INFORMATICA, 2000, Vol. 11, No. 4, 371–380

Adaptive Integration of Stiff ODE

Raimondas ČIEGIS, Olga SUBOČ,
Vilnius Gediminas Technical University
Saulėtekio 11, 2054 Vilnius, Lithuania
e-mail: rc@fm.vtu.lt

Remigijus ČIEGIS
Kaunas Faculty of Humanities Vilnius University
Muitinės 8, 3000 Kaunas, Lithuania
e-mail: remigijus.ciegis@aula.vukhf.lt

Received: November 2000

Abstract. The accuracy of adaptive integration algorithms for solving stiff ODE is investigated. The analysis is done by comparing the discrete and exact amplification factors of the equations. It is proved that the usage of stiffness number of the Jacobian matrix is sufficient in order to estimate the complexity of solving ODE problems by explicit integration algorithms. The complexity of implicit integration algorithms depends on the distribution of eigenvalues of the Jacobian. Results of numerical experiments are presented.

Key words: stiff ODE, adaptive integration, explicit and implicit algorithms.

1. Introduction

We consider the time integration of stiff systems of ODE given in the form

$$\frac{\mathrm{d}U}{\mathrm{d}t} = f(t, U), \quad 0 < t \leqslant T, \tag{1}$$
$$U(0) = U_0,$$

where f is a nonlinear map $f\colon \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$, U is a vector of m components. Many models of real world applications are described by initial value problems for systems of ODE. The reaction term f usually introduces stiffness into the problem. The precise definition of stiffness is not very important for our purposes. We can assume that stiffness means that the problem describes processes with a huge range of characteristic reaction times. Good surveys on stiff systems of ODE are given by Dekker and Verwer (1984), Aiken (1985), Higham and Trefethen (1993), Hairer and Wanner (1996).

Numerical methods for solving systems of ODE can be divided into two large groups, for non stiff and stiff problems. Explicit methods are usually used for integration of non stiff problems, and implicit methods are preferred when ODE are stiff.

The stiffness of initial value problem for a system of ODE obviously depends on the differential equation itself, but we must also take into account the size of the tolerance to be used, the integration interval and the initial values.

One simple stiffness detection technique connects the stiffness of the initial value problem (1) with the stiffness of the Jacobian matrix J. A survey on such techniques is given in (Ekeland *et al.*, 1998).

Most modern integration algorithms are adaptive. They use a stepsize selection strategy that tries in each step to find the largest possible stepsize such that the local truncation error is kept smaller than the user-defined tolerance ε. If the aposteriori estimated local error is larger than ε, the step is rejected, and a smaller stepsize is tried.

The current work is devoted to the investigation of the efficiency of explicit and implicit adaptive integration algorithms for solving linearized systems of ODE. We shall prove that stiffness number of the Jacobian matrix gives important information about stiff ODE but this information is not sufficient in order to evaluate the computational difficulty of stiff ODEs.

The remainder of the paper is organized as follows. Section 2 describes finite difference schemes, gives an analysis of the discretization errors associated with these schemes, and presents stability results. Section 3 describes our adaptive integration technique. Section 4 presents the results of numerical experiments, and Section 5 states our conclusions.

2. Finite–Difference Schemes

As was stated above, the eigenvalues of the Jacobian J of f in (1) give important information about the stiffness of the initial-value problem for ODE. Hence, we consider the following system of linear ODE

$$\begin{aligned}&\frac{\mathrm{d}U}{\mathrm{d}t} + AU = 0, \quad 0 < t \leqslant T,\\ &U(0) = U_0,\end{aligned} \tag{2}$$

here A is $m \times m$ constant matrix. Let assume that A is diagonalizable with real eigenvalues, so that we can decompose it

$$A = RDR^{-1},$$

where

$$D = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)$$

is a diagonal matrix of eigenvalues, and $R = (R_1, R_2, \dots, R_m)$ is a matrix of right eigenvectors, i.e.,

$$AR_j = \lambda_j R_j\,, \quad j = 1, 2, \cdots, m.$$

We will always assume that the eigenvalues of A are positive

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_m,$$

and the system of eigenvectors R is complete, e.g., the initial vector U_0 has the eigenvector expansion

$$U_0 = \sum_{j=1}^{m} \alpha_j R_j.$$

The problem (2) is called *stiff*, if the stiffness number $S = \lambda_m/\lambda_1$ of matrix A is a large number, i.e., $S \gg 1$.

