context of electrical networks) are discussed in [2].

The approach discussed in this paper is based on two-sided a posteriori estimates derived by Ostrowski [7] (see also systematic exposition presented in the books [4, 8]). The algorithm includes natural adaptation of the integration step and provides guaranteed bounds for the accuracy on the time interval $[t_0, t_K]$.

In Sect. 2, we present the main idea of the Picard-Lindelöf method and obtain the conditions which not only provide convergence of the method but also allow applying a posteriori error estimates. However, these estimates cannot be directly used. In practice computations based on the Picard-Lindelöf method we must take into account interpolation and integration errors. This analysis is done in Sect. 3. It leads to error bounds, derived in Sect. 4, which include the interpolation and integration errors. The structure of the algorithm is exposed in Sect. 5, where results of numerical tests are presented.

2 Picard-Lindelöf Method

Assume that the function $\varphi(\xi(t), t)$ (which is allowed to be a vector-valued function) in (1) is continuous with respect to both variables in terms of the continuous norm

$$\|u\|_{C([t_k, t_{k+1}])} := \max_{t \in [t_k, t_{k+1}]} |u(t)| \tag{2}$$

and satisfies the Lipschitz condition in the form

$$\|\varphi(u_2, t_2) - \varphi(u_1, t_1)\|_{C([t_1, t_2])} \leq \mathrm{L}_1 \|u_2 - u_1\|_{C([t_1, t_2])} + \mathrm{L}_2 |t_2 - t_1|, \qquad \forall (u_1, t_1), (u_2, t_2) \in Q, \tag{3}$$

where L_1, L_2 are Lipschitz constants, and

$$Q := \{(\xi, t) \mid \xi \in \mathrm{U},\ t_0 \leq t \leq t_N\}. \tag{4}$$

U is the set of possible values of u which comes from an a priori analysis of the problem. (It is clear that $u_0 \in \mathrm{U}$.)

In the Picard-Lindelöf method, we represent the differential equation in the integral form

$$u(t) = \int_{t_0}^{t} \varphi(u(s),s)\,ds + u_0. \tag{5}$$

Now, the exact solution is a fixed point of (5), which can be found by the iteration method

$$u_j(t) = \int_{t_0}^{t} \varphi(u_{j-1}(s),s)\,ds + u_0. \tag{6}$$

We write in the form $u_j = \mathscr{T} u_{j-1} + u_0$, where $\mathscr{T} : X \to X$ is the integral operator.

It is easy to show that the operator

$$\mathscr{T} u := \int_{t_k}^{t} \varphi(u(\tau),\tau) d\tau + u_{0,k}$$

is q-contractive on $I_k = [t_k, t_{k+1}]$, where I_k is a subinterval of the mesh $\mathscr{F}_K = \cup_{k=0}^{K-1} [t_k, t_{k+1}]$ defined on the interval $[t_0, t_K]$, with respect to the norm $\|u\|_{C(I_k)}$, if the condition

$$q := \mathrm{L}_1 (t_{k+1} - t_k) < 1 \tag{7}$$

is provided.

Therefore, if the interval $[t_{k+1}, t_k]$ is small enough, then the solution can be found by the iteration procedure. In the next sections, we call this method the Adaptive Picard-Lindelöf (APL) method.

3 Application of the Ostrowski Estimates

For the considered problem, the Ostrowski estimate reads as follows:

Theorem 1 ([7]). *Assume that* (7) *is satisfied on* $I_k := [t_k, t_{k+1}]$. *Then, the following estimate holds:*

$$M_j^{\ominus} := \frac{1}{1+q} \|u_j - u_{j+1}\|_{C(I_k)} \leq \|u - u_j\|_{C(I_k)} \leq \frac{q}{1-q} \|u_j - u_{j-1}\|_{C(I_k)} =: M_j^{\oplus}. \tag{8}$$

Remark 1. It is possible to derive more accurate error bounds for $\|u - u_j\|_{C(I_k)}$ by using additional elements of the sequence $\{u_j\}_{j=1}^{\infty}$ that have indexes greater than j:

$$\|u - u_j\|_{C(I_k)} \leq M_j^{\oplus,p} := \frac{1}{1-q^p} \|u_j - u_{j+p}\|_{C(I_k)}. \tag{9}$$

By the mathematical induction method it can be proved that the optimal form of the majorant and minorant based on P correspondent elements of the sequence are as follows:

$$M_j^{\ominus,P} := \sup_{p=1,\dots,P} \left\{ \frac{1}{1+q^p} \|u_j - u_{j+p}\|_{C(I_k)} \right\},$$
$$M_j^{\oplus,P} := \inf_{p=1,\dots,P} \left\{ \frac{1}{1-q^p} \|u_j - u_{j+p}\|_{C(I_k)} \right\}. \tag{10}$$

However, the estimates (8) cannot be directly used because numerical approximations include interpolation and integration errors, which must be taken into account by fully reliable schemes.

