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Partitioned Linear Multistep Method for Long Term Integration of the N-Body Problem

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In this paper an exponential fitted partitioned linear multistep method is developed for the long term integration of the N-body problem. The new method integrates exactly any linear combination of the functions 1, x, x^2, x^3 ,..., x^{2k-1}, exp($\pm wx$) for the coordinates and any linear combination of the functions 1, x, x^2, x^3,..., x^{2k-3}, exp($\pm wx$) for the velocities. Numerical results are produced and compared with a set of well known symplectic and single step methods.

1 Introduction

A lot of effort has been given during the last years for the construction of numerical methods that improve the classical integration. Of special interest is the long-term integration of Hamiltonian systems (such as the propagation of planetary orbits), since it is essential that the discrete methods employed reproduce both qualitatively and quantitatively the underlying dynamics of the continuous system they are supposed to approximate. More precisely, these discrete methods must show the same asymptotic behavior and the same invariants as the exact solution of the problem. Symplectic integrators do conserve the symplectic form $dp \wedge dq$ but in general energy conservation is lost[1].

On the other hand, non symplectic methods, but with properties of symmetry, have been found very adequate for long term propagation of planetary orbits. Quinlan and Tremaine [2] developed high order symmetric multistep methods which although exhibit simplicity and accuracy, they suffer from resonances and instabilities, the origins of which are explained in a great detail by Quinlan [3].

Simos and Vigo-Aguiar [4] showed that exponential fitting, when it is used in symmetric multistep methods, improve the accuracy of the method, especially in long-term integration. Exponential fitting removes the problems that are related to phase-lag observed in methods with constant coefficients, but require an efficient estimation of the frequency of the problem. Simos [4] showed that if we have a general initial value problem of the form

$$y_i'' = -f_i y_i + ... \tag{1}$$

where f_i, i=1(1)M are the coefficients of y_i and M is the number of equations defined, the selection of $\omega_i = \sqrt{|f_i|}$, where ω_i are the frequencies of the problem, produce very accurate solutions.

In the case of propagation of planetary orbits, one can extract a partitioned system of differential equations (one for the coordinates and one for the momenta). In such cases, it has been found that the use of two different methods (partitioned) can overcome instabilities observed when a single method is applied to both equations [5]. A sufficient condition to obtain this in case of linear multistep methods, is that the characteristic polynomials of both applied methods have distinct single roots, except for 1, as we shall see in the later.

In this work, the systematic construction of a partitioned multistep method with exponential fitting is presented. The order of the method can be increased arbitrary. In section 2, we give all the details of the construction as well as the calculation of the local truncation error of the new method. In section 3, we study the stability of the new

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method, when it is applied in the integration of the outer solar system. Numerical results are presented in section 3. The results are compared with a set of well known methods (both symplectic and non symplectic).

2 Construction of the new method

Consider the following partitioned multistep method:

$$\sum_{j=0}^{2k+1}(-1)^{j+1}q_{n+j}=h\sum_{j=0}^{2k}b_jq'_{n+j} \tag{2}$$

for the coordinates and:

$$\sum_{j=0}^{2k-1}(-1)^{j+1}p_{n+j}=h\sum_{j=0}^{2k-2}c_jp'_{n+j} \tag{3}$$

for the momenta. In the above equations, q_{n+j} and p_{n+j} are the estimations of the exact solutions $q(t)$ and $p(t)$ at the time $t=(n+j)h$, where h is the step of the method and q'_{n+j} and p'_{n+j} their corresponding derivatives. The characteristic polynomials of the above methods are:

$$\begin{array}{c}\varrho(z)=\sum_{j=0}^{2k+1}(-1)^{j+1}z^j=\frac{(-z)^{2k+2}-1}{z+1}\\ \hat{\varrho}(z)=\sum_{j=0}^{2k-1}(-1)^{j+1}z^j=\frac{(-z)^{2k}-1}{z+1}\end{array} \tag{4}$$

and their corresponding roots are:

$$\begin{array}{c}z=e^{i\frac{n}{k+1}\pi},n=0..2k+1,n\neq k+1\\ \hat{z}=e^{i\frac{n}{k}\pi},n=0..2k-1,n\neq k\end{array} \tag{5}$$

