Adaptive Composition ODE Solvers Based on Semi-Implicit Integration

Denis N. Butusov, Valerii Y. Ostrovskii, Vitalii Y. Martynov, Dmitrii O. Pesterev, Vyacheslav G. Rybin
Department of Computer Aided Design
Saint Petersburg Electrotechnical University "LETI"
St. Petersburg, Russia
dnbutusov@etu.ru

***Abstract*— The paper considers the algorithms of adaptive integration stepsize control for composition fractal ODE solvers. Several techniques of local truncation error estimation are represented, including a novel commutation analysis method that uses the special properties of semi-implicit integration. It is shown that the application of the stepsize control technique based on commutation error analysis allows to increase the performance of adaptive fractal ODE solvers in comparison to the conventional stepsize control algorithms. The results of computational experiments are given, showing the possibility to preserve the geometric properties of the composition solver when the proposed adaptive stepsize technique is applied.**

***Keywords*— geometric integration; fractal methods; semi-implicit integration; adaptive stepsize; chaotic system; memristive circuit; Bouali system**

I. Introduction

Computer simulation of continuous dynamical systems represented by ordinary differential equations requires the application of numerical integration methods. The most common ODE solvers, e.g. Runge-Kutta and extrapolation methods, usually incorporate adaptive step control algorithms, designed to improve the performance of the solver. However, some dynamical problems require numerical integration methods with special structural properties [1]. These methods are usually called symmetric, geometric or *reflexive* integrators [2]. It is known [3], that certain classes of chaotic dynamical systems require symmetric integration to obtain adequate discrete models due to the phase space volume preservation effects. At the same time, among the known ways to increase the order of accuracy of ODE solver, only composition schemes retain geometric properties of the basic method.

The development of adaptive stepsize control algorithms for composition ODE solvers is still an open problem. The most common *explicit* methods of local error estimation violate the property of reflexivity [4]. Explicit stepsize control algorithms for geometric integrators were proposed in [4–6], but limited performance evaluation was given and only Hamiltonian systems were considered. *Implicit* algorithms, based on the “present” or “future” information about the local truncation error, were introduced in [7, 8]. Nevertheless, for chaotic systems simulation only fractal composition *semi-implicit* methods can exhibit numerical efficiency comparable with single-step explicit Runge-Kutta methods [3]. In this study, several algorithms of adaptive stepsize control, based on the different approaches to the local error estimation, are compared in application to the fractal semi-implicit methods.

As experimental data, we provide the performance plots for several adaptive composition solvers and their reversibility estimation on two test chaotic systems.

The reported study was supported by RFBR, research project No. 17-07-00862.

II. Test systems

To perform numerical simulations, we chose the model of simplest chaotic circuit with memristor [9] and Safieddine Bouali`s 3D chaotic system [10].

The simplest memristive circuit [9] has only three circuit elements and can be represented by the following system of differential equations:

$$\begin{cases} \dot{x} = y \\ \dot{y} = \gamma x - \beta y(z^2 - 1) \\ \dot{z} = -y - \alpha z + yz \end{cases} \qquad (1)$$

The system parameters α = 0.6, β = 0.5, γ = 0.33 correspond to the chaotic mode of oscillations.

Bouali 3D chaotic system model incorporates a cubic term coupled to a quadratic cross-term. This system consists of three equations:

$$\begin{cases} \dot{x} = \alpha x(1-y) - \beta z \\ \dot{y} = -\gamma y(1-x^2) \\ \dot{z} = \mu x \end{cases} \qquad (2)$$

where α = 3, β = 2.2, γ = 1, μ = 0.001. These parameters bring the system to a stable equilibrium point, where it generates a strange attractor appearing as a unique figure with two comparable double wings connected with two paths [10].

