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Clean numerical simulation for some chaotic systems using the parallel multiple-precision Taylor scheme

Pengfei Wang · Yong Liu · Jianping Li

Abstract An improved parallel multiple-precision Taylor (PMT) scheme is developed to obtain clean numerical simulation (CNS) solutions of chaotic ordinary differential equations (ODEs). The new version program is about 500 times faster than the reported solvers developed in the MATHEMATICA, and also 2–3 times faster than the older version (PMT-1.0) of the scheme. This solver has the ability to yield longer solutions of Lorenz equations [up to 5000 TU (time unit)]. The PMT-1.1 scheme is applied to a selection of chaotic systems including the Chen, Rossler, coupled Lorenz and Lü systems. The T_c-M and T_c-K diagrams for these chaotic systems are presented and used to analyze the computation parameters for long-term solutions. The reliable computation times of these chaotic equations are obtained for single- and double-precision computation.

Keywords Taylor scheme · Parallel multiple-precision computation · Chaotic dynamic systems

P. Wang (✉) · Y. Liu
Center for Monsoon System Research, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100190, China
e-mail: wpf@mail.iap.ac.cn

P. Wang · J. Li
State Key Laboratory of Numerical Modeling for Atmospheric Sciences and Geophysical Fluid Dynamics, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100029, China

1 Introduction

Obtaining the true trajectories of chaotic dynamical systems by numerical approaches is not an easy task. Researchers [1–3] have reported that numerical methods can provide approximate trajectories close to reality by applying Riemannian manifolds theory [4]. However, a remaining problem is how well and how long the numerical trajectory approximates the real one [5]. Many studies have documented the sensitivities of computation parameters for numerical solutions of chaotic equations [6–11], and indicate that, in spite of there being no initial errors, the computation is still limited by the maximal effective computation time (T_c) due to round-off error. Li et al. [7] carried out systematic investigations on these phenomena for nonlinear ordinary differential equations (ODEs), by employing numerical experiments and analytical way, and put forward the computational uncertainty principle (CUP). The sensitivity of computed results for chaotic systems is important. For example, previous results [6, 9, 10] have indicated that the maximal effective computation time is approximately 35 LTU (Lorenz time unit) for Lorenz equations under double precision. Nevertheless, studies are still needed to carry out theoretical analyses of data for computation times of longer than 35 LTU. It is important to design a difference solver to provide the correct solution for times beyond 35 LTU, which is the situation for many types of chaotic system [12].

The existence of T_c indicates that if we need the solution of $t = 1000$, single- and double-precision computers are insufficient. In order to overcome the shortcomings of computation precision, a suite of multiple-precision (MP) software [13, 14] has been developed. This library can provide user-defined floating-point precision in the

computation; the similar reliable mathematical libraries are supported by some software such as MAPLE, MATH-EMATICA, and MATLAB. Using MP, it is possible to choose a sufficiently high precision level with a certain step size h to maintain round-off errors that are negligible compared with the truncation error. In such cases, the total computation error is derived mainly from truncation errors. Wang et al. [15] and Liao [10] have shown these MP libraries to solve Lorenz equations, demonstrating that high precision is valuable in terms of obtaining correct numerical solutions.

The effective way to control truncation error is by applying a higher-order method (e.g., the Taylor method) to solve ordinary differential equations (ODEs). A benefit of the Taylor method is that it can easily develop a higher order by applying Moore's method [16, 17] to repeatedly calculate the Taylor coefficients. Barrio [18] studied general issues when applying the Taylor method to ODEs, and analyzed the convergence properties of the method. Liao [10] proposed the "clean numerical simulation" (CNS) method, in which a 400-order Taylor method with 800 significant digits in MATHEMATICA was used to obtain reliable results up to 1100 LTU. However, MATHEMATICA needed around 1 month to finish the computation. Recently, Liao [19] presented a thorough study of the transfer of physical uncertainties in chaotic systems by CNS, and also demonstrated [10, 19, 20] a way to obtain the relation of T_c and the order (M) of the Taylor method. Meanwhile, Barrio et al. [21] used the Taylor method to study Lorenz equations, Kepler systems and Henon–Heiles systems [22], and their results indicated, for a certain predefined time t, the method can obtain highly precise numerical solutions. Kehlet and Logg [23] also gained a reliable chaotic solution of Lorenz equation on the time interval [0, 1000] by applying the 200-order finite element method with 400-digits precision. Therefore, reliable, convergent chaotic results of Lorenz equation can be obtained by two different types of numerical approaches.