Both groups of unknown coefficients (i.e. $b_j, j=0(1)2k+1$ and $c_j, j=1(1)2k-1$) are calculated in the same way. Below we shall present the calculation of b_j' s. The coefficients c_j' s are calculated by simply replacing k with $k-1$. Consider now the function $L(q(t),h)$ given by:

$$L(q(t),h)=\sum_{j=0}^{2k+1}(-1)^{j+1}q(t+jh)-h\sum_{j=0}^{2k}b_jq'(t+jh) \tag{6}$$

Substituting $q(t+jh)$ and $q'(t+jh)$ with their Taylor expansions, we get the following power series for $L(q(t),h)$:

$$L(q(t),h)=\sum_{s=0}^{\infty}C_sq^{(s)}(t)h^s \tag{7}$$

where

$$C_0=\sum_{j=0}^{j=2k+1}(-1)^j=0 \tag{8}$$

and

$$C_s=\frac{1}{s!}\sum_{j=1}^{2k+1}(-1)^{j+1}j^s-\frac{1}{(s-1)!}\sum_{j=0}^{2k}b_jj^{s-1} \tag{9}$$

In order that the method in (2) integrates exactly the function t^m, then $C_0,C_1,...,C_m$ must vanish. In this way, $2k-1$ equations for b_j's can be extracted. The rest two equations for fully determine b_j's can be extracted by the demand that the method (2) integrates exactly the functions exp($\pm iwx$). This gives:

$$\sum_{j=0}^{2k}iue^{iju}b_j=\sum_{j=0}^{2k+1}(-1)^{j+1}e^{iju} \tag{10}$$

and

$$\sum_{j=0}^{2k} iue^{-iju} b_j = \sum_{j=0}^{2k+1} (-1)^j e^{-iju} \tag{11}$$

where $u = wh$. Substituting the calculated values for b_j's in equation (4), the local truncation error of the method is given by:

$$LTE = A_k(q^{(2k+2)} + w^2 q^{(2k)})h^{2k+2} + 0(h^{2k+3}) \tag{12}$$

where the coefficient A_k can be calculated from the Taylor expansion of b_j's considered as functions of h. These two methods will be used in numerical tests. Notice here that, the determinant of the system of equations that give the coefficients, vanishes when $u = 0$. This may lead to heavy cancellations when the frequency w of the problem (in fact the quantity $u = wh$) is too small. In order to avoid this, we have to use the Taylor expansions of the coefficients, considered as functions of u.

3 Stability analysis

It is clear that both methods for coordinates and momenta are stable. In fact, all roots of the characteristic polynomial are simple and are located on the unit circle. In order to account for the stability of the partitioned method, we present the following theorem:

Theorem 3.1 *The partitioned method (2)-(3) is stable if the corresponding characteristic polynomials have no common roots except for 1.*

P r o o f. In order to account for the stability of the partitioned method, we derive some basic results from the theory of general linear multistep methods. For details we refer to chapter 4 of [6] and chapter III of [7]. Consider a differential equation of the form

$$\dot{y} = f(y) \tag{13}$$

A general explicit linear multistep method for solving (13) can be written as:

$$\begin{array}{l} Y_{n+1} = DY_n + hFf(\hat{Y}_{n+1}) \\ \bar{Y}_{n+1} = GY_n + hAf(\hat{Y}_{n+1}) \end{array} \tag{14}$$

where $Y_n := (y_{n+k-1}, ..., y_n)^T$, $\hat{Y}_{n+1} = (y_{n+k}, ..., y_n)^T$ and y_n is the approximate value of $y(x + nh)$. The matrices D and F are given by:

$$D = \begin{pmatrix} -a_{k-1} & -a_{k-2} & ... & -a_0 \\ 1 & 0 & ... & 0 \\ & : & & : \\ & & 1 & 0 \end{pmatrix}, \quad F = \begin{pmatrix} 0 & \beta_{k-1} & ... & \beta_0 \\ 0 & 0 & ... & 0 \\ : & : & & : \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{15}$$

and the matrices G and A:

$$G = \begin{pmatrix} & & D & & \\ 0 & 0 & ... & 0 & 1 \end{pmatrix}, A = \begin{pmatrix} B \\ 0 \end{pmatrix} \tag{16}$$

