

Error Control Strategy in Error Correction Methods

PHILSU KIM

Department of Mathematics, Kyungpook National University, Daegu 702-701, Korea

e-mail : `kimps@knu.ac.kr`

SUNYOUNG BU*

Institute for Mathematical Convergence, Kyungpook National University, Daegu 702-701, Korea

e-mail : `syboo@knu.ac.kr`

ABSTRACT. In this paper, we present the error control techniques for the error correction methods (ECM) which is recently developed by P. Kim et al. [8, 9]. We formulate the local truncation error at each time and calculate the approximated solution using the solution and the formulated truncation error at previous time for achieving uniform error bound which enables a long time simulation. Numerical results show that the error controlled ECM provides a clue to have uniform error bound for well conditioned problems [1].

1. Introduction

We consider numerical solutions for the ordinary differential equation (ODE) well conditioned initial value problem (IVP) [1]

$$(1.1) \quad \frac{d\phi}{dt} = f(t, \phi(t)), \quad t \in [t_0, t_f], \quad \phi(t_0) = \phi_0.$$

Many numerical techniques [2, 3, 12] have been developed for the accurate and efficient solution of the well conditioned IVPs, including linear multi-step methods,

* Corresponding Author.

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Runge-Kutta methods and operating splitting techniques, etc. In this paper, we present a technique to improve the efficiency of the error correction method (ECM) recently introduced by P. Kim, X. Piao, and S. Kim [8, 9, 10]. ECM is a variation on the deferred correction methods [3, 4] which allow for the construction of stable and extremely high order solutions and is designed to avoid the iteration process for nonlinear problems. To avoid the unnecessary iteration process, a deferred correction equation is converted to an asymptotical linear ODE based on the local platform. It turns out that ECM can have the excellent super-convergence $O(h^{2p+2})$ if one can make a local platform $y(t)$ to the true solution on each time step such that the local residual error $f(t, y(t)) - y'(t)$ has the asymptotic behavior $O(h^p)$, where p is any positive integer. Note that the p -stage implicit Runge-Kutta(RK) method can achieve the order of accuracy $2p$ (see [5]) and it requires solving a simultaneous system of equations at each time step by a costly Newton-type iteration.

The primary goal of this paper is to introduce an error control mechanism to improve its efficiency of ECM. There have been several approaches [6, 7, 11] to control numerical errors derived from existing numerical methods, such as adaptive time stepping, global error control and long time error estimation, etc. These approaches have a common framework to estimate the error and solution - the solution at each time is approximated by using the solution at the previous time step and the error is estimated only for controlling time step size to satisfy the stability region for a given method. In this paper, we propose a new technique to estimate the solution and the local truncation error at each time for achieving uniform error bound which enables a long time simulation. Unlike the existing mechanism to estimate the solutions and errors, the approximated solution ϕ_{m+1} at t_{m+1} is calculated by using both the approximated solution ϕ_m and the estimated error e_m at the previous time t_m . That is, an estimated error e_m at the previous step is needed to estimate the solution ϕ_{m+1} at the next step. In other words, for further approximations, we recursively need the estimation for a local truncation error e_{m+1} at t_{m+1} .

This paper is organized as follows. In Sec. 2, we describe how to control the error controlled ECM formula. Preliminary numerical results are presented in Sec. 3 to give numerical evidences for the theoretical analysis. Finally in Sec. 4, we summarize our results and discuss applications of the new techniques.

2. Abstract for Error Controlled Error Correction Methods

In this section, we briefly review the algorithm ECM and introduce a new error control methodology having uniform error bound for well conditioned problem.

