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High-precision numerical solution of ODE with high-order Taylor methods in parallel

R. Barrio[a], F. Blesa[b] and M. Lara[c]

Grupo de Mecánica Espacial

[a]Dept. Matemática Aplicada, Univ. Zaragoza, 50015 Zaragoza, Spain.

[b]Dept. Física Aplicada, Univ. Zaragoza, 22071 Huesca, Spain.

[c]Real Observatorio de la Armada, 11110 San Fernando, Spain.

rabarrio@posta.unizar.es, fblesa@posta.unizar.es, mlara@roa.es

Abstract

In this paper we study a variable order formulation of the Taylor method for the numerical solution of ODE when a very high precision of the solution is required. Finally, simulations on a parallel computer Sun UltraSPARC-II with 4 processors are shown.

1 Introduction

The Taylor method is one of the oldest numerical methods for solving ordinary differential equations (it was already used by Newton and Euler). The formulation is quite simple. Let us consider the initial value problem:

$$\frac{d\mathbf{y}(t)}{dt} = \mathbf{f}(t, \mathbf{y}(t)), \qquad \mathbf{y}(t_0) = \mathbf{y}_0, \qquad \mathbf{y} \in \mathbb{R}^s,\ t \in \mathbb{R}\,.$$

Now, the value of the solution at t_i (that is, $\mathbf{y}(t_i)$) is approximated from the n-th degree Taylor series of $\mathbf{y}(t)$ at $t = t_i$ (obviously the function $\mathbf{f}$ need to be a smooth function, in this paper we consider that $\mathbf{f}$ is analytic). So, denoting $h_i = t_i - t_{i-1}$,

$$\begin{aligned}
&\mathbf{y}(t_0) = \mathbf{y}_0,\\
&\mathbf{y}(t_i) \simeq \mathbf{y}_i = \mathbf{y}_{i-1} + \frac{d\mathbf{y}(t_{i-1})}{dt}\, h_i + \frac{1}{2!}\,\frac{d^2\mathbf{y}(t_{i-1})}{dt^2}\, h_i^2 + \ldots + \frac{1}{n!}\,\frac{d^n\mathbf{y}(t_{i-1})}{dt^n}\, h_i^n.
\end{aligned}$$

Therefore, the problem is reduced to the determination of the Taylor coefficients $\{d^j\mathbf{y}(t_{i-1})/dt^j\}$. In this paper we follow the method used in [13] of recurrent power series.

2 Variable-order variable-stepsize formulation of Taylor methods

The Taylor method presents several peculiarities. One of them is the easy formulation as a variable-step and variable-order method. In the literature the variable-order formulation has been only used in very few codes due to the difficulties of changing the order in Runge-Kutta methods. In this paper we analyse the VSVO formulation of Taylor methods. Another interesting property of Taylor methods is that it gives us directly a dense output, that is, the solution is an approximation of the function that we can evaluate everywhere, as in collocation methods [3].

Besides, when it is interesting to calculate with hundreds of digits, as in the determination of initial conditions for periodic problems [12], determination of physical constants, etc, Taylor methods, just by increasing the degree n, permits high-precision integrations. Obviously, when we look for high-precision results we also need to use a multiple-precision software.

In the practical implementation of a numerical method for the solution of ODEs the use of variable stepsizes is a crucial point because it permits to automatise the control of the error. Several formulations of variable-stepsize Taylor methods can be found in [4, 8, 11, 13] where the radius of convergence of the power series is calculated by means of different methods. Here we use the approach given in [4].

Once we have obtained the solution of the ODE as a power series we need to calculate the interval into which our approximation to the solution is within the allowed tolerance ϵ. If we denote $\mathbf{Y}_j = 1/j!\, d^j\mathbf{y}(t_{i-1})/dt^j$ and by defining $k(\epsilon, n) = \epsilon^{1/(n+1)}$, we obtain the new stepsize h as

$$h = \texttt{fac} \cdot \min\left\{ k(\epsilon, n)\, \|\mathbf{Y}_n\|_\infty^{-1/n},\ k(\epsilon, n+1)\, \|\mathbf{Y}_{n+1}\|_\infty^{-1/(n+1)} \right\}, \tag{1}$$

being `fac` a safety factor.

In a variable order implementation of the Taylor's method, it is necessary to know "a priori" an estimation of both, the computational time and the stepsize for a fixed error tolerance ϵ, for the different orders. On our own, we fixed the order increment to p, that is, our possibilities are: $n-p$, n or $n+p$, being n the order of the last step in the numerical integration. In this paper we use the variable-order formulation given in [4] (another VO formulation is presented in [11]).

3 Numerical tests

In this section we present several numerical tests done on a Sun UltraSPARC-II. All the numerical tests have been done using the multiple-precision library `mpf90` [2].