The eigenvalues of the matrix D are exactly the roots of the characteristic polynomial of the linear method. Since we are concerned for weakly stable methods, $D^k = I$. Consider now the composition of k consequtive steps (with step size h/k) as a new method. This is again a linear method

$$\begin{array}{l} Y_{n+1} = Y_n + hBf(\hat{Y}_{n+1}) \\ \hat{Y}_{n+1} = CY_n + hEf(\hat{Y}_{n+1}) \end{array} \tag{17}$$

where

$$B = \frac{1}{k}(D^{k-1}F, D^{k-2}F, ..., DF, F)$$

$$C = \begin{pmatrix} G \\ GD \\ : \\ GD^{k-1} \end{pmatrix}$$

$$E = \frac{1}{k}\begin{pmatrix} A & & & \\ GF & A & & \\ : & & & \\ GD^{k-2}F & GD^{k-3} & ... & A \end{pmatrix}$$

Notice that the method (17) is a single step method, so if we replace the second equation of (17) for $\hat{Y}$ in the first and taking the limit $h \to 0$, it follows that the method is consistent with the "augmented differential equation"

$$\dot{Y} = Bf(CY) \tag{18}$$

Consider now again the method (2). The results are the same for the method (3) if we replace k with k-1. We have

$$D^j = \begin{pmatrix} 0_{j-1} & & & I_{j-1} \\ 1 & -1 & ... & -1 \quad 1 \\ I_{2k-j} & & & 0_{2k-j} \end{pmatrix} \tag{19}$$

where I_p is the identity matrix with p rows and 0_p is the zero matrix with p rows. Then

$$D^j F = \begin{pmatrix} & & 0_{j-1} & & \\ 0 & \beta_{2k} & ... & \beta_1 & \beta_0 \\ 0 & \beta_{2k} & ... & \beta_1 & \beta_0 \\ & & 0_{2k-j} & & \end{pmatrix} \tag{20}$$

Consider now the vector $e = (1, 1, ...1)^T$. Then

$$De = e, Ce = e \tag{21}$$

and

$$Be = \frac{1}{2k+2}\left(2\sum_{j=0}^{j=2k}\beta_j\right)e = e \tag{22}$$

from the consistency of the method. Then, if $y(t)$ is a solution of (13), the vector $Y = ey(t)$ is a solution of (18) since

$$Bf(CY) = Bf(Cey(t)) = Bef(y(t)) = ef(y(t)) = e\dot{y}(t) = \dot{Y}$$

Consider now the outer solar system. The Hamiltonian of the system is

$$H(q,p) = \frac{1}{2}\sum_{i=0}^{5}\frac{1}{m_i}{p_i}^T p_i - \frac{1}{2}G\sum_{i=0}^{5}\sum_{j=0,j\neq i}^{5}\frac{m_i m_j}{\|q_i - q_j\|} \tag{23}$$

and the partitioned system of differential equations is

$$\dot{p}_r = g_r(q), \quad \dot{q}_r = f_r(p) \tag{24}$$

where

$$g_r(q) = -Gm_r \sum_{i=0, i\neq r}^{5} m_i \frac{q_r - q_i}{\|q_r - q_i\|^3}, \quad f_r(p) = \frac{p_r}{m_r} \tag{25}$$