2.1. General description

Let $x(t)$ be a given local approximation for the solution $\phi(t)$ defined on the integration step $[t_m, t_{m+1}]$ such that

$$(2.1) \quad R^x(t) := f(t, x(t)) - x'(t) = O(h^p), \quad t \in [t_m, t_{m+1}]$$

for some positive number p . Then the difference $\psi^x(t) = \phi(t) - x(t)$ satisfies a linear ODE

$$(2.2) \quad \psi^x(t)' = J^x(t)\psi^x(t) + R^x(t) + \frac{1}{2}\psi^x(t)^2\gamma_0(t), \quad t \in [t_m, t_{m+1}],$$

where $J^x(t) := f_\phi(t, x(t))$ and $\gamma_0(t) = f_{\phi\phi}(t, \theta_1 x(t) + (1 - \theta_1)\phi(t))$ with $\theta_1 \in (0, 1)$. Let us define the integrating factor

$$(2.3) \quad \mathcal{E}^x(t) := \exp\left(\int_t^{t_{m+1}} J^x(\xi)d\xi\right).$$

By multiplying (2.2) by the integrator factor $\mathcal{E}^x(t)$, and integrating the resulting equation in $[t_m, t_{m+1}]$, one may get

$$(2.4) \quad \psi^x(t_{m+1}) = C^x(\alpha_m) + \mathcal{E}^x(t_m)(\psi^x(t_m) - \alpha_m) + \frac{1}{2} \int_{t_m}^{t_{m+1}} \gamma_0(\xi)\mathcal{E}^x(\xi)(\psi^x(\xi))^2 d\xi,$$

where α_m is a given approximation for $\psi^x(t_m)$ and

$$(2.5) \quad C^x(\alpha_m) = \mathcal{E}^x(t_m)\alpha_m + \int_{t_m}^{t_{m+1}} \mathcal{E}^x(\xi)R^x(\xi)d\xi.$$

Note that by the definition of $\mathcal{E}^x(t)$ defined in (2.3), we can easily check that $C^x(\psi^x(t_m))$ can be calculated by the solution of the following ODE with the initial condition,

$$(2.6) \quad \begin{aligned} \vartheta^x(t)' &= \mathcal{J}^x(t)\vartheta^x(t) + R^x(t) \quad t \in [t_m, t_{m+1}] \\ \vartheta^x(t_m) &= \alpha_m, \end{aligned}$$

that is, $C^x(\psi^x(t_m)) = \vartheta^x(t_{m+1})$. It is approximated by using the existing numerical method and the solution $\phi(t_{m+1})$ is calculated by

$$(2.7) \quad \begin{aligned} \phi(t_{m+1}) &= \psi^x(t_{m+1}) + x(t_{m+1}) \\ &= \vartheta^x(t_{m+1}) + x(t_{m+1}) + \mathcal{E}^x(t_m)(\psi^x(t_m) - \alpha_m) \\ &\quad + \frac{1}{2} \int_{t_m}^{t_{m+1}} \mathcal{E}^x(\xi)(\psi^x(\xi))^2\gamma_0(\xi)d\xi. \end{aligned}$$

Remark 1. There are two assumptions. The first one is that α_m is well approximated close to $\psi^x(t_m)$ and the other one is that $\psi^x(t_m)$ is sufficiently small. It implies that the two remaining terms of $\phi(t_{m+1})$ are small enough and $\phi(t_{m+1})$ can be approximated up to the magnitude of $\int_{t_m}^{t_{m+1}} \mathcal{E}^x(\xi)(\psi^x(\xi))^2\gamma_0(\xi)d\xi$.

Based on the mechanism to derive for $\psi^x(t_{m+1})$ and $\phi(t_{m+1})$, we now describe a general methodology for error controlled ECM. Suppose that the approximations ϕ_m and e_m are given for the true solution $\phi(t_m)$ and its actual error E_m at time t_m ,

respectively. To approximate $\phi(t)$, we define $y_m(t)$ as $x(t)$ such that $y_m(t_m) = \phi_m$, that is, $\psi^{y_m}(t_m) = E_m$, so e_m is suitable for α_m as an approximation for $\psi^{y_m}(t_m)$. Since $C^{y_m}(e_m)$ is a solution of the ODE system as explained in (2.6), the existing numerical method using p th order is employed to approximate $\phi(t_{m+1})$. Let $\vartheta_{m+1}^{y_m}$ be the solution of the ODE system,