Let us discuss this issue within the paradigm of a single (e.g., the first) step of the APL:

$$u_1(t) = \int_{t_0}^{t} \varphi(u_0(\tau),\tau)d\tau,\ t \in [t_0,t_1], \tag{11}$$

where u_0 is the initial approximation defined as a piecewise affine function on the mesh $\Omega_{S_k} = \cup_{s=0}^{S_k-1}[z_s, z_{s+1}]$ on the interval $[t_0,t_1]$.

If $q < 1$ and u_1 is computed exactly, then

$$\|u_1(t) - u(t)\|_{C([t_0,t_1])} \leq \frac{q}{1-q} \|u_1(t) - u_0(t)\|_{C([t_0,t_1])}. \tag{12}$$

However, in general, u_1 is approximated by a piecewise affine continuous function

$$\overline{u_1}(t) = \pi u_1 \in CP^1([z_s, z_{s+1}]), \quad s = 0,\dots,S_k - 1, \tag{13}$$

where π is the projection operator $\pi : C \rightarrow CP^1([t_0,t_1])$ satisfying the relation $\pi\, u(z_s) = \overline{u}(z_s)$. Thus, on the right-hand side of (12) we can estimate as follows:

$$\|u_1(t) - u_0(t)\|_{C([t_0,t_1])} \leq \|\overline{u_1}(t) - u_0(t)\|_{C([t_0,t_1])} + \|\overline{u_1}(t) - u_1(t)\|_{C([t_0,t_1])}. \tag{14}$$

Here $\|\overline{u_1}(t) - u_1(t)\|_{C([t_0,t_1])} = \|\overline{e_1}\|_{C([t_0,t_1])}$ is an interpolation error. In general, this term is unknown, but we can estimate it using an interpolation error estimate.

Numerical integration generates other errors which must be taken into account. Indeed, the values $\overline{u}(z_s)$, $s = 0,\dots,S_k$, cannot be found exactly. Hence, at every node z_s instead of $\overline{u_1}(z_s)$ we have $\widehat{u_1}(z_s)$. Now, (14) implies

$$\|u_1(t) - u_0(t)\|_{C([t_0,t_1])} \leq \|\widehat{u_1}(t) - u_0(t)\|_{C([t_0,t_1])} + \\ + \|\widehat{u_1}(t) - \overline{u_1}(t)\|_{C([t_0,t_1])} + \|\overline{u_1}(t) - u_1(t)\|_{C([t_0,t_1])}, \tag{15}$$

where $\|\widehat{u_1}(t) - \overline{u_1}(t)\|_{C([t_0,t_1])} = \|\widehat{e_1}\|_{C([t_0,t_1])}$ is the integration error.

4 Estimates of Interpolation and Integration Errors

4.1 Interpolation Error

We study the difference between u_1 and $\overline{u_1}$, where $\overline{u_1}$ is the linear interpolant of u_1 defined at the points $\{z_s\}_{s=0}^{S_k}$:

$$u_1(z_s) = \overline{u_1}(z_s) = \int_0^{z_s} \varphi(u_0(t),t)\,dt. \tag{16}$$

For all $z \in [z_s, z_{s+1}]$,

$$\overline{u_1}(z) = u_1(z_s) + \frac{u_1(z_{s+1}) - u_1(z_s)}{\Delta_s}(z - z_s). \tag{17}$$

Then,

$$\begin{aligned}
\overline{e} = \overline{u_1}(z) - u_1(z) = \\
= \left[\int_0^{z_s} \varphi(u_0(t),t)\,dt + \frac{\int_{z_s}^{z_{s+1}} \varphi(u_0(t),t)dt}{\Delta_s}(z - z_s)\right] - \int_0^{z} \varphi(u_0(t),t)\,dt = \\
= \frac{z - z_s}{\Delta_s}\int_{z_s}^{z_{s+1}} \varphi(u_0(t),t)dt - \int_{z_s}^{z} \varphi(u_0(t),t)\,dt.
\end{aligned} \tag{18}$$

Taking into account that u_0 is affinely interpolated, consider the last integral on the right-hand side of (18)

$$\int_{z_s}^{z} \varphi(u_0(t),t)\,dt = \int_{z_s}^{z} \varphi\left(u_{0,s} + \frac{u_{0,s+1} - u_{0,s}}{\Delta_s}(t - z_s), t\right)dt. \tag{19}$$