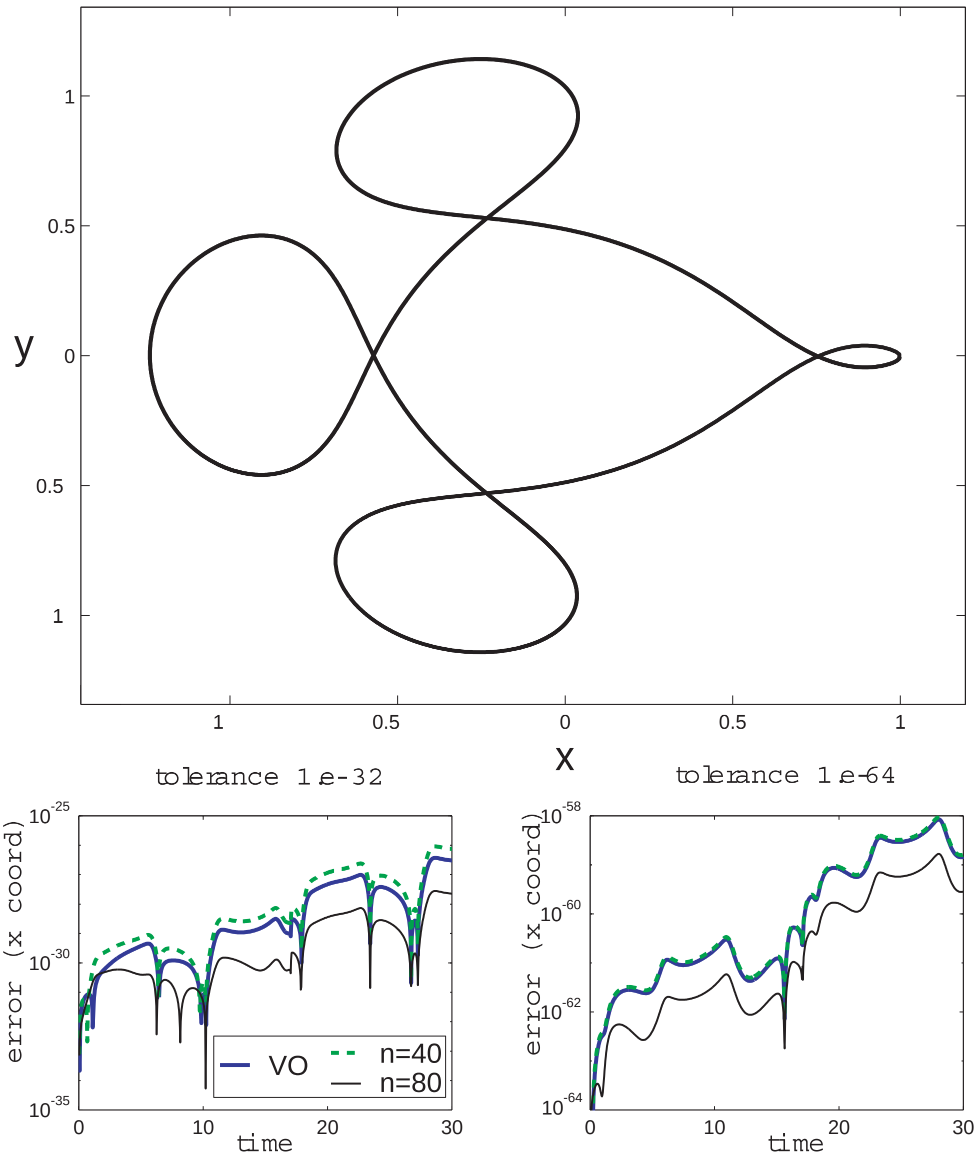

Figure 1: Evolution of the coordinates x, y of the Arenstorf orbits and the errors in the x-coordinate by considering different precision levels and using fixed and variable-order (VO) formulations.

- Arenstorf orbits [1] is a particular case of the restricted three body problem. One consider two bodies of masses $1-\mu$ and μ in circular rotation in a plane and a third body of negligible mass moving around in the same plane. The equations are [15]

$$
\begin{aligned}
x'' &= x + 2y' - \mu' \frac{x+\mu}{D_1} - \mu \frac{x-\mu'}{D_2}, \\
y'' &= y - 2x' - \mu' \frac{y}{D_1} - \mu \frac{y}{D_2},
\end{aligned}
$$

$$
\begin{cases}
D_1 = ((x+\mu)^2 + y^2)^{3/2}, \qquad D_2 = ((x-\mu')^2 + y^2)^{3/2}, \\
x_0 = 0.994, \quad y_0 = 0, \quad x'_0 = 0, \quad y'_0 = -2.0015851063790825, \\
\mu = 0.012277471, \qquad \mu' = 1-\mu.
\end{cases}
$$

In the figure 1 we present the evolution of the coordinates x and y for $t \in [0, 30]$. The orbit is periodic of period 17.065216560157962. On the figures on the bottom we show the differences between fixed and variable-order formulations. The fixed order simulations have been done with $n = 40$ and $n = 80$ for different tolerance levels. From the tests we observe the correct behaviour of the VO formulation.

