ABSOLUTELY STABLE EXPLICIT SCHEMES FOR REACTION SYSTEMS

Eun-Hee Park [1] , Chang-Ock Lee [1] , Jae Boum Youm [2] and Chae Hun Leem [3]

1) *Division of Applied Mathematics, KAIST, Daejeon, 305-701, Korea*

2) *Department of Physiology, College of Medicine, Inje University, Busan, 614-735, Korea*

3) *Department of Physiology, College of Medicine, University of Ulsan, Seoul, 138-736, Korea*

Corresponding Author : Chang-Ock Lee, colee@amath.kaist.ac.kr

Co-corresponding Author : Chae Hun Leem, leemch@amc.seoul.kr

ABSTRACT

Many phenomena of interest in physiology and biochemistry are characterized by reactions among several chemical species and diffusion in various mediums (see [4–7]). In a closed system, both reactions and diffusion are governed by a system of ordinary differential equations (ODEs)

$$\dot{\mathbf{y}}(t) = M\mathbf{y}(t), \tag{1}$$

which guarantees conservation of the total amount of $\mathbf{y}(t)$ for any $t \geq 0$. Since we are concerned with the steady-state solution as well as the transient in simulations of very large systems of chemical reactions or molecular dynamics, we need to take the overall computational cost into consideration. Many physiologists and biochemists prefer explicit methods to implicit methods since implementation of the explicit methods is easier than the others. The popular methods for reaction systems are simple explicit schemes such as Euler's method, Runge-Kutta method, etc. However, it is well-known that conditional stability, the typical weak point of explicit methods, is very fatal for stiff problems. In the past few decades, many studies on numerical methods for stiff ODEs have been done in various aspects (see [1–3]).

The aim of this talk is to present two absolutely stable explicit schemes which are applicable to a general reaction system (1). The proposed methods are motivated by the simple exact solver for a reversible reaction. In spite of their explicitness, we have unconditional stability, that is, stability without any condition on the step size. Furthermore, we proved the convergence of the proposed methods; one is of first order and the other is of second order.

REFERENCES

1. J.C. Butcher and H. Podhaisky, *On error estimation in general linear methods for stiff ODEs*, Appl. Numer. Math., 56(2006), pp. 345-357.
2. K. Eriksson, C. Johnson, and A. Logg, *Explicit time-stepping for stiff ODEs*, SIAM J. Sci. Comput., 25(2003), pp. 1142-1157.
3. A. Iserles, *Composite methods for numerical solution of stiff systems of ODE's*, SIAM J. Numer. Anal., 21(1984), pp. 340-351.
4. J. Keener and J. Sneyd, *Mathematical physiology*, Springer-Verlag, New York, 1998.

5. M.W.J.M. Musters, J.B. Basssingthwaighte, V. Panday, N.A.W. van Riel, and G.J. van der Vusse, *Computational modeling of cardiac fatty acid uptake and utilization*, In: Lipobiology, G.J. van den Vusse ed., Elsevier, Amsterdam, 2004, pp. 173-224.
6. N.C. Price and R.A. Dwek, *Principles and problems in physical chemistry for biochemists*, Oxford University Press, Oxford, 1979.
7. W. Simon, *Mathematical techniques for biology and medicine*, Dover Publications, New York, 1986.