Operationally, obtaining long-term numerical solutions for chaotic dynamic systems not only depends on the precision and step size of the difference method, but is also depend on the time cost of the solution process. Wang et al. [24] compared the time cost of a 4-order Runge–Kutta (RK4) method and Taylor method, and their analysis clearly indicated higher-order methods can decrease computation time exponentially, and are thus more effective. Nevertheless, this higher-order Taylor method is still time-consuming, and while it works with very high precision, it is a feature that makes the application of this method to chaotic systems less attractive. Wang et al. [24] proposed the parallel multiple-precision

(PMT) scheme to reduce the computation time and managed to achieve an acceptable improvement. Moreover, the final computation result should be reliably validated. In this study, the validation scheme used in Ref. [24] is applied.

In this study, we propose an improved version of the PMT scheme and analyze its efficiency, and then apply the method to some classical chaotic systems. In applying the PMT method, each system's maximal effective computation time (MECT) is investigated for double and single precision. The reference reliable long-term solutions of the systems are listed in the electric supplementary material.

2 The improved parallel multiple-precision Taylor scheme and its performance

Here, we demonstrate the improved PMT scheme by solving Lorenz's [25] equation

$$
\begin{cases}
\dfrac{dx}{dt} = -\sigma x + \sigma y, \\[4pt]
\dfrac{dy}{dt} = Rx - y - xz, \\[4pt]
\dfrac{dz}{dt} = xy - bz,
\end{cases}
\tag{1}
$$

where R, σ, b ($R = 28.0$, $\sigma = 10.0$, $b = 8/3$) are constants, and t is a nondimensional time. The truncated Taylor scheme at p-order ($p \equiv M$) with step size h is

$$
\begin{cases}
x_{n+1} = x_n + \sum_{k=1}^{p} \alpha_k h^k, \\[4pt]
y_{n+1} = y_n + \sum_{k=1}^{p} \beta_k h^k, \\[4pt]
z_{n+1} = z_n + \sum_{k=1}^{p} \gamma_k h^k,
\end{cases}
\tag{2}
$$

where $\alpha_k = \frac{1}{k!}\frac{d^k x(t_n)}{dt^k}$, $\beta_k = \frac{1}{k!}\frac{d^k y(t_n)}{dt^k}$ and $\gamma_k = \frac{1}{k!}\frac{d^k z(t_n)}{dt^k}$ are k-th Taylor coefficients. According to Moore [16, 17], Barrio et al. [18] and Liao [10], the coefficients can be calculated by a recurrence procedure. The initial coefficients are

$$
\begin{cases}
\alpha_0 = x_n, \\
\beta_0 = y_n, \\
\gamma_0 = z_n;
\end{cases}
$$

then, by applying the relation from Eq. (1), the first steps of α_k, β_k and γ_k are

$$
\begin{cases}
\alpha_1 = -\sigma \alpha_0 + \sigma \beta_0, \\
\beta_1 = R\alpha_0 - \beta_0 - \alpha_0 \gamma_0, \\
\gamma_1 = \alpha_0 \beta_0 - b\gamma_0,
\end{cases}
$$

and the ($k+1$)-th coefficients are

$$\begin{cases} \alpha_{k+1} = \dfrac{1}{k+1}(-\sigma\alpha_k + \sigma\beta_k), \\[2mm] \beta_{k+1} = \dfrac{1}{k+1}\left(R\alpha_k - \beta_k - \sum_{i=0}^{k}\alpha_{k-i}\gamma_i\right), \\[2mm] \gamma_{k+1} = \dfrac{1}{k+1}\left(\sum_{i=0}^{k}\alpha_{k-i}\beta_i - b\gamma_k\right). \end{cases} \quad (3)$$

The relation in Eq. (3) indicates that each α_{k+1}, β_{k+1} and γ_{k+1} is computed from the previous α_k, β_k and γ_k. Thus, the computation procedure is more like an explicit scheme, and will save much computation time.