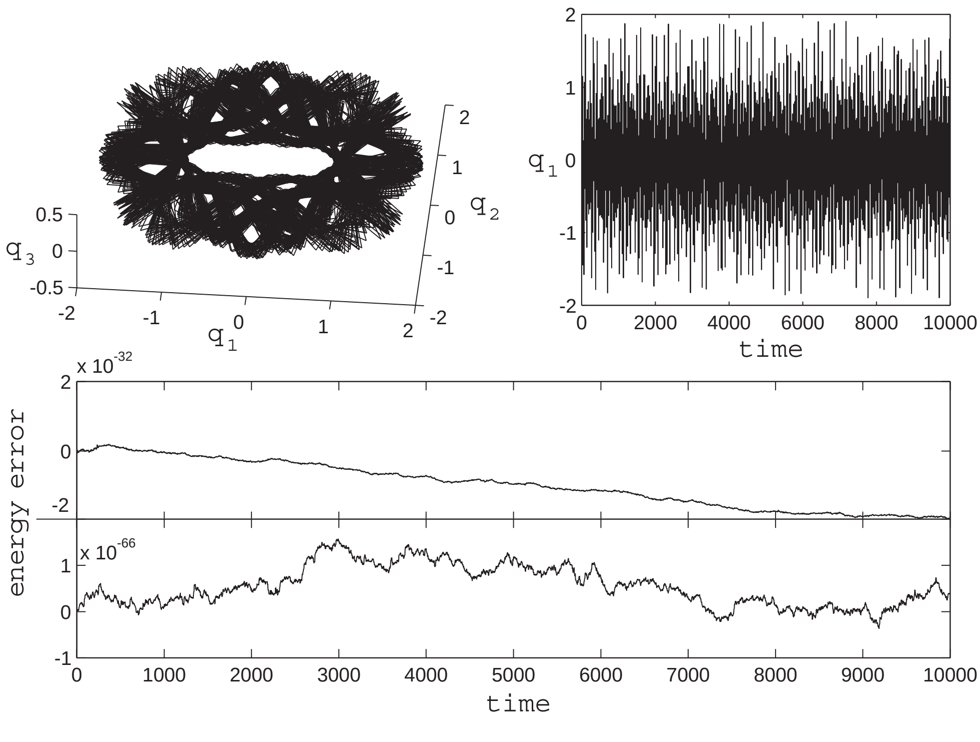

Figure 2: Evolution of the position coordinates q_1, q_2, q_3 of the Galactic problem and the errors in the energy by considering different precision levels.

- A galactic dynamics model [6]. This problem is a Hamiltonian problem with coordinates q_1, q_2, q_3 and momenta p_1, p_2, p_3. The Hamiltonian function for this problem and the initial conditions have been fixed to obtain $\mathcal{H} = 2$) are

$$\mathcal{H} = \frac{1}{2}\,(p_1^2 + p_2^2 + p_3^2) + \Omega\,(p_1\,q_2 - p_2\,q_1) + A\,\ln\left(C + \frac{q_1^2}{a^2} + \frac{q_2^2}{b^2} + \frac{q_3^2}{c^2}\right),$$

$$\begin{cases} a = 1.25, \quad b = 1, \quad c = 0.75 \quad A = 1, \quad C = 1, \quad \Omega = 0.25, \\ q_1(0) = 2.5, \quad q_2(0) = q_3(0) = 0, \\ p_1(0) = 0, \quad p_2(0) = \dfrac{1}{40}\left(25 + \sqrt{6961 - 3200\,\ln 5}\right), \quad p_3(0) = 0.2. \end{cases}$$

In the figure 2 we present the spatial evolution of the coordinates q_1, q_2, q_3 for $t \in [0, 10000]$. On the figures on the bottom we show the errors in the energy for different tolerance levels. In all the tests we have used the VO formulation.

