The Effective Order of Singly–Implicit Methods for Stiff Differential Equations

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ABSTRACT

Singly-implicit Runge-Kutta methods (SIRK) are designed for stiff differential equations. The existing code *STRIDE* based on these methods has been shown to be efficient for stiff problems, especially for high dimensional problems. However, SIRK methods with order greater than 2 possess the undesirable property that some of their abscissae are outside the integration interval. In order to improve the numerical behaviour of SIRK methods, we need to overcome this drawback. While retaining the original advantages of SIRK methods as much as possible, it would be advantageous to have more free parameters in choosing the coefficients for these methods.

Recently, two generalizations of SIRK methods were introduced to overcome this difficulty. One is the so-called "DESI" (Diagonally Extended Singly-Implicit Runge-Kutta) method in which some additional diagonally implicit stages are added to the corresponding classical SIRK method. It turns out that there is more freedom in choosing the abscissae because of these extra stages. The other generalization is the so-called "ESIRK" (Effective order Singly-Implicit Runge-Kutta) method which adopts the idea of "effective order" so that the desirable free parameters come from "perturbed" initial values. The first approach has been verified to be a successful generalization. The existing variable order code *DESI* was shown to be more efficient than *STRIDE*, and competes well with the BDF (Backward Differentiation Formulae) code *LSODE* for many stiff problems (Butcher, Cash, Diamantakis [24] 1996).

For the second approach, the numerical behaviour of ESIRK methods with variable stepsize, is closely related to the choice of the abscissae. In this thesis, it is shown that the classical SIRK methods are not the best choice with respect to the local truncation error. We analyze the numerical behaviour of the ESIRK methods both theoretically and experimentally. The choices of the abscissae for these methods are investigated. It is found that except when $s = 2$ (s is the number of stages in the method), the numerical results obtained with equally spaced abscissae in $[0, 1]$ are better than the corresponding SIRK methods for

$s = 3, \ldots, 6, 8$. Several alternative choices are also given. Some experimental variable-stepsize ESIRK codes are designed and are compared with the famous IRK codes *SDIRK4*, *RADAU5* and the BDF code *LSODE*. The numerical results show that ESIRK methods are successful generalizations of the SIRK methods and are good candidates as solvers for stiff problems.

In attempting to increase the efficiency of ESIRK methods, the idea of adding some additional diagonal stages is proposed. The generalizations of the ESIRK methods, called "EDESI" (Effective order Diagonally Extended Singly-Implicit Runge-Kutta) methods, are shown to be promising in solving stiff problems and are also successful generalizations of DESI and ESIRK methods.

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Contents

List of Figures

List of Tables