We discretize the system of ODE (2) on the nonuniform difference grid

$$\omega_\tau = \{t_n\colon\ t_n = t_{n-1} + \tau_n, \quad n = 1, 2, \cdots, N\}.$$

Let $V^n = V(t_n)$ denotes approximation of the solution $U(t_n)$ at the discrete grid points.

For the time integration we consider the following schemes (see, Richtmyer and Morton, 1967; Stetter, 1973; Butcher, 1987):

Forward Euler scheme:

$$\frac{V^n - V^{n-1}}{\tau_n} + AV^{n-1} = 0. \tag{3}$$

Backward Euler scheme:

$$\frac{V^n - V^{n-1}}{\tau_n} + AV^n = 0. \tag{4}$$

Centered Euler scheme:

$$\frac{V^n - V^{n-1}}{\tau_n} + A\frac{V^n + V^{n-1}}{2} = 0. \tag{5}$$

Rosenbrock scheme: (see, Shirkov, 1984)

$$\begin{aligned} &\frac{W^n}{\tau_n} + A\left(\frac{1+i}{2}W^n + V^{n-1}\right) = 0,\\ &V^n = V^{n-1} + \operatorname{Re} W^n, \quad i = \sqrt{-1}. \end{aligned} \tag{6}$$

2.1. *Local Truncation Error*

As was stated in Section 1, most adaptive integration algorithms try to keep the local truncation error constant and smaller than a user-defined tolerance ε.

The local truncation error Ψ^n is defined replacing V^n in a difference scheme by the exact solution U^n at the corresponding point. It is obvious that Ψ^n is a measure how well the difference scheme approximates the differential equation locally. Assuming that exact solutions are smooth and expanding some terms of Ψ^n in Taylor series about U^n we get the following well-known results.

Lemma 2.1. *Let assume that $U \in C^2(0,T)$, then $|\Psi^n| = O(\tau)$ for the forward and backward Euler schemes. If $U \in C^3(0,T)$, then $|\Psi^n| = O(\tau^2)$ for the centered Euler and Rosenbrock schemes.*

2.2. *Stability*

The Lax equivalence theorem says, that for a consistent linear method, *stability* is necessary and sufficient for convergence (see, Richtmyer and Morton, 1967). We consider the eigenvectors expansion of the discrete function

$$V^n = \sum_{j=1}^{m} v_j^n R_j. \tag{7}$$

If we put (7) into a finite difference scheme, we obtain m decoupled equations

$$v_j^n = \rho_j(\tau\lambda_j) v_j^{n-1}, \quad j = 1, 2, \cdots, m.$$

Then we define the *amplification factor* of the difference scheme as

$$\rho(\tau) = \max_{1 \leqslant j \leqslant m} |\rho_j(\tau\lambda_j)|.$$

The finite difference scheme is stable provided

$$\rho(\tau) \leqslant 1. \tag{8}$$

In some applications it is important to guarantee that the asymptotical behavior of the discrete solution is the same as for the exact solution. The finite difference scheme is said to be asymptotically stable provided (see, Samarskij, 1988)

$$\rho(\tau) = |\rho_1(\tau\lambda_1)| < 1.$$

Asymptotical stability analysis of large number of finite difference schemes for PDE is given by Čiegis (1991).

The finite difference scheme is said to be positive provided

$$\rho_j(\tau\lambda_j) \geqslant 0, \quad j = 1, 2, \cdots, m.$$

Such condition is very important for solving problems, which describe mass conservation in chemical reactions.