Define

$$\lambda = \frac{t - z_s}{\Delta_s} = \frac{t - z_s}{z_{s+1} - z_s}, \tag{20}$$

where z_s and z_{s+1} are nodes of the mesh defined in Section 3. Substitute $t = z_s + (z_{s+1} - z_s)\lambda$ to $\varphi(u_0(t),t)$

$$\begin{aligned}
\varphi\left(u_{0,s} + \frac{u_{0,s+1} - u_{0,s}}{\Delta_s}(t - z_s), t\right) = \\
= \varphi(u_{0,s} + (u_{0,s+1} - u_{0,s})\lambda, z_s + \lambda(z_{s+1} - z_s)) = \\
= \varphi(\lambda u_{0,s+1} + (1 - \lambda)u_{0,s}, \lambda z_{s+1} + (1 - \lambda)z_s).
\end{aligned} \tag{21}$$

Let

$$\widetilde{\varphi}_{[s,s+1]} := \varphi_s + \frac{\varphi_{s+1} - \varphi_s}{\Delta_s}(t - z_s), \tag{22}$$

where $\varphi_s = \varphi(u_{0,s}, z_s)$ and $\varphi_{s+1} = \varphi(u_{0,s+1}, z_{s+1})$. Using (20), we rewrite (22)

$$\widetilde{\varphi}_{[s,s+1]} = \varphi_s + (\varphi_{s+1} - \varphi_s)\lambda = \lambda\varphi_{s+1} + (1-\lambda)\varphi_s. \tag{23}$$

Thus, we can derive the following estimate with the help of (23) and (3):

$$\begin{aligned}
&\left|\varphi\left(u_{0,s} + \frac{u_{0,s+1}-u_{0,s}}{\Delta_s}(t-z_s), t\right) - \widetilde{\varphi}_{[s,s+1]}\right| \leq \\
&\leq |\varphi(\lambda u_{0,s+1} + (1-\lambda)u_{0,s},\ \lambda z_{s+1} + (1-\lambda)z_s) - \lambda\varphi_{s+1} + (1-\lambda)\varphi_s| \leq \\
&\leq (1-\lambda)\Big[\mathrm{L}_{1,s}\,|\lambda u_{0,s+1} + (1-\lambda)u_{0,s} - u_{0,s}| + \\
&\qquad\qquad + \mathrm{L}_{2,s}\,|\lambda z_{s+1} + (1-\lambda)z_s - z_s|\Big] + \\
&\quad + \ \lambda\Big[\mathrm{L}_{1,s}|\lambda u_{0,s+1} + (1-\lambda)u_{0,s} - u_{0,s+1}| + \\
&\qquad\qquad + \mathrm{L}_{2,s}|\lambda z_{s+1} + (1-\lambda)z_s - z_{s+1}|\Big] \leq \\
&\leq 2\lambda(1-\lambda)\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}|z_{s+1}-z_s|\right] \\
&\leq 2\frac{(z_{s+1}-t)(t-z_s)}{\Delta_s^2}\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\Delta_s\right].
\end{aligned} \tag{24}$$

We decompose (19)

$$\begin{aligned}
&\int_{z_s}^{z} \varphi(u_0(t),t)dt = \\
&\quad = \int_{z_s}^{z} \widetilde{\varphi}_{[s,s+1]}(t)dt + \int_{z_s}^{z} \left[\varphi(u_{0,s} + \frac{u_{0,s+1}-u_{0,s}}{\Delta_s}(t-z_s), t) - \widetilde{\varphi}_{[s,s+1]}\right] dt.
\end{aligned} \tag{25}$$

Let us denote the first integral on the right-hand side of (25) by $\widetilde{i}_s(z)$. Then,

$$\widetilde{i}_s(z) := \int_{z_s}^{z} \left(\varphi_s + \frac{\varphi_{s+1}-\varphi_s}{\Delta_s}(t-z_s)\right) dt \ = (z-z_s)\left[\varphi_s + \frac{\varphi_{s+1}-\varphi_s}{2\Delta_s}(z-z_s)\right]. \tag{26}$$

The second integral on the right-hand side of (25) is estimated with the help of (24):

$$\begin{aligned}
&\int_{z_s}^{z} \left|\varphi\left(u_{0,s} + \frac{u_{0,s+1}-u_{0,s}}{\Delta_s}(t-z_s), t\right) - \widetilde{\varphi}_{[s,s+1]}\right| dt \leq \\
&\quad \leq \frac{2\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\Delta_s\right]}{\Delta_s^2} \int_{z_s}^{z} (t-z_s)(z_{s+1}-t)dt = \\
&\quad = \frac{2\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\Delta_s\right]}{\Delta_s^2} \int_{z_s}^{z} (t-z_s)(z_s+\Delta_s-t)dt = \\
&\quad = \frac{2\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\Delta_s\right]}{\Delta_s^2} (z-z_s)^2 \left[\frac{\Delta_s}{2} - \frac{z-z_s}{3}\right] = \\
&\quad = \frac{\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\Delta_s\right]}{3\Delta_s^2} (z-z_s)^2(2z_s + 3\Delta_s - 2z).
\end{aligned} \tag{27}$$