$$(2.8) \quad C^{y_m}(\alpha_m) = \vartheta_{m+1}^{y_m}(t_{m+1}) = \vartheta_{m+1}^{y_m} + R_p,$$

where R_p is the truncation error derived from the p th order numerical methods and $R_p = C_p h^{p+1} + O(h^{p+2})$ with an appropriate constant C_p . Therefore, $\phi(t_{m+1})$ is represented by

$$(2.9) \quad \begin{aligned} \phi(t_{m+1}) &= \vartheta_{m+1}^{y_m} + C_p h^{p+1} + O(h^{p+2}) + y_m(t_{m+1}) + \mathcal{E}^{y_m}(t_m)(\psi^{y_m}(t_m) - e_m) \\ &\quad + \frac{1}{2} \int_{t_m}^{t_{m+1}} \mathcal{E}^{y_m}(\xi)(\psi^{y_m}(\xi))^2 \gamma_0(\xi) d\xi. \end{aligned}$$

Let us define ϕ_{m+1} an approximation for $\phi(t_{m+1})$, then, it can be written by

$$(2.10) \quad \phi_{m+1} = \vartheta_{m+1}^{y_m} + y_m(t_{m+1}).$$

Then the actual error is given by

$$(2.11) \quad E_{m+1} = R_p + \mathcal{E}^{y_m}(t_m)(\psi^{y_m}(t_m) - e_m) + \frac{1}{2} \int_{t_m}^{t_{m+1}} \mathcal{E}^{y_m}(\xi)(\psi^{y_m}(\xi))^2 \gamma_0(\xi) d\xi.$$

Recall that unlike the existing mechanism, $\phi(t_{m+1})$ depends on e_m as well as ϕ_m , so does ϕ_{m+1} . To complete the formula, based on the assumption that two remaining term of E_{m+1} are sufficiently small, we need a methodology to estimate E_{m+1} so that the dominated term of E_{m+1} in (2.11) can be estimated. For this, reason, we will need (2.4) with another local platform $z_m(t)$ to satisfy $z_m(t_{m+1}) = \phi_{m+1}$ for estimating E_{m+1} . Notice that

$$(2.12) \quad \begin{aligned} \psi^{z_m}(t_m) &= \phi(t_m) - z_m(t_m) \\ &= \phi_m + e_m - z_m(t_m) + E_m - e_m. \end{aligned}$$

On the assumption that e_m is very close to E_m , we can set $\alpha_m = \phi_m + e_m - z_m(t_m)$ for an approximation of $\psi^{z_m}(t_m)$. Then, we will solve (2.6) again with the initial condition $\phi_m + e_m - z_m(t_m)$ and $z_m(t)$ using an existing numerical method having q th order and E_{m+1} is estimated by

$$(2.13) \quad \begin{aligned} E_{m+1} = \psi^{z_m}(t_{m+1}) &= \vartheta_{m+1}^{z_m} + R_q + \mathcal{E}^{z_m}(t_m)(\psi^{z_m}(t_m) - \alpha_m) \\ &\quad + \frac{1}{2} \int_{t_m}^{t_{m+1}} \mathcal{E}^{z_m}(\xi)(\psi^{z_m}(\xi))^2 \gamma_0(\xi) d\xi \end{aligned}$$

where $R_q = C_q h^{q+1} + O(h^{q+2})$. With an assumption that two remaining terms of E_{m+1} in (2.13) are sufficiently small, E_{m+1} is well approximated by e_{m+1} and its

quantity is

$$(2.14) \quad e_{m+1} = \vartheta_{m+1}^{z_m}$$

Since E_{m+1} in (2.13) is approximated for the dominated term of E_{m+1} in (2.11), the q th order numerical method is chosen so it can fully estimate the magnitude of $R_p = C_p h^{p+1} + O(h^{p+2})$. Also, e_{m+1} is estimated by using the calculated values ϕ_m, ϕ_{m+1} and e_m and is used for estimating the solution at the next time step.