Table 1

Stability of finite difference schemes for the linear problem (2)

Scheme	ρ_j	Stability	Asympt. stability	Positivity
(3)	$1-\tau\lambda_j$	$\tau \leqslant \frac{2}{\lambda_m}$	$\tau < \frac{1}{\lambda_m}$	$\tau \leqslant \frac{1}{\lambda_m}$
(4)	$\frac{1}{1+\tau\lambda_j}$	∞	∞	∞
(5)	$\frac{1-0.5\tau\lambda_j}{1+0.5\tau\lambda_j}$	∞	$\tau < \frac{2}{\sqrt{\lambda_1\lambda_m}}$	$\tau \leqslant \frac{2}{\lambda_m}$
(6)	$\frac{1}{1+\tau\lambda_j+0.5\tau^2\lambda_j^2}$	∞	∞	∞

The amplification factors and stability conditions of finite difference schemes (3)-(6) are listed in Table 1.

It follows from Table 1 that the backward Euler and Rosenbrock schemes satisfy unconditionally all stability requirements. The centered Euler scheme is unconditionally stable with respect to the stability definition (8), but we need to put restrictions on stepsize τ in order to preserve positivity and asymptotical stability of its solution.

3. Adaptive Integration Algorithm

We use the following stepsize selection strategy

$$\tau_n = \min(\tau_{n1}, \tau_{n2}, \tau_0), \tag{9}$$

where τ_0 is a user-defined maximal stepsize, τ_{n1} is the largest possible stepsize such that the appropriate stability requirement is satisfied, e.g.,

$$\rho(\tau_{n1}) \leqslant 1,$$

and τ_{n2} is the largest possible stepsize such that the local discretization error is smaller than a user-defined tolerance

$$|(\rho_j(\tau_{n2}\lambda_j) - \mathrm{e}^{-\tau_{n2}\lambda_j})v_j^{n-1}| \leqslant \varepsilon, \quad j = 1, 2, \cdots, m. \tag{10}$$

By using such definition of the local discretization error we estimate the error introduced during one integration step starting with the initial value V_j^{n-1}. Then the exact solution of ODE is given by

$$u_j^n = \mathrm{e}^{-\tau_{n2}\lambda_j} v_j^{n-1},$$

and the solution of finite difference scheme is given by

$$v_j^n = \rho_j(\tau_{n2}\lambda_j)v_j^{n-1}.$$

A similar definition of the local discretization error was used in Shirkov (1984). The local discretization error is closely connected to the local truncation error, defined in Section 2. For example, the local truncation error of the forward Euler scheme is given by

$$\Psi_j^n = \frac{1}{\tau_n}(\mathrm{e}^{-\tau_n\lambda_j} - \rho_j(\tau_n\lambda_j))u_j^{n-1}.$$

We shall investigate computational costs of this adaptive integration algorithm by making direct computational experiments with various test problems. Matrix A is selected artificially with the goal to describe important cases of stiff ODE.

4. Numerical Experiments

In this section we solve two different types of stiff ODE. The definition of stiffness number S depends only on minimal and maximal eigenvalues of matrix A. Hence in the first set of test problems we use 2×2 matrix A with two eigenvalues

$$\lambda_1 = 1, \quad \lambda_2 = 10^k, \quad k = 3, 4, 5, 6. \tag{11}$$

In the second example we use $m \times m$ matrix A with the same stiffness number $S = 10^6$ but with different distributions of eigenvalues:

$$\begin{aligned} &m = 2, \quad \lambda_1 = 1, \quad \lambda_2 = 10^6,\\ &m = 3, \quad \lambda_1 = 1, \quad \lambda_2 = 10^3, \quad \lambda_3 = 10^6,\\ &m = 4, \quad \lambda_1 = 1, \quad \lambda_2 = 10^2, \quad \lambda_3 = 10^4, \quad \lambda_3 = 10^6,\\ &m = 5, \quad \lambda_j = 10^{j-1}, \quad j = 1, 2, \cdots, 7. \end{aligned} \tag{12}$$

The problem (2) is solved in the interval $[0, 6]$ and the tolerance ε is set to 10^{-4}. In all numerical experiments, we take $\tau_0 = 0.2$ as the maximal allowed stepsize in the adaptive stepsize selection algorithm (9).