The parallel scheme of Wang et al. [24] is regarded as version 1.0, and in this paper we propose a new coefficient computation method and parallel scheme as version 1.1. The time cost for this Taylor scheme is depend on the computation time of α_k, β_k and γ_k; when computing the solution from the n-th step to the $(n+1)$-th step, the coefficient α_k needs $3p$ float-point operations (here, operations including multiplication and division), while β_k needs $2p + \frac{p(p+1)}{2}$ operations and γ_k needs $2p + \frac{p(p+1)}{2}$ operations, the total of computation times are $7p + p(p+1)$. The computation time cost thus following $T_w \propto p^2$, and therefore parallel scheme is useful for improving the performance.

From Eq. (3), we have a time cost of p^2, but the computation of β_{k+1}, which sums items in $\sum_{i=0}^{k}\alpha_{k-i}\gamma_i$, can be separate it to N CPUs for parallel computation. Each CPU will carry out $\frac{p(p+1)}{2N}$ operations when summing the items in $\sum_{i=0}^{k}\alpha_{k-i}\gamma_i$, and now the total computation time become $T_w \propto p^2/N$. Since the communication speed limited by hardware, the parallel efficiency is generally under 100 %. Table 1 summarizes the performance results for PMT-1.1.

Using the improved PMT scheme, it has the ability to compute the reliable solution for $t = 1200$ within 0.8 h, and this speed is 500 times faster than that reported by L09, and is also 2–3 times faster than version 1.0 of the PMT scheme. Moreover, this new parallel scheme uses less computer memory, and thus we can carry out more complex computations than with the old version. The reliable solutions up to $t = 5000$ are listed in Table S1 (online).

Table 1 Performance of PMT-1.1 for Lorenz equations ($t = 1200$, $K = 2666$, $p = 400$)

CPU	V1.1 time (h)	V1.0 time (h)	L09 time(h)
1	9.98	32.91	461
5	2.23	7.52	–
10	1.33	4.13	–
20	1.13	2.46	–
50	0.83	1.48	–

3 Application of the PMT method to solve some classical chaotic systems

3.1 Chen system

Chen et al. [26] found a chaotic system defined by

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = -ax + ay, \\[2mm] \dfrac{\mathrm{d}y}{\mathrm{d}t} = (c-a)x + cy - xz, \\[2mm] \dfrac{\mathrm{d}z}{\mathrm{d}t} = xy - bz, \end{cases} \quad (4)$$

where $a = 35$, $b = 3$, $c = 28$, and the initial values are $(x_0, y_0, z_0) = (-3, 2, 20)$.

Applying the PMT scheme to solve this equation, the Taylor coefficient recurrence formulas are

$$\begin{cases} \alpha_0 = x_n, \\ \beta_0 = y_n, \\ \gamma_0 = z_n, \end{cases} \begin{cases} \alpha_{k+1} = \dfrac{1}{k+1}(-a\alpha_k + a\beta_k), \\[2mm] \beta_{k+1} = \dfrac{1}{k+1}\left((c-a)\alpha_k + c\beta_k - \sum_{i=0}^{k}\alpha_{k-i}\gamma_i\right), \\[2mm] \gamma_{k+1} = \dfrac{1}{k+1}\left(\sum_{i=0}^{k}\alpha_{k-i}\beta_i - b\gamma_k\right). \end{cases}$$

We can obtain the relation of maximal computation time versus order ($T_c - M$ diagram), while keeping the precision K ascertained value (e.g., $K = 666$ bits, $M = 20$–100, interval 10). In a similar procedure, we can obtain the relation of maximal computation time versus precisions ($T_c - K$ diagram) with $M = 32$, $K = 50$–200 and interval 10.

Figure 1a indicates that if we want to obtain a reliable solution of the Chen equation to 1000 TU, a 1000-order Taylor method is necessary. At the same time, Fig. 1b tells us the computation must have precision of at least 3000 bits. By analyzing the diagrams of $T_c - M$ and $T_c - K$ we can obtain the necessary computation parameter for chaotic dynamic systems, and this procedure makes the reliable computation of chaotic dynamic systems operable. Table S2 (online) lists the reliable reference solutions of the Chen equation.