III. Fractal composition methods

Let Φ_h be a basic reflexive method and $\delta_1, \ldots, \delta_s$ be real numbers. Then the composition with stepsizes $\delta_1 h, \delta_2 h, \ldots, \delta_s h$, where $\delta_1 + \ldots + \delta_s = 1$, i.e.

$$\psi_h = \Phi_{\delta_s h} \circ \ldots \circ \Phi_{\delta_s h},$$

978-1-5386-5824-6/18/$31.00 ©2018 IEEE

is called the *composition* method ψ_h. The aim of composition is to increase the accuracy order of the finite-difference scheme while preserving desirable geometrical properties [1] of the basic method, e.g. reflexivity. Fig. 1 shows a graphical interpretation of the 7-stage composition method of the 6th order.

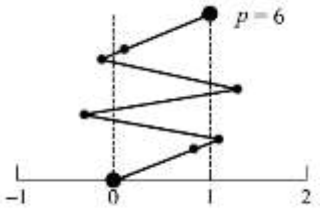

Fig. 1. The sub-steps plot for *s7or6* composition scheme

The classical approach for calculating coefficients δ is the formula proposed by H. Yoshida [11]. However, Yoshida composition methods possess the weak stability and low numerical efficiency. In [12] M. Suzuki proposed a modified method for calculating the coefficients δ:

$$\delta_c = -\frac{(s-1)^{1/(n+1)}}{s-(s-1)^{1/(n+1)}-1}, \qquad \delta_s = \frac{1}{s-(s-1)^{1/(n+1)}-1} \tag{3}$$

where s is the total number of stages of the composition scheme, e.g. s = 3, 5, 7…; n is the order of the base method; δ_c is the coefficient for the central stage and δ_s are the coefficients for all other stages.

The described approach allows one to construct a composition ODE solver of arbitrary accuracy order with an odd number of stages. To increase the accuracy order of the integration scheme, the process should be iterated by dividing each stage into sub-stages with the same coefficients δ, hence the name *fractal* methods was given.

Let us consider two fractal algorithms of order 4, based on second-order basic method and having five (*s5or4*) and seven (*s7or4*) stages. The coefficient values of the *s5or4* method are:

$$\delta_3 = -\frac{4^{1/3}}{4-4^{1/3}}, \qquad \delta_{1,2,4,5} = \frac{1}{4-4^{1/3}} \tag{4}$$

Similarly, the coefficients of the *s7or4* method are:

$$\delta_4 = -\frac{6^{1/3}}{6-6^{1/3}}, \qquad \delta_{1,2,3,5,6,7} = \frac{1}{6-6^{1/3}} \tag{5}$$

IV. ADAPTIVE STEPSIZE CONTROL

In this section, we investigate the stepsize control algorithms. All described approaches share the same idea of changing the stepsize on each integration step depending on the estimation of local truncation error. The overall stepsize control algorithm is looped and each iteration consists of four steps:

1. Solve a system with the current stepsize;
2. Estimate the local truncation error;
3. Use the estimated local error value to calculate new step with following formula [1]:

$$h_{new} = 0.94h\left(0.65\frac{tol}{err}\right)^{\frac{1}{2k-1}} \tag{3}$$

where h_{new} is the new size of integration step, h is the current stepsize, *tol* is the required absolute or relative tolerance, *err* is the local error estimation, $2k$ is the accuracy order of composition scheme;

4. The algorithm exit the loop when $err \le tol$ or when the amount of iterations exceed the certain limit.

The most important procedure in the stepsize control is the estimation of the local truncation error. In this study we consider four different approaches to estimate the local error.

1. Half-step estimation (HSE): this conventional method estimates the local error as the difference between two parallel solutions obtained with the same method but different stepsizes h and $h/2$.
2. Reverse step estimation (RSE): this method estimates the local error as the difference between the "forward" solution obtained with step h and "backward" solution obtained with negative step $-h$.
3. The method of commutation error estimation (CEE): this method estimates the local error as the difference between the solutions obtained by two solvers of the same order but with different basic method *switch matrix* [13].
4. Method order estimation (MOE): this method calculates the local error estimation as a difference between two parallel solutions obtained by a pair of solvers of different accuracy order. In our study, it was assumed that the first method is *s7or4* and the second method is *s7or6* solver.