4.1. *Spectral Stability*

In this section we use the general stability condition (8). Table 2 presents the numbers of steps required for different integration algorithms to solve the first test problem (11).

It is easy to see that the stepsize of the explicit Euler scheme is restricted due to stability requirements and the number of steps depends linearly on the stiffness of matrix A. It follows from this example that the stiffness number S can not be used to estimate costs of implicit adaptive integration algorithms. We note that second order accurate integration schemes (i.e., the centered Euler and Rosenbrock schemes) are computationally more efficient than the first order accurate backward Euler scheme.

In Table 3 we present the numbers of steps required for different integration algorithms to solve the second test problem (12).

Table 2
Number of integration steps for solving Example 1

k	FES	BES	CES	ROS
3	3133	271	59	66
4	30133	272	59	66
5	300130	272	59	66
6	3000103	272	59	66

Table 3
Number of integration steps for solving Example 2

m	FES	BES	CES	ROS
2	3000103	272	59	66
3	3000103	408	84	95
4	3000108	529	107	122
7	3000172	718	145	170

It follows from results given in Table 3 that the number of integration steps for implicit integration schemes depends linearly on the number of clusters in the distribution of matrix A eigenvalues. After resolving accurately the transition of jth component, the stepsize increases in accordance with the size of $(j+1)$th eigenvalue. The centered Euler scheme was most efficient for this test problem, but the other unconditionally stable schemes (i.e., the backward Euler and Rosenbrock schemes) were also efficient.

4.2. *Asymptotical Stability*

In this section we investigate the efficiency of adaptive integration schemes when the asymptotical behavior of the solution is most important. Hence we change the stability condition in the stepsize selection algorithm and define τ_{n1} in accordance with the requirement

$$\rho(\tau) = |\,\rho_1(\tau\lambda_1)|.$$

As it follows from Table 1, this new condition makes impact only on the explicit and centered Euler schemes. In Table 4 we present results of numerical experiments for the second test problem (12).

The centered Euler scheme solves the problem in more steps than the backward Euler and Rosenbrock schemes, but still can be used in numerical simulations.

Table 4
Experiments with asymptotically stable difference schemes

m	FES	BES	CES	ROS
2	6000069	272	3025	66
3	6000069	408	3046	95
4	6000069	529	3053	122
7	6000119	718	3078	170

Table 5
Experiments with difference schemes satisfying the positivity condition

m	FES	BES	CES	ROS
2	6000069	272	2999991	66
3	6000069	408	2999991	95
4	6000069	529	2999991	122
7	6000119	718	2999992	170

4.3. *Positivity of Difference Schemes*

Many real-life problems of computational chemistry, ecology, atmosferic transport-chemistry lead to initial-value problems for ODE. The vector U defines concentrations of different species and all its components must be nonnegative. In this section we investigate the efficiency of adaptive integration algorithms with τ_{n1} chosen in accordance with the positivity requirement for the amplification factor of the difference scheme

$$\rho_j(\tau_1 \lambda_j) \geqslant 0.$$

As it follows from Table 1, this positivity condition makes impact only on the centered Euler schemes. In Table 5 we present results of numerical experiments for the second test problem (12).

These results show that the centered Euler scheme is only twice faster than the forward Euler scheme if positivity of solution must be guaranteed.

5. Conclusions

In this paper we have investigated the efficiency of adaptive integration algorithms for solving stiff initial-value ODE. It is proved that the stiffness number of the Jacobian matrix J gives a sufficient information to estimate the computational costs of explicit schemes.