Table 2 lists the wall-clock times of the PMT method to solve the Chen equation with $t = 1000$ TU using different parameters. The three cases show that the parallel method provides valuable speed-up until the CPU number reaches 50. Moreover, when the computation workload increases (C>B>A), the speed-up increases from 12.1 to 30.0. This indicates the more computation workload there is, the more effective the parallel scheme.

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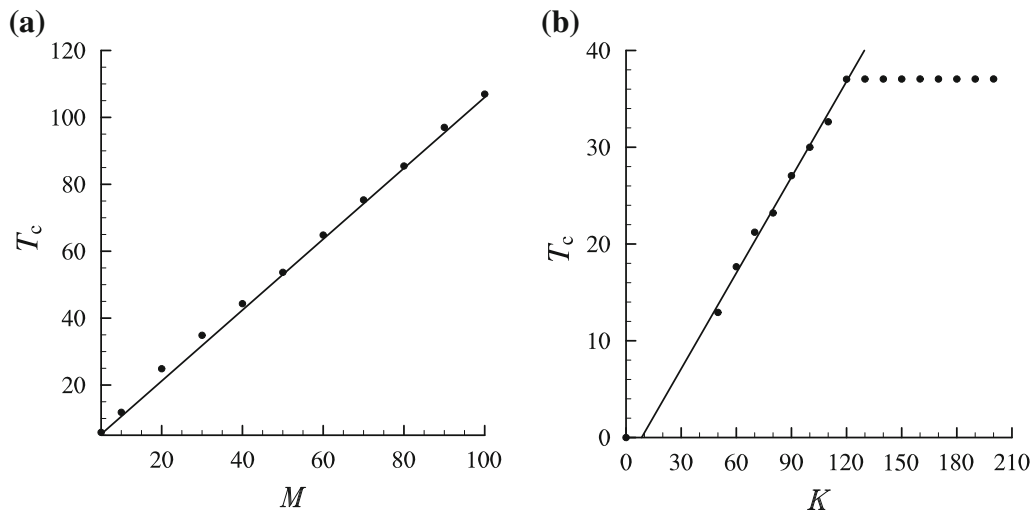Chin. Sci. Bull. (2014) 59(33):4465–4472

(a)

(b)

Fig. 1 (a) The $T_c - M$ diagram of the Chen equation, with $K = 666$; the line is $T_c = 1.06M$. (b) The $T_c - K$ diagram of the Chen equation, with $M = 32$; the line is $T_c = 0.33K - 2.8$. The unit of precision K is binary bits

Table 2 Performance of PMT-1.1 for Chen equations

CPU	A time (h)	B time (h)	C time (h)
1	9.05	88.81	152.85
5	2.19	18.65	32.00
10	1.21	9.81	16.65
20	0.87	5.62	9.25
50	0.75	3.30	5.08
Speedup	12.10	26.90	30.00

The parameters for case A are $t = 1000$, $K = 2666$, $M = 400$; for case B are $t = 1000$, $K = 3500$, $M = 1000$; and for case C are $t = 1000$, $K = 4000$, $M = 1200$

3.2 Rossler system

Rossler [27] chaotic systems are described by

$$\begin{cases} \dfrac{dx}{dt} = -y - z, \\ \dfrac{dy}{dt} = x + ay, \\ \dfrac{dz}{dt} = b + z(x - c), \end{cases} \qquad (5)$$

where $a = 0.2$, $b = 0.2$, $c = 5.7$, and the initial values are $(x_0, y_0, z_0) = (0, -6.78, 0.02)$.

The Taylor coefficient recurrence formulas for Eq. (5) are

$$\begin{cases} \alpha_0 = x_n, \\ \beta_0 = y_n, \\ \gamma_0 = z_n, \end{cases} \begin{cases} \alpha_{k+1} = \dfrac{1}{k+1}(-\beta_k - \gamma_k), \\ \beta_{k+1} = \dfrac{1}{k+1}(\alpha_k + a\beta_k), \\ \gamma_{k+1} = \dfrac{1}{k+1}\left(\sum_{i=0}^{k} \alpha_{k-i}\gamma_i - c\gamma_k\right). \end{cases}$$

Figures 2a and b indicate that if we want to obtain a reliable solution to the Rossler equation to 1000 TU, a 17-order Taylor method and 120-bits precision are necessary. Table S3 (online) lists the reliable reference solutions of the Rossler equation.