We can extend now the above result to a general explicit partitioned method of the type

$$\begin{aligned} Q_{n+1} &= DQ_n + hFf(V_{n+1}) \\ P_{n+1} &= \hat{D}P_n + h\hat{F}g(U_{n+1}) \end{aligned} \tag{26}$$

which is consistent with the "partitioned augmented differential equation"

$$\dot{Q} = Bf(\hat{C}P), \quad \dot{P} = \hat{B}g(CQ) \tag{27}$$

Notice here that there is an integer m such that $D^m = I$ and $\hat{D}^m = I$. We linearize the above system of equations around $Q(t) = eq(t)$ and $P(t) = \hat{e}p(t)$, and consider the variational equation

$$\begin{aligned} d\dot{Q} &= B\hat{C}f_p(q,p)dP \\ d\dot{P} &= \hat{B}Cg_q(q,p)dQ \end{aligned} \tag{28}$$

Let now λ_j, w_j, w_j^* be the eigenvalues and (right and left) eigenvectors of D and $\hat{\lambda}_j, \hat{w}_j, \hat{w}_j^*$ the eigenvalues and (right and left) eigenvectors of $\hat{D}$. All λ's and $\hat{\lambda}$'s are distinct and $\lambda_j \neq \hat{\lambda}_i$ except for $\lambda_1 = \hat{\lambda}_1 = 1$. Observe that from the definition of B and $\hat{B}$ it follows that

$$w_j^* B\hat{C}\hat{w}_i = \frac{1}{m} w_j^* F\hat{w}_i \lambda_j^{-1} \sum_{l=0}^{m-1} \left(\frac{\hat{\lambda}_i}{\lambda_j}\right)^l = \nu\delta_{j1}\delta_{i1} \tag{29}$$

and

$$\hat{w}_j^* \hat{B}Cw_i = \frac{1}{m} \hat{w}_j^* \hat{F}w_i \hat{\lambda}_j^{-1} \sum_{l=0}^{m-1} \left(\frac{\lambda_i}{\hat{\lambda}_j}\right)^l = \kappa\delta_{j1}\delta_{i1} \tag{30}$$

since $\lambda^m = \hat{\lambda}^m = 1$ and thus the sum in the above equations vanishes except for the case $i = j = 1$. The general solution of (28) can be written

$$(dQ)(t) = \sum_{j=1}^{2k+1} \eta_j(t) w_j, (dP)(t) = \sum_{j=1}^{2k-1} \zeta_j(t)\hat{w}_j \tag{31}$$

If we take now the derivatives of the above relations and multiply (28) from left with w_j ($\hat{w}_j$) we find

$$\begin{aligned} \dot{\eta}_1 &= \nu f_p(q,p)\zeta_1 \\ \dot{\zeta}_1 &= \kappa g_q(q,p)\eta_1 \\ \dot{\eta}_j &= 0, j \neq 1 \\ \dot{\zeta}_j &= 0, j \neq 1 \end{aligned} \tag{32}$$

which are stable equations (the first two of them constitutes the variational equations of the outer solar system, which is supposed to be stable, while the other two are trivially stable). Summarizing, we have found that the augmented partitioned differential equations (which are consistent with our method) are stable and thus the stability of our method is guaranteed.

□

4 Numerical results

The method is tested in the integration of the outer soloar system. Initial values obtained from [7]. Masses are relative to the sun, so that the sun has mass 1. We have taken $m_{sun} = 1.00000597682$ to take account for the inner planets. Distances are in astronomical units (1A.U.=149597 870 km), times in earth days and the gravitational constant $G = 2.95912208286 \cdot 10^{-4}$. Initial values correspond to September 5, 1994 at 0h00 [5]. The new method was tested in two versions (PEFM2 with k=2 and PEFM3 with k=3) with four other methods i.e. the symplectic Euler, the implicit midpoint, the Bulirsch-Stoer [8] and the fourth order symplectic Neri-Candy-Rozmus [9]. Since there is no reference exact solution, the comparison was based on the error produced by each method to the energy and the angular momentum of the outer solar system as a function of computational time needed for each method. The integration time was 200,000 earth days.