Theorem 2. *Assume that the the local platforms $y_m(t)$ and $z_m(t)$ were set up to have magnitudes $O(h^{p_1})$ and $O(h^{q_1})$, respectively. The actual error E_{m+1} has uniform error bound and its magnitude is*

$$(2.15) \quad E_{m+1} \sim O(h^{\min(p+1, q+1, 2p_1+1, 2q_1+1)}).$$

Proof. Recall (2.13)

$$(2.16) \quad |E_{m+1} - e_{m+1}| \leq \mathcal{E}^{z_m}(t_m)|E_m - e_m| + O(h^{q+1}) + O(h^{2q_1+1}).$$

We let $E_0 = e_0 = 0$ and the inequality leads us

$$(2.17) \quad |E_m - e_m| \leq \frac{(\mathcal{E}^{z_m})^m - 1}{\mathcal{E}^{z_m} - 1} O(h^{\min(q+1, 2q_1+1)}).$$

From Eq. (2.11),

$$(2.18) \quad \begin{aligned} |E_{m+1}| &\leq O(h^{p+1}) + \mathcal{E}^{z_m}(t_m)|E_m - e_m| + O(h^{q+1}) + O(h^{2q_1+1}) \\ &\leq O(h^{p+1}) + O(h^{\min(q+1, 2q_1+1)}) + O(h^{2p_1+1}) \\ &\leq O(h^{\min(p+1, q+1, 2p_1+1, 2q_1+1)}). \end{aligned} \quad \square$$

For well conditioned problem, Theorem can be simply interpreted to the following corollary.

Corollary 3. *Assume that the the local platforms $y_m(t)$ and $z_m(t)$ were set up to have magnitudes $O(h^{p_1})$ and $O(h^{q_1})$, respectively. For well conditioned problem, the actual error E_{m+1} has uniform error bound and its magnitude is*

$$(2.19) \quad E_{m+1} = C_1 h^{\min(p+1, q+1, 2p_1+1, 2q_1+1)}.$$

where C_1 is an appropriate constant.

Proof. Recall (2.13)

$$(2.20) \quad |E_{m+1} - e_{m+1}| \leq \mathcal{E}^{z_m}(t_m)|E_m - e_m| + C_q h^{q+1} + O(h^{2q_1+1}).$$

Since we are solving the well conditioned problem, $\mathcal{E}^{z_m}(t_m) \leq 1$,

$$(2.21) \quad |E_m - e_m| \leq O(h^{\min(q+1, 2q_1+1)}).$$

From Eq. (2.11),

(2.22)

$$\begin{aligned} |E_{m+1}| &\leq C_p h^{p+1} + \mathcal{E}^{z_m}(t_m) |E_m - e_m| C_q h^{q+1} + O(h^{2q_1+1}) \\ &\leq C_p h^{p+1} + O(h^{\min(q+1, 2q_1+1)}) + O(h^{2p_1+1}) \\ &\leq C_1 h^{\min(p+1, q+1, 2p_1+1, 2q_1+1)}. \end{aligned}$$

□

2.2. Practical explicit algorithm

Based on the general description of the methodology, we concretely present the algorithm using the first and second local platforms and existing numerical methods - the second and third Runge-Kutta methods (RK2 and RK3) to estimate solutions, respectively. To begin with the simplest case, we let $y_m(t)$ be the Euler's polygon defined by

$$(2.23) \quad y_m(t) := \phi_m + (t - t_m)f(t_m, \phi_m), \quad t \in [t_m, t_{m+1}].$$

As described in the previous subsection, the difference $\psi^{y_m}(t) = \phi(t) - y_m(t)$ and (2.5) lead to the following ODE system

$$(2.24) \quad \begin{aligned} \vartheta^{y_m}(t)' &= f(t, \psi^{y_m}(t) + y_m(t)) - y_m'(t) \quad t \in [t_m, t_{m+1}] \\ \vartheta^{y_m}(t_m) &= e_m. \end{aligned}$$