3.3 Coupled Lorenz system

Boffetta et al. [28] proposed a coupled Lorenz system when studying the predictability of different timescale systems. The equations are

$$\begin{cases} \dfrac{dx}{dt} = -ax + ay, \\ \dfrac{dy}{dt} = r_s x - y - xz - \varepsilon_s XY, \\ \dfrac{dz}{dt} = xy - bz, \\ \dfrac{dX}{dt} = c(-aX + aY), \\ \dfrac{dY}{dt} = c(r_f X - Y - XZ) + \varepsilon_f Xy, \\ \dfrac{dZ}{dt} = c(XY - bZ), \end{cases} \qquad (6)$$

where $a = 10$, $b = \frac{8}{3}$, $r_s = 28$, $r_f = 45$, $c = 10$; the coupled coefficients are $\varepsilon_s = 10^{-2}$, $\varepsilon_f = 10$; and the initial values are $(x_0, y_0, z_0) = (5, 5, 10)$ and $(X_0, Y_0, Z_0) = (5, 5, 10)$. The first three and last three equations of Eq. (6) are called slow and fast dynamic systems, respectively. Boffetta et al. [28] indicated that if the coupled coefficients are all 0, the slow and fast dynamic systems' maximal Lyapunov exponents are $\lambda_1^s = 0.905$ and $\lambda_1^f = 12.17$ respectively, and when coupled together it is $\lambda_1 = 11.5$.
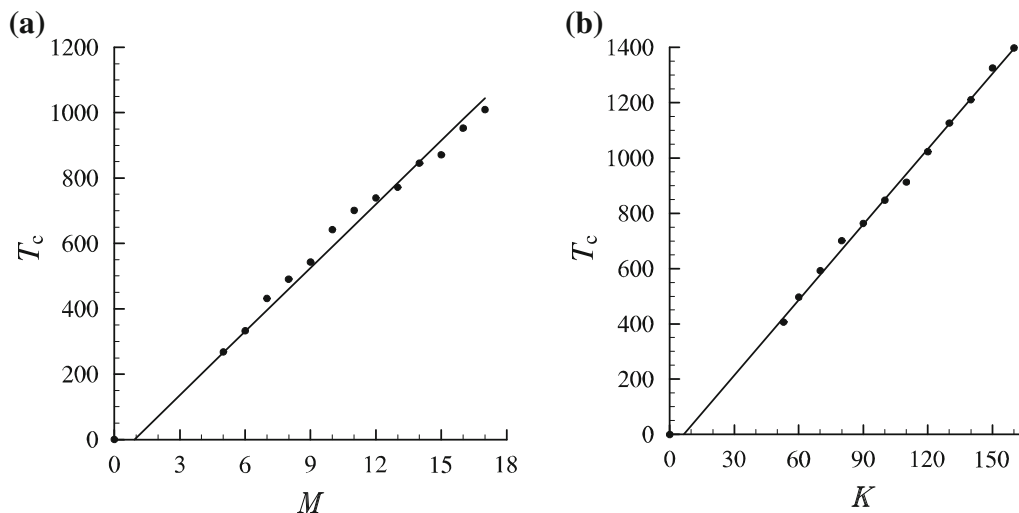
Fig. 2 The same as Fig. 1, but for the Rossler equation. (a) $T_c - M$ diagram with $K = 666$; the line is $T_c = 65M - 60$. (b) $T_c - K$ diagram with $M = 32$; the line is $T_c = 9.1K - 60$