Since

$$\max_{z\in[z_s,z_{s+1}]}(z-z_s)^2(2z_s+3\Delta_s-2z)=\Delta_s^3, \tag{28}$$

we find that

$$\begin{aligned}\int_{z_s}^{z}\left|\varphi(u_{0,s}+\frac{u_{0,s+1}-u_{0,s}}{\Delta_s}(t-z_s),t)-\widetilde{\varphi}_{[s,s+1]}\right|dt \le \\ \le \frac{\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}|+\mathrm{L}_{2,s}\Delta_s\right]\Delta_s^3}{3\Delta_s^2} = \\ = \frac{\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}|+\mathrm{L}_{2,s}\Delta_s\right]\Delta_s}{3}.\end{aligned} \tag{29}$$

We represent the interpolation error (18) using (26),

$$\begin{aligned}\overline{u_1}(z)-u_1(z)=\frac{z-z_s}{\Delta_s}\int_{z_s}^{z_{s+1}}\varphi(u_0(t),t)dt-\int_{z_s}^{z}\varphi(u_0(t),t)dt= \\ =\frac{z-z_s}{\Delta_s}\widetilde{i}_s(z_{s+1})-\widetilde{i}_s(z)+\varepsilon_1(z)+\varepsilon_2(z),\end{aligned} \tag{30}$$

where

$$\begin{aligned}\varepsilon_1=\int_{z_s}^{z_{s+1}}\left|\varphi(u_{0,s}+\frac{u_{0,s+1}-u_{0,s}}{\Delta_s}(t-z_s),t)-\widetilde{\varphi}_{[s,s+1]}\right|dt, \\ \varepsilon_2=\int_{z_s}^{z}\left|\varphi(u_{0,s}+\frac{u_{0,s+1}-u_{0,s}}{\Delta_s}(t-z_s),t)-\widetilde{\varphi}_{[s,s+1]}\right|dt.\end{aligned} \tag{31}$$

Thus, we estimate the interpolation error as follows:

$$\begin{aligned}\overline{e}=\|\overline{u}_1(z)-u_1(z)\|_{C([z_s,z_{s+1}])}\le \\ \le \max_{z\in[z_s,z_{s+1}]}\left|\frac{z-z_s}{\Delta_s}\widetilde{i}_s(z_{s+1})-\widetilde{i}_s(z)\right|+\max_{z\in[z_s,z_{s+1}]}|\varepsilon_1(z)+\varepsilon_2(z)|.\end{aligned} \tag{32}$$

For the first term on the right hand side of (32) we have (see (26))

$$\begin{aligned}\max_{z\in[z_s,z_{s+1}]}\left|\frac{z-z_s}{\Delta_s}\widetilde{i}_s(z_{s+1})-\widetilde{i}_s(z)\right|dt\le\frac{|\varphi_{s+1}-\varphi_s|}{2\Delta_s}\max_{z\in[z_s,z_{s+1}]}|(z-z_s)(z_{s+1}-z)|\le \\ \le\frac{|\varphi_{s+1}-\varphi_s|}{2\Delta_s}\frac{\Delta_s^2}{4}=\frac{1}{8}|\varphi_{s+1}-\varphi_s|\Delta_s.\end{aligned} \tag{33}$$

For the second term, we have (see (29))

$$\max_{z\in[z_s,z_{s+1}]}|\varepsilon_1(z)+\varepsilon_2(z)|\le 2\frac{\Delta_s\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}|+\mathrm{L}_{2,s}\Delta_s\right]}{3}. \tag{34}$$

Hence, the overall estimate of the interpolation error has the form

$$\|\overline{u}_1(z)-u_1(z)\|_{C([z_s,z_{s+1}])} \leq \frac{\varphi_{s+1}-\varphi_s}{8}\Delta_s + \frac{2}{3}\Delta_s\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\,\Delta_s\right]. \quad (35)$$

4.2 Integration Error

The interpolation error estimate (35) does not account for the fact that computations of the integral are performed approximately. It is not difficult to evaluate the integration errors by noting that for a Lipschitz function $f(t)$ the error encompassed in the simplest trapezoidal quadrature formula

$$\int_{t_0}^{t_1} f(t)dt \simeq \frac{f(t_0)+f(t_1)}{2}(t_1-t_0) \quad (36)$$

can be estimated as follows:

$$e_{int} \leq \frac{L}{4}(t_1-t_0)^2 - \frac{1}{4L}[f(t_1)-f(t_0)]^2. \quad (37)$$

Then, it is not difficult to show that the integration error can be estimated as

$$\|\widehat{u}_1(t)-\overline{u}_1(t)\|_{C([z_s,z_{s+1}])} \leq \frac{\mathrm{L}_s}{4}\Delta_s^2 - \frac{1}{4\mathrm{L}_s}[\varphi_{s+1}-\varphi_s]^2, \quad (38)$$

where $\mathrm{L}_s = \mathrm{L}_{1,s}\,l_s + \mathrm{L}_{2,s}$. (Here, l_s is the slope of the piecewise function on every interval $[z_s,z_{s+1}]$, $s=0,...,S_k-1$.)