One can see that among these estimation techniques there are approaches based on "present" information about local error as well as methods, considering "past" information. We performed the comparative study of four represented stepsize control algorithms in a series of computational experiments.

V. EXPERIMENTAL RESULTS

The purpose of our investigation was to find the best local error estimation technique for adaptive stepsize control while simulating chaotic dynamical systems (1) and (2).

We used following simulation parameters in our computational experiments: simulatuon time t = 40, max stepsize h_{max} = 1, min stepsize h_{min} = 0.001.

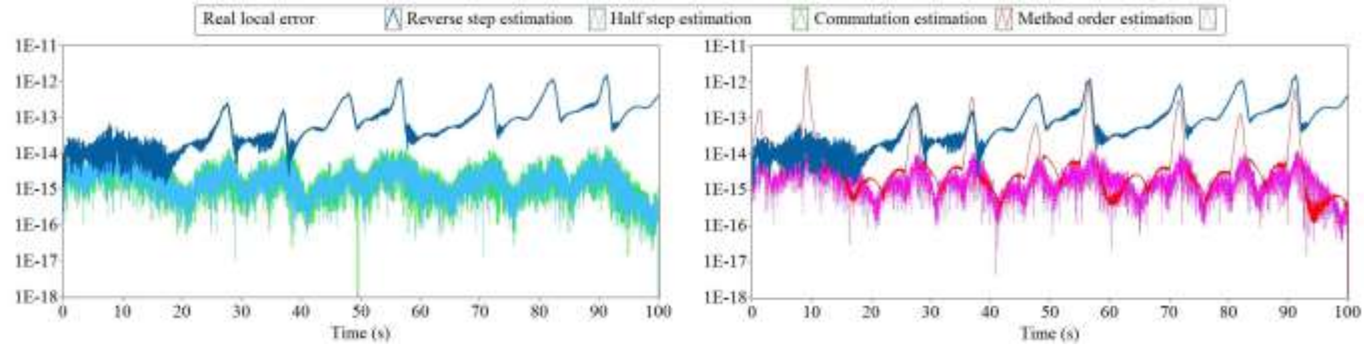

Fig. 2. The precision of various local truncation error estimation techniques

The solution tolerance *tol* was varied within the range from 10^{-5} to 10^{-10}. We used the semi-mplicit basic CD methods [13] with Suzuki [12] fractal coefficients.

The first experiment was the overall test of error estimation techniques (Fig. 2), carried out to investigate how close each method of error estimation is to the real values of local truncation error. One can see that the commutation error estimation method gives the best results, and it can be assumed that it may show best performance in the further tests.

The second type of experiment was the investigation of the numerical efficiency of adaptive fractal solvers with various stepsize control algorithms. The performance plots representing the relationship between the global error and elapsed computational time are shown in Fig. 3.

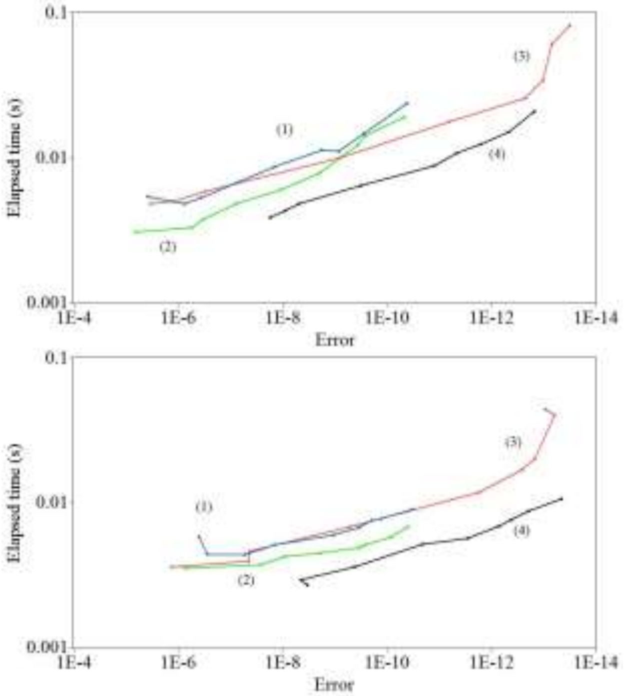

Fig. 3. The perfomance plots for simulation of memristive circuit and Bouali chaotic system by (1) – adaptive fractal ODE solver with RSE control; (2) – ODE solver with HSE control, (3) – ODE solver with CEE control, (4) – ODE solver with MOE control.