The Taylor coefficients can be computed start with $\alpha_0 = x_n$, $\beta_0 = y_n$, $\gamma_0 = z_n$, $\alpha_0^f = X_n$, $\beta_0^f = Y_n$, $\gamma_0^f = Z_n$, and the recurrence formulas are

$$
\begin{cases}
\alpha_{k+1} = \dfrac{1}{k+1}(-a\alpha_k + a\beta_k), \\[2mm]
\beta_{k+1} = \dfrac{1}{k+1}\left(r_s\alpha_k - \beta_k - \displaystyle\sum_{i=0}^{k}\alpha_{k-i}\gamma_i\right) \\[2mm]
\qquad\quad - \dfrac{1}{k+1}\varepsilon_s\displaystyle\sum_{i=0}^{k}\alpha_{k-i}^f\beta_i^f, \\[2mm]
\gamma_{k+1} = \dfrac{1}{k+1}\left(\displaystyle\sum_{i=0}^{k}\alpha_{k-i}\beta_i - b\gamma_k\right), \\[2mm]
\alpha_{k+1}^f = \dfrac{c}{k+1}(-a\alpha_k^f + a\beta_k^f), \\[2mm]
\beta_{k+1}^f = \dfrac{c}{k+1}\left(r_f\alpha_k^f - \beta_k^f - \displaystyle\sum_{i=0}^{k}\alpha_{k-i}^f\gamma_i^f\right) \\[2mm]
\qquad\quad + \dfrac{1}{k+1}\varepsilon_f\displaystyle\sum_{i=0}^{k}\alpha_{k-i}^f\beta_i, \\[2mm]
\gamma_{k+1}^f = \dfrac{c}{k+1}\left(\displaystyle\sum_{i=0}^{k}\alpha_{k-i}^f\beta_i^f - b\gamma_k^f\right),
\end{cases}
$$

Figures 4a and b and Fig. 3a and b indicate that if we want obtain a reliable solution of the coupled Lorenz system to 1000 TU, a 5000-order Taylor method and 17000-bits precision are necessary. The coupled Lorenz system is more complex than the Lorenz equation and Chen equation; the computation (wall-clock) time is 10 times longer, and we only list the first 100 TU reliable solutions in Table S4 (online).

3.4 Lü system

Lü and Chen [29] discovered a chaotic system whose properties are between those of the Lorenz system and Chen system. This Lü equation is an important link between these two types of system in canonical Lorenz equation theory. The equations of the Lü system are

$$
\begin{cases}
\dfrac{dx}{dt} = -ax + ay, \\[2mm]
\dfrac{dy}{dt} = cy - xz, \\[2mm]
\dfrac{dz}{dt} = xy - bz,
\end{cases}
\tag{7}
$$

where $a = 36$, $b = 3$, $c = 20$, and the initial values are $(x_0, y_0, z_0) = (-3, 2, 20)$.

The Taylor coefficient recurrence formulas for Eq. (7) are

$$
\begin{cases}
\alpha_0 = x_n, \\
\beta_0 = y_n, \\
\gamma_0 = z_n,
\end{cases}
\quad
\begin{cases}
\alpha_{k+1} = \dfrac{1}{k+1}(-a\alpha_k + a\beta_k), \\[2mm]
\beta_{k+1} = \dfrac{1}{k+1}\left(c\beta_k - \displaystyle\sum_{i=0}^{k}\alpha_{k-i}\gamma_i\right), \\[2mm]
\gamma_{k+1} = \dfrac{1}{k+1}\left(\displaystyle\sum_{i=0}^{k}\alpha_{k-i}\beta_i - b\gamma_k\right).
\end{cases}
$$