4.3 Guaranteed Error Bounds for Picard-Lindelöf Method

Thus, on every subinterval $[z_s,z_{s+1}]$ the interpolation error can be estimated with the help of (35). Then, for whole interval $[t_0,t_1] := \cup_{s=0}^{S_k-1}[z_s,z_{s+1}]$ the interpolation error estimate is the following:

$$\|\overline{u}_1(t)-u_1(t)\|_{C([t_0,t_1])} \leq$$
$$\leq \sum_{s=0,\dots,S_k-1} \frac{\varphi_{s+1}-\varphi_s}{8}\Delta_s + \frac{2}{3}\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}| + \mathrm{L}_{2,s}\Delta_s\right]\Delta_s. \quad (39)$$

Analogously, for the integration error

$$\|\overline{u}_1(t)-\widehat{u}_1(t)\|_{C([t_0,t_1])} \leq \sum_{s=0,\dots,S_k-1} \frac{\mathrm{L}_s}{2}\Delta_s^2 - \frac{1}{2\mathrm{L}_s}[\varphi_{s+1}-\varphi_s]^2. \quad (40)$$

Then, the inequality (15) implies the estimate

$$\|u_1(t)-u_0(t)\|_{C([t_0,t_1])} \leq \|\widehat{u}_1(t)-u_0(t)\|_{C([t_0,t_1])}+ \\ + \sum_{s=0,\dots,S_k-1}\left(\frac{\varphi_{s+1}-\varphi_s}{8}\Delta_s+\frac{2}{3}\Delta_s\left[\mathrm{L}_{1,s}|u_{0,s+1}-u_{0,s}|+\mathrm{L}_{2,s}\Delta_s\right]\right)+ \\ + \sum_{s=0,\dots,S_k-1}\left(\frac{\mathrm{L}_s}{2}\Delta_s^2-\frac{1}{2\mathrm{L_s}}\left[\varphi_{s+1}-\varphi_s\right]^2\right). \quad (41)$$

After j steps of the iterations we obtain

$$\|u_{j+1}(t)-u_j(t)\|_{C([t_0,t_1])} \leq \mathrm{M}^{\oplus,1}_{j+1}(\widehat{u}_j) := \\ \|\widehat{u}_{j+1}(t)-\widehat{u}_j(t)\|_{C([t_0,t_1])}+E^1_{interp}+E^1_{integr}, \quad (42)$$

where

$$E^1_{interp} := \sum_{s=0,\dots,S_k-1}\left(\frac{\varphi(\widehat{u}_{j,s+1},z_{s+1})-\varphi(\widehat{u}_{j,s},z_s)}{8}\Delta_s+ \\ +\frac{2}{3}\Delta_s\left[\mathrm{L}_{1,s}|\widehat{u}_{j,s+1}-\widehat{u}_{j,s}|+\mathrm{L}_{2,s}\Delta_s\right]\right) \quad (43)$$

and

$$E^1_{integr} := \sum_{s=0,\dots,S_k-1}\left(\frac{\mathrm{L_s}}{2}\Delta_s^2-\frac{1}{2\mathrm{L_s}}\left[\varphi(\widehat{u}_{j,s+1},z_{s+1})-\varphi(\widehat{u}_{j,s},z_s)\right]^2\right), \quad (44)$$

where for $j=0$ the function $\widehat{u}_j$ is taken as a piecewise affine interpolation of u_0, and for $j \geq 1$ it is taken from the previous iteration step.

The quantity $\mathrm{M}^{\oplus,1}_j$ is fully computable, and it shows the overall error associated with the step number j on the first interval.

Remark 2. Estimate of the overall error related to the interval $[t_0,t_K]$ includes all errors computed on the intervals. In other words the error associated with $[t_0,t_{k-1}]$ is appended to the error on $[t_{k-1},t_k]$ (which formally follows from the fact that the initial condition on $[t_{k-1},t_k]$ includes errors on the previous intervals).

Thus, we have shown that fully guaranteed and computable bounds can indeed be derived for the problem (1) with the Lipschitz function φ, i.e. for every finite time interval $[t_0,t_K]$ and for every a priori required accuracy ε an approximate solution of the problem can be found by the APL method discussed above.

5 APL Algorithm and Numerical Examples

Let ε be a required accuracy of an approximate solution. Then, practical computation can be performed by Algorithm 1.