One can see that adaptive fractal solver that uses the difference between two parallel composition schemes of different order as the local error estimation, shows the best results. However, the method that estimates the local error by commutation analysis technique also shows good results and even allow simulating the memristive circuit system with more precision. The solvers that use reverse step and half-step error estimation tend to underestimate the real value of truncation error and are much less efficient.

Let us describe the third group of computational experiments, introducing the tools to measure the preservation of the geometric properties of fractal finite-difference scheme when an adaptive stepsize is applied. Reversibility plot shows how far the solution can go backward in time before exceeding the certain accuracy limit. The horizontal axis of reversibility plot represents the tolerance values that were set for current simulation. In our study, the accuracy limit was set to 1%. Since the adaptive backward solution of ODEs requires the development of novel formula for step control, we simplified the procedure by using the reversed step arrays instead. The purpose of this experiment was to show how various adaptive fractal composition schemes could preserve the reversibility of the basic method depending on the implemented local error estimation technique. Reversibility plots for both test systems are shown in Fig. 4. One can see, that fractal solver, controlled by the CEE method, shows superior reversibility amongst other three algorithms and outperform the method with MOE step control.

The possible explanation of this fact is that parallel solvers, implemented in the algorithm of commutation error estimation, have very similar stability regions, which is not true for MOE control technique. On a negative stepsizes the latter fact may cause low convergence of the algorithm and therefore, the reflexivity break. The two remaining step control algorithms totally failed the reversibility test. None of them can be efficiently used with the negative timestep or preserve the geometric properties of composition scheme when using a variable stepsize. These results are in a good agreement with those obtained in [4] for Hamiltonian systems simulation.

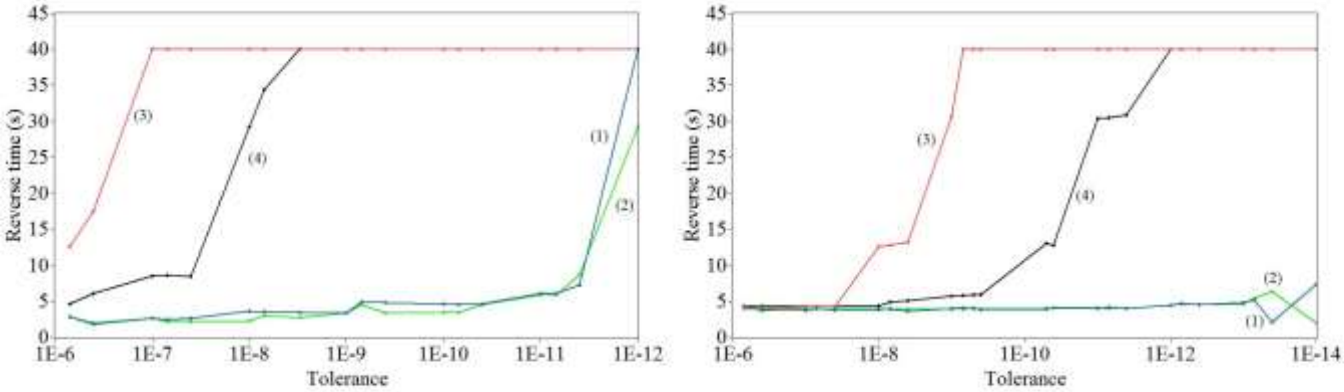

Fig. 4. The reversibility plots for the memristive circuit and Bouali chaotic system. (1) – adaptive fractal ODE solver with RSE step control; (2) – ODE solver with HSE step control, (3) – ODE solver with CEE step control, (4) – ODE solver with MOE step control