Figure 1 shows the maximum error in total energy ($|E - E_0|/|E_0|$ where E is the total energy and E_0 is the total initial energy). The method PEFM3 is about three times faster from the Bulirsch-Stoer one and more than one order of magnitude faster from the other methods. Notice here that one of the major advantages of our method is that the computational cost produced by increasing k is very small, since in every step of our method, only one derivative is calculated. The additional computational time produced by increasing k is limited to shift operations and the computation of the coefficients of the method (from complicated trigonometric functions). This can be handled efficiently by calculating only two of the coefficients by the trigonometric relations (ie b_{2k} and b_{2k-1}), while the other coefficients can be calculated by simple algebraic expression (as functions of b_{2k} and b_{2k-1}).

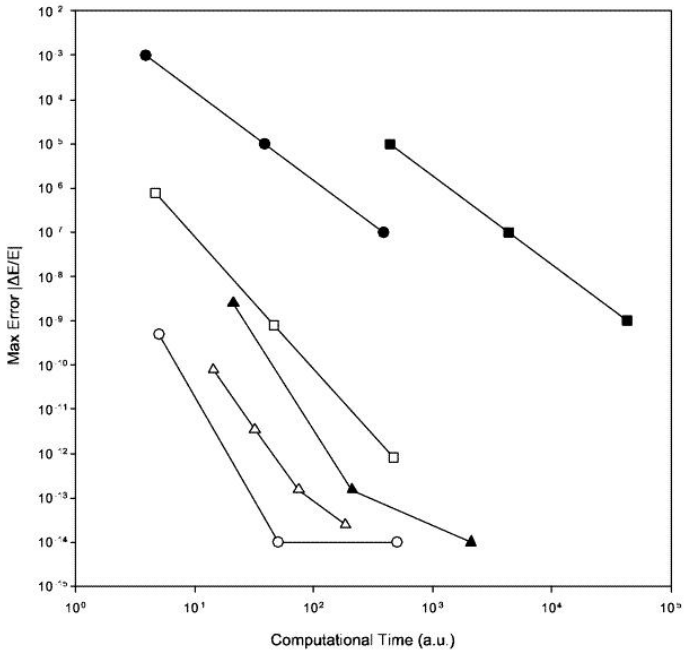

Fig. 1 Maximum error in total energy for integration of the outer solar system for 200,000 days. empty square-PEFM2, empty circle-PEFM3, solid circle-Symplectic Euler, solid square-Implicit Midpoint, empty triangle-Bulirish-Stower, solid triangle-Nery-Candy-Rozmus.

5 Conclusions

In this paper, a partitioned multistep method with exponential fitting was developed for the long-term integration of the outer solar system. We have given explicitly the way for the construction of the new method, the order of which can be increased arbitrarily. Stability analysis is also presented. Numerical examples indicate that the

new method is more efficient as far as the energy conservation of the outer solar system is concerned, than well known methods used for long-term integration of orbital problems, both symplectic and non symplectic.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

References

[1] Z. Ge and J.E. Marsden, Phys. Lett. A, **133**, 134 (1988).
[2] G.D. Quinlan and S. Tremaine, Astronomical Journal, **100**, 1694 (1990).
[3] G.D. Quinlan, astro-ph/9901136, (1999).
[4] T.E. Simos and J. Vigo-Aguiar, Computer Physics Communications, **140**, 358 (2001).
[5] E. Hairer, C. Lubich and G. Wanner, Geometric Numerical Integration, Structure-Preserving Algorithms for Ordinary Differential Equations, Springer Series in Computational Mathematics, Vol. 31 Springer, Berlin (2002).
[6] J.C. Butcher, The Numerical Analysis of Ordinary Differential Equations, Wiley, New York (1987).
[7] E. Hairer, S.P. Nørsett and G. Wanner, Solving Ordinary Differential Equations I. Nonstiff Problems, Springer Series in Computational Mathematics, Vol. 8, Springer-Verlag Second revised edition (1993).
[8] J. Stoer and R. Bulirsch, Introduction to Numerical Analysis,
[9] F.J. Vesely, Computational Physics - An Introduction, Kluwer-Plenum (2001). New York: Springer-Verlag (1980).