Algorithm 1 The algorithm of the APL method

Input: ε {required accuracy on the interval}, u_0 {input initial boundary condition}
$\mathscr{F}_K = \bigcup_{k=0}^{K-1} [t_k, t_{k+1}]$ { constructed by *Mesh Generation Procedure*}
$\varepsilon^k = \frac{\varepsilon}{K}$ {obtain accuracy of the approximate solution on interval $[t_k, t_{k+1}]$}
$\Omega_{S_k} = \bigcup_{s=0}^{S_k-1} [z_s, z_{s+1}]$ {initial mesh for each subinterval}
for $k = 1$ to K **do**
  $j = 0$
  do
    if $k = 1$
      $a = u_0$
    else
      $a = v^{k-1}(t_{k-1})$
    endif
    $v_j^k = \textit{Integration Procedure}(\varphi, v_{j-1}^k, S_k) + a$
    calculate E_{interp}^k and E_{integr}^k by using (43) and (44)
    $M_j^{\oplus,k} = \|v_j^k - v_{j-1}^k\|_{C([t_{k-1},t_k])} + E_{interp}^k + E_{integr}^k$
    $e_j^{\oplus} = \frac{q}{1-q} M_j^{\oplus,k}$
    if $E_{interp}^k + E_{integr}^k > \varepsilon_k$
      $S_k = 2\,S_k$ {refine the mesh Ω_{S_k}}
    endif
    $j = j + 1$
  while $e_j^{\oplus} > \varepsilon^k$
  $v^k = v_j^k$ {approximate solution on the interval $[t_{k-1}, t_k]$}
  $e^{\oplus,k} = e_j^{\oplus}$ {error bound achieved for the interval $[t_{k-1}, t_k]$}
end for
Output: $\{v^k\}_{k=1}^K$ {approximate solution}
  $\{e^{\oplus,k}\}_{k=1}^K$ {error bounds estimates on sub intervals}

In general, the algorithm should start with the generation of a suitable mesh (i.e., select time intervals). Here, we do not discuss this question in detail, but only note that the *Mesh Guaranteed Procedure* must adapt the mesh to the nature of $\varphi(u(t),t)$, which requires information about U (see (4)). In practise, such information can be obtained by solving the problem (1) numerically with the help of some heuristic (e.g., Runge-Kutta) method on a coarse mesh.

The APL algorithm is a cycle over all the intervals of the mesh $\mathscr{F}_K = \cup_{k=0}^{K-1} [t_k, t_{k+1}]$. On each subinterval, the algorithm is realized as a subcycle (whose index is j). In the subcycle, we apply the PL method and try to find an approximation that meets the accuracy requirements imposed (i.e., the accuracy must be higher than ε^k). Initial data are taken from the previous step (for the first step, the initial condition is defined by u_0).

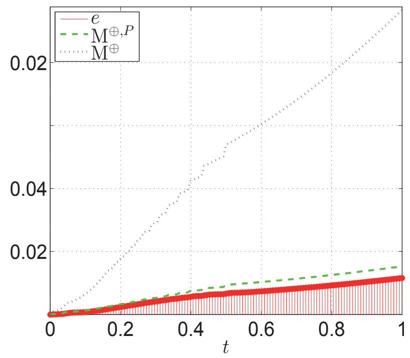


Fig. 1 The error and error majorants

After computing an approximation on $[t_k, t_{k+1}]$ we use our majorant and find a guaranteed upper bound (which includes the interpolation and integration errors). Iterations are continued unless the required accuracy ε^k has been achieved. After that we save the results and proceed to the next interval.

Note that in Algorithm 1, we do not discuss in detail the process of integration on an interval, which is performed on a local mesh with a certain amount of subintervals (whose size is Δ_s). In principle, it may happen that the desired level of accuracy, ε^k, is not achieved with the Δ_s selected. This fact will be easily detected because interpolation and integration errors will dominate and do not allow the overall error to decrease below ε^k. In this case, Δ_s must be reduced, and computations on the corresponding interval must be repeated.

Example 1. Consider the problem

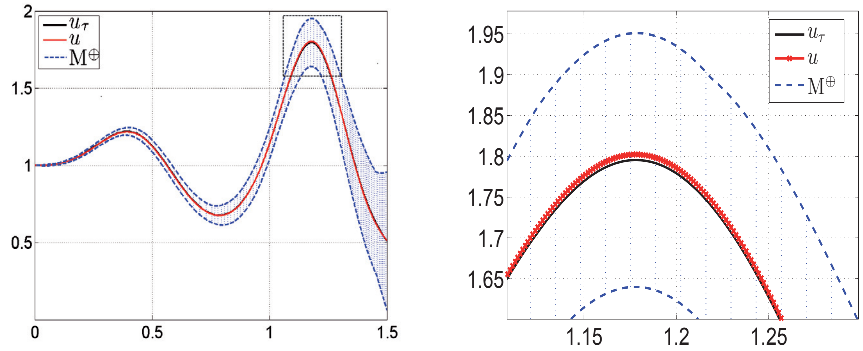
$$\begin{aligned} \frac{du}{dt} &= 4ut\sin(8t), \quad t \in [0, 3/2], \\ u(0) &= u_0 = 1 \end{aligned} \tag{45}$$