Figures 5a and b indicate that if we want to obtain a reliable solution of the Lü system to 1000 TU, a 600-order Taylor method and 2000-bits precision are necessary. Table S5 (online) in the appendix lists the reliable reference solutions of the Lü equation.
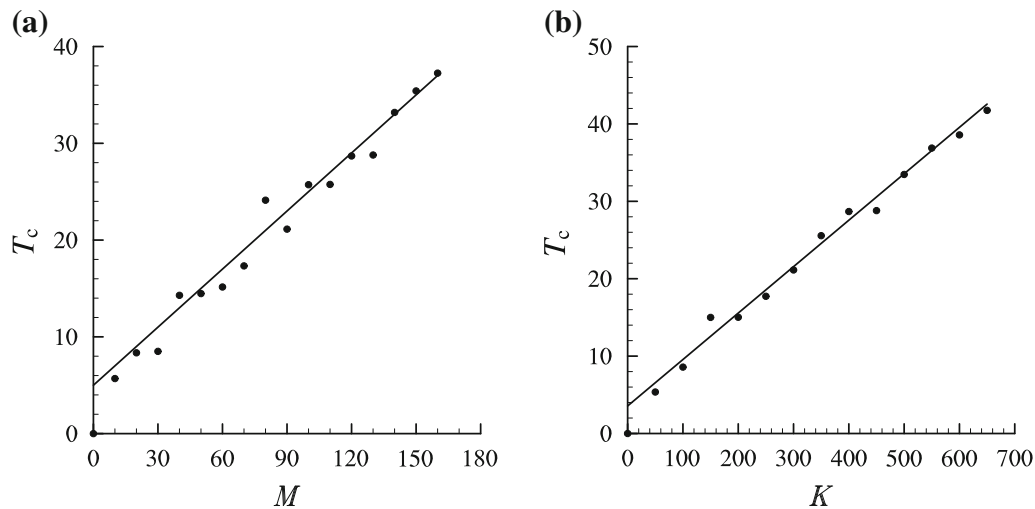
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Fig. 3 The same as Fig. 1, but for coupled Lorenz systems. (**a**) $T_c - M$ diagram for slow dynamics with $K = 666$; the line is $T_c = 0.2M + 5$. (**b**) $T_c - K$ diagram for slow dynamics with $M = 200$; the line is $T_c = 0.06K + 3.56$
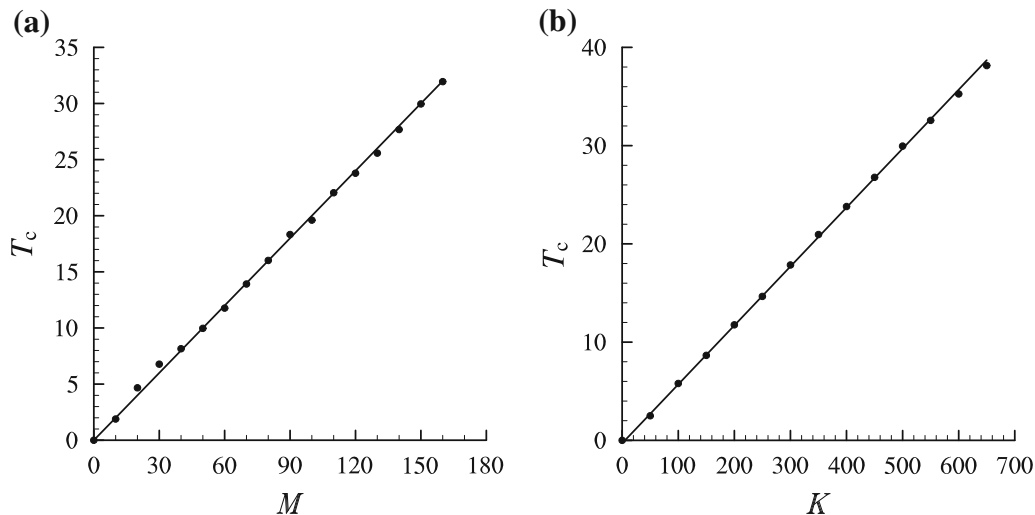

Fig. 4 The same as Fig. 3, but for fast dynamic systems. (**a**) $T_c - M$ diagram for fast dynamics with $K = 666$; the line is $T_c = 0.2M$. (**b**) $T_c - K$ diagram for fast dynamics with $M = 200$; the line is $T_c = 0.06K - 0.3$

4 Discussion and conclusion

An improved parallel multiple-precision Taylor (PMT) scheme based on Wang et al. [24] has been presented in this paper. The improved computation of the Taylor coefficients and less memory usage increase the computation speed, with results indicating the performance of the newer scheme is about 2–3 times faster than PMT-1.0.