VI. Conclusion

In this study, we considered theoretical and experimental features of adaptive fractal composition ODE solvers based on semi-implicit integration. Several methods of the integration step control, based on different techniques for local truncation error estimation, were implemented and studied in a series of computational experiments. The computational efficiency of semi-implicit fractal solvers was investigated and represented through the efficiency plots. The adaptive fractal solver that uses the MOE local error estimation has shown the best computational performance among other methods, and the solver with adaptive timestep based on the novel CEE local error analysis took the second place. Reversibility plot was introduced as a tool to study the efficiency of adaptive fractal solvers in backward integration procedures. It was shown that the estimation of local truncation error by the explicit techniques causes the loss of geometric properties of the solver. The commutation analysis of the local truncation error appear to be the promising technique for implementing highly effective time-reversible solvers of chaotic ODEs.

The development of adaptive stepsize algorithm for backward integration and the experimental study of the adaptive composition solvers on a negative simulation times will be the purpose of our further research.

References

[1] Hairer E., Lubich C., Wanner G. *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*. Springer Science & Business Media, 2006. V. 31.

[2] Kahan W, Li R.C. Composition constants for raising the orders of unconventional schemes for ordinary differential equations. *Mathematics of Computation of the American Mathematical Society*, 1997, V. 66, no. 219, pp. 1089-1099. DOI: 10.1090/S0025-5718-97-00873-9.

[3] Butusov D.N., Goryainov S.V., Andreev V.S., Barashok K.I., Kozak M.N. Fractal Composition ODE Solvers Based on Semi-implicit Methods *Proc. XXI IEEE International Conference on Soft Computing and Measurements (SCM)*, Saint Petersburg, 2018.

[4] Hairer E., Gustaf S. Explicit, time reversible, adaptive step size control. *SIAM Journal on Scientific Computing*, 2005, V. 26, no. 6, pp. 1838-1851. DOI: 10.1137/040606995.

[5] Huang W., Leimkuhler B. The adaptive Verlet method. *SIAM Journal on Scientific Computing*, 1997, V. 18., no. 1, pp. 239-256. DOI: 10.1137/S1064827595284658.

[6] Holder T., Leimkuhler B., Reich S. Explicit variable step-size and time-reversible integration. *Applied Numerical Mathematics*, 2011, V. 39, no. 3-4, pp. 367-377. DOI: 10.1016/S0168-9274(01)00089-7.

[7] Hut P., Makino J., McMillan S. Building a better leapfrog. *The Astrophysical Journal*, 1995, no. 443, pp. L93-L96. DOI: 10.1086/187844.

[8] Stoffer D. Variable steps for reversible integration methods. *Computing*, 1995, V. 55, no. 1, pp. 1-22. DOI: 10.1007/BF02238234.

[9] Muthuswamy B., Chua L. O. Simplest chaotic circuit. *International Journal of Bifurcation and Chaos*, 2010, V. 20, no. 05, pp. 1567-1580. DOI: 10.1142/S0218127410027076.

[10] Bouali S. A 3D Strange Attractor with a Distinctive Silhouette. The Butterfly Effect Revisited. *arXiv preprint arXiv:1311.6128*, 2013.

[11] Yoshida H. Construction of higher order symplectic integrators. *Physics Letters A*, 1990, V. 150, no. 5-7, pp. 262-268. DOI: 10.1016/0375-9601(90)90092-3.

[12] Suzuki M. Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Physics Letters A*, 1990, V. 146, no. 6, pp. 319-323. DOI: 10.1016/0375-9601(90)90962-N.

[13] Butusov, D. N., T. I. Karimov, and V. Y. Ostrovskii. Semi-implicit ODE solver for matrix Riccati equation. *Proc. IEEE NW Russia Young Researchers in Electrical and Electronic Engineering Conference (EIConRusNW)*, Saint Petersburg, 2016, pp. 168-172. DOI: 10.1109/EIConRusNW.2016.7448146.