with the exact solution

$$u = e^{\frac{1}{16}\sin(8t) - \frac{1}{2}t\cos(8t)}.$$

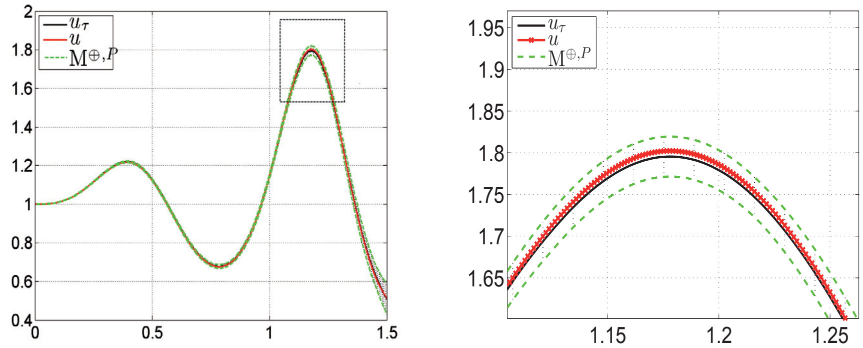
In Fig. 1, we depict the error (bold dots), error bounds computed by the Ostrowski estimates (dotted line) and by the advanced form of the estimate (dashed line). In order to make the results more transparent, we depict the approximate solution together with the zone which contains the exact solution (see Figs. 2(a) and 3(a)). The form of this (shaded) zone is determined by the a posteriori estimates.

Thus, the APL method computes two-sided guaranteed bounds containing the exact solution. It may happen that the desired level of accuracy has been exceeded at some moment $t' < t_K$ and further Picard-Lindelöf iterations are unable to reduce the error. This situation may arise if the amount of internal points used for numerical integration on each interval is too small. In this case, we must enlarge the number of internal nodes (which will reduce integration and interpolation errors) and repeat



(a) (b)

Fig. 2 (a) Exact and approximate solutions with guaranteed bounds of deviation computed by the Ostrowski estimate. (b) A zoomed interval of exact and approximate solutions with bounds of deviation computed by the majorant.



(a) (b)

Fig. 3 (a) Exact and approximate solutions with guaranteed bounds of deviation computed by the advanced form of the estimate. (b) A zoomed interval of exact and approximate solutions with bounds of deviation computed by the majorant.

the computations. Numerical results illustrated in Figs. 2(a) and 3(a) show that the advanced majorant provides much sharper bounds of the deviation.

Values of the components of the estimate (the first term, the *estimate of* $\|\overline{e}\|$ and the *estimate of* $\|\widehat{e}\|$ from (42)) are presented in Table 1. We see that in this example the values of S_k were selected properly, so that interpolation and integration error estimates are insignificant with respect to the first term.

Example 2. The APL method works with stiff problems as well. Consider the classical stiff equation

Table 1 Components of the general estimate

Estimate of $\|e_j\|$	Estimate of $\|\bar{e_j}\|$	Estimate of $\|\hat{e}_j\|$
2.2658e-002	8.6160e-008	9.5725e-008
4.6095e-002	1.8847e-007	5.8148e-007
5.4949e-002	2.5299e-007	5.9301e-007
7.4818e-002	2.5768e-007	2.3618e-006
9.5993e-002	3.0190e-007	2.3699e-006
1.0302e-001	3.4216e-007	2.3807e-006
1.5427e-001	4.8963e-007	2.4320e-006
1.5647e-001	6.1877e-007	2.4999e-006
2.3495e-001	9.4891e-007	2.6183e-006
2.7145e-001	9.8935e-007	2.6328e-006
3.0533e-001	9.9923e-007	2.6373e-006
3.2838e-001	1.0158e-006	2.6404e-006
4.4629e-001	1.0182e-006	2.6517e-006

$$\begin{aligned} \frac{du}{dt} &= 50\cos(t) - 50u, \quad t = [0,1], \\ u(0) &= u_0 = 1 \end{aligned} \tag{46}$$

with the exact solution

$$u = \frac{1}{2501}e^{-50t} + \frac{2500}{2501}\cos(t) + \frac{50}{2501}\sin(t).$$