Through applying the PMT scheme, we were able to complete reliable computation of the Chen equation, Rossler equation, Lü equation, and the coupled Lorenz system. Each of these chaotic systems possesses different properties, and the different maximal Lyapunov exponents in particular will cause numerical errors to increase at

different speeds. The PMT method obtains each system's $T_c - M$ and $T_c - K$ diagrams, and then obtains the reliable reference solutions for these systems. These reference solutions can be used to verify the user's numerical program. Moreover, through analysis the reference solutions, we can obtain the T_c of each chaotic system for single and double precision.

Table 3 list the effective computation time for the five chaotic systems. Compared with the Lorenz system, the T_c of the Chen system is much shorter (mainly caused by the properties of the chaotic system itself) and the numerical error accumulation is much faster. On the contrary, the T_c of the Rossler system is much longer than the Lorenz system, indicating the error does not increase as quickly,
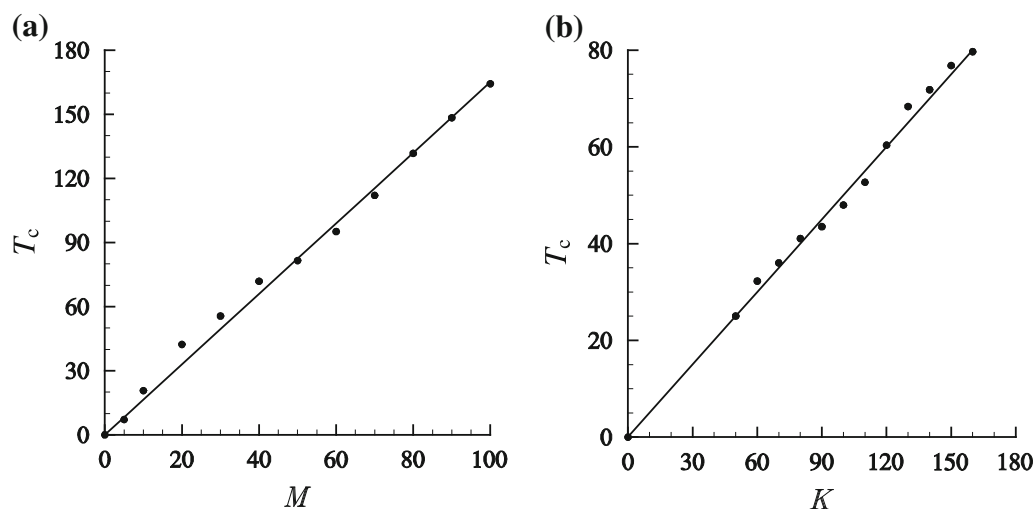
Fig. 5 The same as Fig. 1, but for the Lü system. (a) $T_c - M$ diagram for the Lü system with $K = 666$; the line is $T_c = 1.65M$. (b) $T_c - K$ diagram for the Lü system with $M = 100$; the line is $T_c = 0.5K$

Table 3 The effective computation time for each system

Chaotic system	T_c (single precision)	T_c (double precision)
Lorenz system	16.8	35.4
Chen system	6.3	14.6
Rossler system	136.6	406.6
Lü system	7.1	32.3
Coupled Lorenz system (slow dynamics)	5.3	5.7
Coupled Lorenz system (fast dynamics)	1.05	2.6

scheme is suitable for computation of the chaotic systems focused upon in the present paper, but the capacity of the PMT method is not only limited to these chaotic systems. The PMT scheme is not complex, but can obtain very precise computational results. Thus, it is a scheme with encouraging prospects for application.

and thus we can obtain the solution more easily. The performance of the Lü system is similar to the Chen system.

The coupled Lorenz system has a different T_c for slow and fast dynamics. It seems that, owing to the coupled process, the T_c for slow dynamics is much shorter than the uncoupled Lorenz system, while with fast dynamics the T_c is even shorter. The T_c values of these coupled systems are 1.05 TU and 2.6 TU, respectively. These small T_c values mean the general double-precision computer cannot obtain reliable solution longer than 2.6 TU, and thus analysis of this system and the conclusions drawn from it in terms of the predictability problem should pay attention to the numerical error.

The parallel performance of the improved PMT scheme has been demonstrated for the Lorenz and Chen systems, with the time cost and speed-up of many CPUs indicating the newer PMT scheme performs better than the older one. This parallel efficiency increase is even larger when computation with larger M and K is carried out. The PMT

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