To solve the ODE system (2.24), we simply use the 2nd order Runge-Kutta (RK2). For any step size $h > 0$,

$$(2.25) \quad \psi_{m+1}^{y_m} = e_m + K_2,$$

with

$$(2.26) \quad \begin{aligned} K_1 &= h[f(t, e_m + y_m(t_m)) - y_m'(t_m)] \\ K_2 &= h[f(t, e_m + \frac{K_1}{2} + y_m(t_m + \frac{h}{2})) - y_m'(t_m + \frac{h}{2})] \end{aligned}$$

and

$$(2.27) \quad \vartheta^{y_m}(t_{m+1}) - \vartheta_{m+1}^{y_m} = R_2,$$

which R_2 is a truncation error with the estimation using RK2 and its magnitude is $O(h^3)$. ϕ_{m+1} is represented by

$$(2.28) \quad \phi_{m+1} = \phi_m + e_m + f(t_m + \frac{h}{2}, \phi_m + e_m + \frac{h}{2}f(t_m, \phi_m + e_m)),$$

and the actual error E_{m+1} is

$$(2.29) \quad E_{m+1} = R_2 + \mathcal{E}^{y_m}(E_m - e_m) + O(h^5).$$

Lemma 4. *The truncation error R_2 derived from RK2 is calculated as*

$$(2.30) \quad R_2 = \frac{h^3}{24} \tilde{\phi}(t_m)''' + \frac{h^3}{8} \tilde{\phi}(t_m)'' f_\phi + O(h^4).$$

Proof. From Eq. (2.27) and the Taylor expansion of $\psi^{y_m}(t_{m+1})$,

$$(2.31) \quad \begin{aligned} R_2 &= \vartheta^{y_m}(t_{m+1}) - \vartheta_{m+1}^{y_m} \\ &= \frac{h^3}{24} (f_{tt} + 2f_{t\phi}f + f_{\phi\phi}f^2 + 4f_\phi f_t + 4f_\phi f_\phi f) + O(h^4) \\ &= \frac{h^3}{24} \tilde{\phi}(t_m)''' + \frac{h^3}{8} \tilde{\phi}(t_m)'' f_\phi + O(h^4) \end{aligned}$$

where $\tilde{\phi}(t_m)' = f$, $\tilde{\phi}(t_m)'' = f_t + f_\phi f$, and $\tilde{\phi}(t_m)''' = f_{tt} + 2f_{t\phi}f + f_{\phi\phi}f^2 + f_\phi f_t + f_\phi f_\phi f$ at time t_m . \square

Therefore, E_{m+1} is summarized as follows

$$(2.32) \quad E_{m+1} = \frac{h^3}{24} \tilde{\phi}(t_m)''' + \frac{h^3}{8} \tilde{\phi}(t_m)'' f_\phi + \mathcal{E}^{y_m}(E_m - e_m) + O(h^4).$$

Recall that unlike the existing mechanism, $\phi(t_{m+1})$ depends on e_m as well as ϕ_m , so does ϕ_{m+1} . To complete the formula, we need another methodology to estimate E_{m+1} . For this reason, we introduce another local platform $z_m(t)$ to satisfy $z_m(t_{m+1}) = \phi_{m+1}$ for estimating E_{m+1} as follows:

$$(2.33) \quad z_m(t) = \phi_{m+1} + (t - t_{m+1})f(t_{m+1}, \phi_{m+1}) + \frac{(t - t_{m+1})^2}{2} f_j^1 f^j(t_{m+1}, \phi_{m+1}),$$

where the Einstein summation symbol $f_j^1 f^j$ means $f_t + f_\phi f$ and is estimated as

$$(2.34) \quad f_j^1 f^j = \frac{2}{h} \left(f(t_{m+1}, \phi_{m+1}) - f(t_{m+\frac{1}{2}}, \phi_{m+1} - \frac{h}{2} f(t_{m+1}, \phi_{m+1})) \right).$$