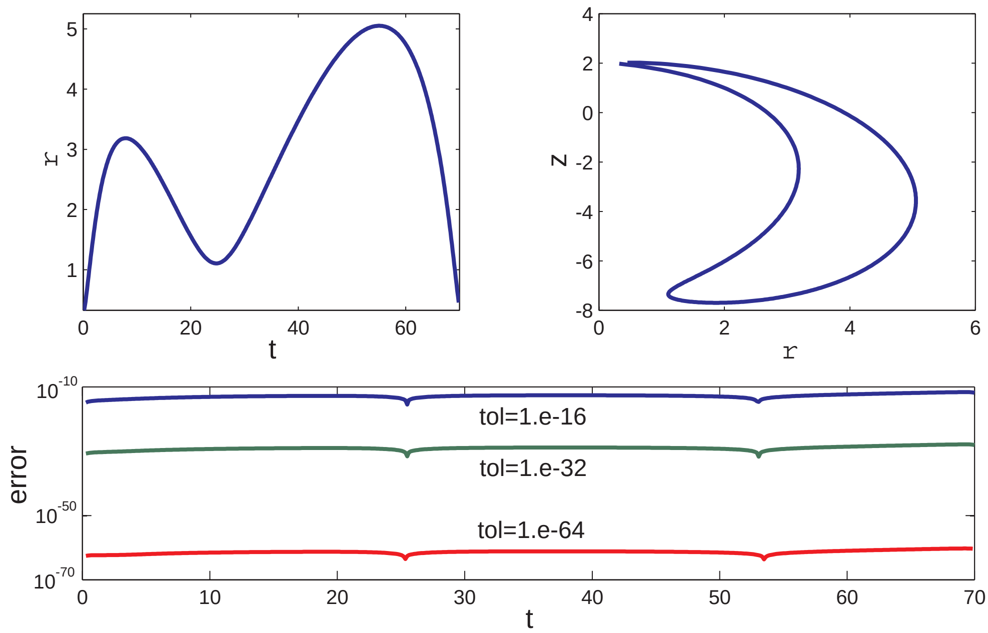

Figure 3: Evolution of the cylindrical coordinates ρ, z of the main problem problem and the errors in the ρ coordinate by considering different precision levels.

- The main problem in artificial satellite theory. Due to the axial symmetry, the problem accepts the polar component Λ of the angular momentum as integral. Other parameters of the problem are the gravitational constant μ of the planet, the oblateness coefficient J_2 and the scaling factor α that is the equatorial radius of the planet. The Hamiltonian function in cylindrical coordinates is

$$\mathcal{H} = \frac{1}{2}\,(P^2 + \frac{\Lambda^2}{\rho^2} + Z^2) - \frac{\mu}{r} + \frac{\alpha^2\,J_2\,\mu\,P_2(u)}{r^3}$$

where $u = z/r$, $r = \sqrt{\rho^2 + z^2}$ and $P_2(x) = (3\,x^2 - 1)/2$ is the Legendre polynomial of degree 2. In the simulations we have used the initial values

$$\begin{aligned} \rho(0) &= 0.3 \qquad & z(0) &= 2. \\ P(0) &= 0. \qquad & Z(0) &= -1. \end{aligned}$$

In the figure 3 we present the evolution of the cylindrical coordinates ρ, z of the main problem problem and in the figure on the bottom the errors in the ρ coordinate by considering different precision levels. As above, in all the tests we have used the VO formulation and the final error are in the tolerance level.

4 Parallel implementation

It is important to remark that high-precision methods will need high-precision computations and, therefore, the computational effort is quite large. In this situation a parallel implementation can be very useful. In the generation of the Taylor series it is possible in some problems to group some subseries in a form suitable for parallel computers. In order to validate the results we have done several numerical tests on a Sun UltraSPARC-II with 4 processors of 480 MHz using Message Passing Interface (MPI) as parallel environment and using Fortran90.

Table 1: Time, speed-up S_p and efficiency E_p in the parallel solution of the Pleiades problem.

Time (seconds)	bits=16	32	64	128
1 processor	31.84	40.74	142.87	741.51
2 processors	20.02	24.98	80.09	406.39
4 processors	14.86	18.29	45.89	217.84
Speed-up (S_p)	bits=16	32	64	128
2 processors	1.59	1.63	1.78	1.82
4 processors	2.14	2.23	3.11	3.40
Efficiency (E_p)	bits=16	32	64	128
2 processors	0.78	0.82	0.89	0.91
4 processors	0.54	0.56	0.78	0.85

The parallel implementation of Taylor series is not an easy task. Moreover, in most of the situations it is not possible because for an efficient implementation we have to divide the Taylor series in almost equal independent parts. The number of communications among processors is high, we need, for a n degree Taylor method, $n+1$ communications in each integration step, one per each degree, in order to compute all the series. Therefore, this parallel alternative will only be interesting for high-precision demands.

In the Table 1 we present the running time with p processors (T_p), the speed-up $S_p = T_1/T_p$ and the efficiency $E_p = T_1/(p \cdot T_p)$ for a 4-star case of the Pleiades problem. Note that the efficiency tends to 1.

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