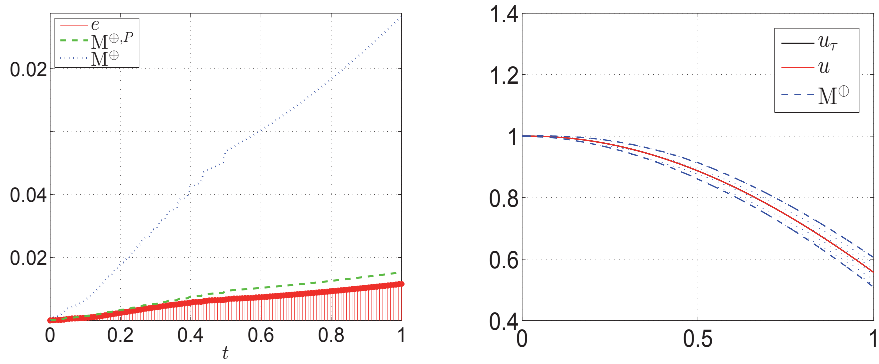
Analogously to the previous example, in Fig. 4(a) the general error (lines with dots on the top) estimated by the Ostrowski estimate (dotted line) and the advanced form of the estimate (dashed line) are illustrated. Another way to depict obtained results is shown in Fig. 4(b).

Example 3. The APL method can also be applied to stiff systems of ODEs. As an example, we consider the system

$$\begin{cases} \frac{du_1}{dt} = 998u_1 + 1998u_2, \\ \frac{du_2}{dt} = -999u_1 - 1999u_2, \\ u_1(t_0) = 1, u_2(t_0) = 1, \\ t \in [0, 5 \cdot 10^{-3}] \end{cases}$$

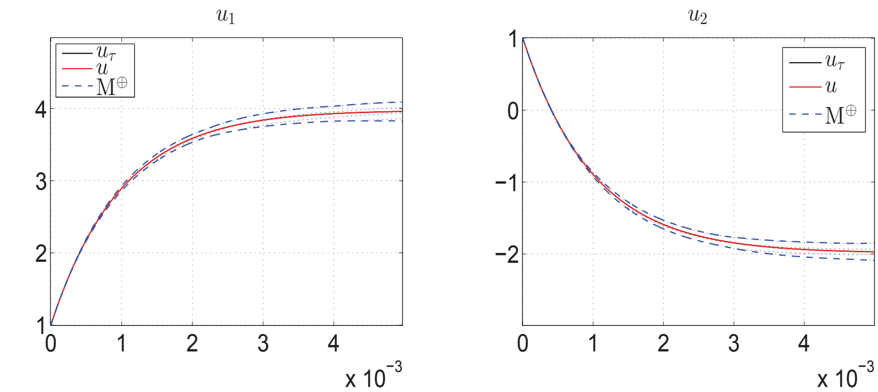
with the exact solutions $u_1 = 4e^{-t} - 3e^{-1000t}$ and $u_2 = -2e^{-t} + 3e^{-1000t}$. In Figs. 5(a), 5(b), 6(a) and 6(b), we present the same type of information (behavior of the solution and guaranteed bounds) as in the previous examples.

We note that for stiff equations getting an approximate solution with guaranteed and sharp error bounds requires much larger expenditures than in relatively simple



(a) (b)

Fig. 4 (a) Error and error majorants. (b) Exact and approximate solutions with a guaranteed deviation bound.



(a) (b)

Fig. 5 Exact solutions and approximate solutions of the system and guaranteed error bounds computed by the Ostrowski method.

Examples 1 and 2. This result is not surprising because (as it is quite natural to expect) for such type of problems fully reliable computations will be much more expensive.

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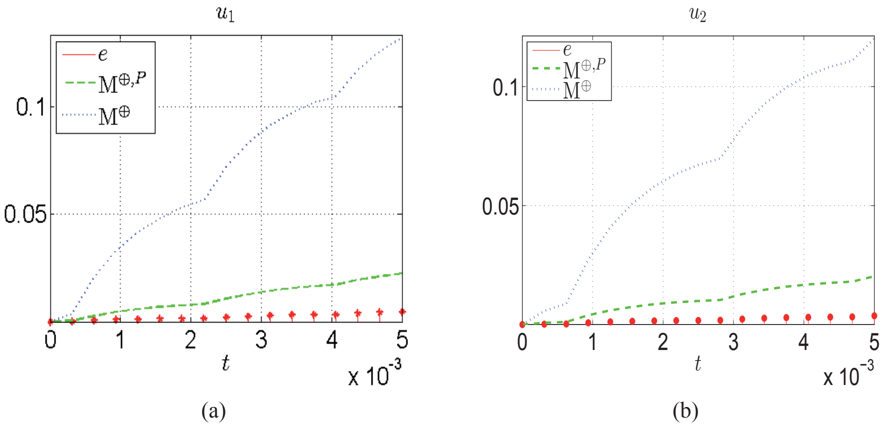

Fig. 6 The error and error majorants for the solutions u_1, u_2 of the system.

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