Notice that the initial condition of $\psi^{z_m}(t_m)$ is considered as

$$(2.35) \quad \psi^{z_m}(t_m) = \phi(t_m) - z_m(t_m) + O(h^4) = \phi_m + e_m - z_m(t_m) + O(h^4).$$

With $\vartheta_m^{z_m} = \phi_m + e_m - z_m(t_m)$, the 3rd order Runge-Kutta (RK3) method is applied to solve the ODE system derived from the local platform $z_m(t)$ as done for (2.6). For any step size $h > 0$,

$$(2.36) \quad \begin{aligned} K_1 &= h[f(t, \psi_m^{z_m} + y_m(t_m)) - z_m'(t_m)] \\ K_2 &= h\left[f\left(t, \psi_m^{z_m} + \frac{K_1}{2} + z_m\left(t_m + \frac{h}{2}\right)\right) - z_m'\left(t_m + \frac{h}{2}\right)\right] \\ K_3 &= h\left[f\left(t, \psi_m^{z_m} - K_1 + 2K_2 + z_m(t_m + h)\right) - z_m'(t_m + h)\right] \\ \vartheta_{m+1} &= \vartheta_m^{z_m} + \frac{1}{6}(K_1 + 4K_2 + K_3). \end{aligned}$$

Hence, E_{m+1} is expanded as

$$(2.37) \quad E_{m+1} = \vartheta_{m+1}^{z_m} + R_3 + \mathcal{E}^{y_m}(E_m - e_m) + O(h^7).$$

where R_3 is a local truncation error derived from RK3 and its magnitude is $O(h^4)$. By Taylor expansion of e_{m+1} at (t_m, ϕ_m) ,

$$(2.38) \quad e_{m+1} = \frac{h^3}{24} \tilde{\phi}(t_m)''' + \frac{h^3}{8} \tilde{\phi}(t_m)'' f_\phi + O(h^4 + h^3 e_m + e_m^2)$$

Summarizing (2.29) and (2.37), one may complete the algorithm as follows.

$$(2.39) \quad \begin{aligned} \phi_{m+1} &= \phi_m + hf(t_m, \phi_m) + \vartheta_{m+1}^{y_m}, & m \geq 0, \\ e_{m+1} &= \vartheta_{m+1}^{z_m}, & m \geq 0; \quad e_0 = 0. \end{aligned}$$

3. Numerical Results

In this section, preliminary numerical results are presented to compare the efficiency of the error controlled ECM to the 3rd order RK method.

3.1. Nonlinear ODE system

For the first numerical example, we consider the non-stiff and nonlinear problem

$$(3.1) \quad \frac{d\phi}{dt} = \frac{\kappa\phi(t)(1-\phi(t))}{2\phi(t)-1}, \quad t \in (0, 200]; \quad \phi(0) = \frac{5}{6}$$

whose analytic solution is $\phi(t) = \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{5}{36} \exp(-\kappa t)}$ with a parameter $\kappa = 1/200$. For the time stepping, we use the explicit scheme(RK2/RK3) for error controlled ECM and we march from $t_0 = 0.0$ to $t_{final} = 200.0$ with fixed step size $\Delta t = 0.2$.

At first, we demonstrate the error behavior of the error controlled ECM and compare it with the 3rd order Runge Kutta (RK3) method since error controlled ECM has the 3rd order. We plot the relative errors in the whole simulation time interval as depicted in Fig. 1(a) and show the accuracy of error controlled ECM is much better than the existing 3rd order method and the error grows much more gentle. As seen in Fig. 1(b), convergence results are presented for both the error controlled ECM and the existing 3rd order Runge-Kutta method for different step size selections. The plot indicate the order of the error controlled ECM is close to the expected order 3 since RK2 and RK3 are used to estimate the solution and the truncation error for error controlled ECM framework.

3.2. ODE system

As observed the previous example, the numerical convergence order of the error controlled ECM using RK2/RK3 is greater than 3, but less than 4. Hence, in our second example, not only RK3 method, but the 4th order method (RK4) is also compared with our results.