The computational complexity of implicit integration algorithms depends on the distribution of eigenvalues of the Jacobian matrix. It is proved that unconditional stability of difference schemes is more important than the order of local truncation error. Numerical results obtained solving two sets of test problems demonstrate that the backward Euler and Rosenbrock schemes are most efficient and accurate.

References

Aiken, R.(1985). *Stiff Computation*. Oxford University Press, Oxford, England.

Butcher, J.C. (1987). *The Numerical Analysis of Ordinary Differential Equations: Runge-Kutta and General Linear Methods*. Wiley, New York.

Čiegis, Raim., Rem. Čiegis (1991). Asymptotical stability of economical difference schemes. *Lith. Math. Journal*, **31**, 535–548.

Dekker, K., J. Verwer (1984). *Runge-Kutta Methods for Stiff Nonlinear Differential Equations*. North Holland.

Ekeland, K., B. Owren, E. Øines (1998). Stiffness detection and estimation of dominant spectra with explicit Runge-Kutta methods. *ACM Transactions on Mathematical Software*, **24**, 368–382.

Hairer, E., G. Wanner (1996). *Solving Ordinary Differential Equations II*, 2nd ed., Springer.

Higham, D., L. Trefethen (1993). Stiffness of ODE's. *BIT*, **33**, 285–303.

Richtmyer, R.D., K.W. Morton (1967). *Difference Methods for Initial-Value Problems*, Wiley-Interscience.

Samarskij, A.A. (1988). *The Theory of Difference Schemes*, Nauka, Moscow. (in Russian)

Shirkov, P.D. (1984). On accuracy of monotonic schemes for systems of stiff differential equations. *Zh. Vychisl. Matem. i Matem. Fiziki*, **24**, 1577–1580 (in Russian).

Stetter, H.J. (1973). *Analysis of Discretization Methods for Ordinary Differential Equations*. Springer-Verlag, New-York.

Raim. Čiegis has graduated from Vilnius University Faculty of Mathematics in 1982. He received the PhD degree from the Institute of Mathematics of Belorussian Academy of Science in 1985 and the degree of Habil. Doctor of Mathematics from the Institute of Mathematics and Informatics, Vilnius in 1993. He is a professor and the head of Mathematical Modelling department of Vilnius Gediminas Technical University. His research interests include numerical methods for solving nonlinear PDE, parallel numerical methods and mathematical modelling in nonlinear optics, biophysics, technology.

Rem. Čiegis has graduated from Kaunas Technological University, Faculty of Engineering Chemistry in 1982. He received the PhD degree in economics from the Vilnius University. He is an assoc. professor of Vilnius University, Kaunas Faculty of Humanities. His research interests include mathematical modelling of problems dealing with sustainable economics and ecology.

O. Subač has graduated from Vilnius University Faculty of Mathematics. She received her B.Sc. in 1996 and M.Sc. in 1998. Now she is a PhD student at Vilnius Gediminas Technical University. Her research interests include numerical algorithms for solving PDE and mathematical modelling of bioreaction processes.

Diferencialinių lygčių standžiųjų sistemų adaptyvusis integravimas

Raimondas ČIEGIS, Remigijus ČIEGIS, Olga SUBOČ

Šiame darbe nagrinėjamas adaptyviųjų integravimo algoritmų efektyvumas, kai sprendžiamos standžiosios paprastųjų diferencialinių lygčių sistemos. Lokalioji vieno žingsnio paklaida įvertinama palyginant diferencialinės lygties ir jos aproksimacijos augimo daugiklius. Parodyta, kad išreikštinių integravimo algoritmų kaštus galima pakankamai tiksliai įvertinti remiantis sistemos jakobiano sąlygotumo skaičiumi. Neišreikštinių integravimo algoritmų skaičiavimo kaštai priklauso ne nuo matricos sąlygotumo skaičiaus, bet nuo matricos tikrinių reikšmių sankaupos taškų skaičiaus.