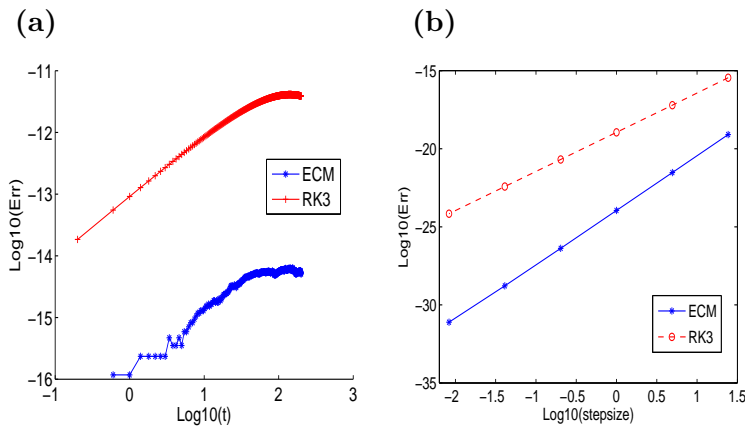


Figure 1: Comparison of the (a) error behavior and (b) convergence order for Error Controlled ECM 23 and 3rd order Runge Kutta (RK3)

The problem considered in this example is

$$(3.2) \quad \begin{aligned} y'(t) &= \lambda(t - p(t))^2 - p'(t) \\ y(0) &= p(0) \end{aligned}$$

where $y(t)$ and $p(t)$ can be vectors of dimension N and the exact solution is $y(t) = p(t)$ and $\lambda = 1.0$. In this example, we choose $N = 1$ and $\cos(t)$ as $p(t)$. We demonstrate the (relative) error behavior of the error controlled ECM by computing the solution from $t_0 = 0$ to $t_{final} = 20\pi$ with time step size $\Delta t = \pi/60$. Fig. 2 shows that the error of error controlled ECM is gradually growing with ,whereas other existing methods (RK3 and RK4) have linear growth of the error.

4. Conclusion and Further Discussion

A new mechanism to control error for well-conditioned problems is developed in ECM framework. Unlike the traditional way to approximate solutions singly using an approximated solution at the previous time step, we suggest formulating a local truncation error and approximating the solutions using both the approximated solution and local truncation error at the previous step. Numerical results show that the error controlled ECM provides a possible vision to obtain uniform error bound which has never been achieved in existing numerical methods and which enables a long time simulation.

To improve the performance of the error controlled ECM, several extensions are currently being pursued. Since the main purpose of this study is to enable a long time simulation by minimizing the local accumulated error, the generalization of the error controlled ECM has been applied to real long time simulator such as real power systems, etc. Numerical results are very promising and a paper reporting

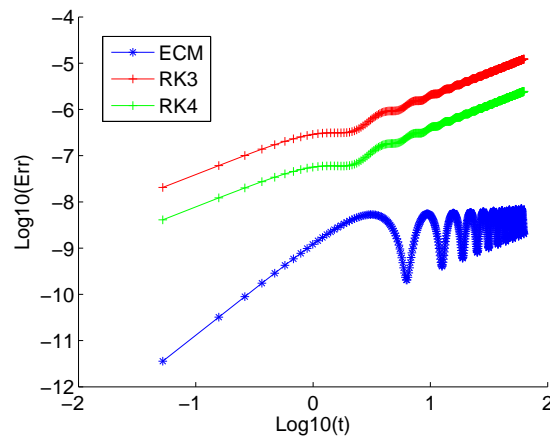


Figure 2: Comparison of Error Behavior for error controlled ECM with for other existing methods (RK3 and RK4)

on this result is in preparation. Another work to pursue is to apply this technique to stiff system, and investigate the stability analysis for the system. The other possibility for further efficiency of error controlled ECM is to increase accuracy by employing higher order techniques to estimate the solution and the local truncation error. Results along these directions will be reported in the future.

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