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**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

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$s = 3, \dots, 6, 8$ . 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 "EDES" (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

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Review of singly-implicit Runge-Kutta methods . . . . .	1
1.2	The aims and the framework of this thesis . . . . .	9
<b>2</b>	<b>Numerical methods for stiff differential equations</b>	<b>11</b>
2.1	Stiff problems . . . . .	12
2.2	Stability requirements . . . . .	17
2.3	Implicit Runge–Kutta methods . . . . .	23
<b>3</b>	<b>Singly–Implicit Methods</b>	<b>37</b>
3.1	Butcher’s transformation . . . . .	38
3.2	SIRK methods and their stability . . . . .	44
3.3	The transformation matrix . . . . .	48
3.4	DESI methods . . . . .	52
<b>4</b>	<b>The effective order of SIRK methods</b>	<b>63</b>
4.1	Effective order . . . . .	64
4.2	Effective order conditions for SIRK methods . . . . .	76



4.3	Doubly Companion Matrices . . . . .	87
4.4	ESIRK methods . . . . .	99
4.5	Variable stepsize for ESIRK methods . . . . .	113
4.6	Study of a systematic stepsize change pattern . . . . .	118
4.6.1	Local truncation error . . . . .	122
4.6.2	Stability considerations . . . . .	142
4.7	Error estimation for changing stepsize and order . . . . .	150
4.8	Implementation and some numerical results . . . . .	166
<b>5</b>	<b>The design of an EDESI integrator</b>	<b>191</b>
5.1	Construction of EDESI methods . . . . .	192
5.2	Variable step-size for EDESI methods . . . . .	206
5.3	Implementation . . . . .	211
5.4	Numerical results . . . . .	214
<b>A</b>	<b>Mathematica and Matlab programs</b>	<b>245</b>
A.1	Transformation matrix $T = WV$ for ESIRK methods . . . . .	245
A.2	Stability function $R(z, r)$ . . . . .	249
A.3	Local truncation error . . . . .	253
A.3.1	Error ratio $\varepsilon(r, c)$ . . . . .	253
A.3.2	Normalized error constant $\widehat{C}(r, c)$ . . . . .	255
	<b>Bibliography</b>	<b>258</b>

# List of Figures

1.1	Runge-Kutta methods for stiff problems . . . . .	8
2.1	The components of the Robertson problem (2.6) . . . . .	15
2.2	The first component of the Van der Pol problem (2.7) with $\theta = 10^6$	17
2.3	The second component of (2.7) with $\theta = 10^6$ . . . . .	17
4.1	Integration procedure for effective order methods . . . . .	66
4.2	Effective order method $\phi$ and the starting method $\psi$ . . . . .	67
4.3	Order-2 SIRK: $-$ , $[\frac{7-4\sqrt{2}}{3}, 1]$ : $+$ , $[0, 1]$ : $\dots$ , order-3 SIRK: $--$ , $[0, \frac{1}{5}, 1]$ : $\times$ , $[0, \frac{1}{2}, 1]$ : $\circ$ . . . . .	109
4.4	Order-2 SIRK: $-$ , $[\frac{7-4\sqrt{2}}{3}, 1]$ : $+$ , $[0, 1]$ : $\dots$ , order-3 SIRK: $--$ , $[0, \frac{1}{5}, 1]$ : $\times$ , $[0, \frac{1}{2}, 1]$ : $\circ$ . . . . .	109
4.5	Variable stepsize scheme for ESIRK methods . . . . .	113
4.6	Stepsize changing pattern for studying stability function of variable stepsize ESIRK methods . . . . .	120
4.7	$s = 2$ , Graph of $\bar{\varepsilon}(c_1) = \frac{\partial^2}{\partial r^2} \varepsilon(r, c_1) _{r=1}$ . . . . .	124
4.8	$s = 2$ , error ratio $\varepsilon(r, c_1)$ of variable stepsize against constant stepsize	125
4.9	$s = 3$ , $c_1 = 0$ , $y$ -axis : $\bar{\varepsilon}(c_2) = \frac{\partial^2}{\partial r^2} \varepsilon(r, c_2) _{r=1}$ , $x$ -axis : $c_2$ . . . . .	126
4.10	$s = 3$ , error ratio $\varepsilon(r, c)$ of variable stepsize/constant stepsize . . .	126

4.11  $s = 3, c_1 = -1, y\text{-axis} : \bar{\varepsilon}(c_2) = \frac{\partial^2}{\partial r^2} \varepsilon(r, c_2)|_{r=1}, x\text{-axis} : c_2 \dots\dots\dots 127$

4.12  $s = 3, \text{error ratio } \varepsilon(r, c) \text{ of variable stepsize/constant stepsize} \dots\dots\dots 127$

4.13 The error ratio  $\varepsilon(r, c)$  for ESIRK methods  $(0, \frac{1}{2}, 1), (-1, 0, 1)$ . The curve  $\varepsilon(r, c)$  for  $(-1, 0, 1)$  is concave down when  $r \in (0.844405, 1.18427)$  and is only smaller than the the curve of  $(0, \frac{1}{2}, 1)$ , when  $r \in (0.65, 1.53846)$ .  $\dots\dots\dots 128$

4.14 Order-2 SIRK, ESIRK methods  $(0, 1), (\frac{7-4\sqrt{2}}{3}, 1) \dots\dots\dots 129$

4.15 Order-2 SIRK, ESIRK methods  $(0, 1), (\frac{7-4\sqrt{2}}{3}, 1) \dots\dots\dots 131$

4.16 Order-3 SIRK, ESIRK methods  $(0, \frac{1}{2}, 1), (0, \frac{1}{5}, 1) \dots\dots\dots 131$

4.17 Second derivative of the normalized error constant  $\widehat{C}(r, c_1)|_{r=1}$  for  $s = 2 \dots\dots\dots 133$

4.18 Normalized error constant  $\widehat{C}(r, c)$  for  $s = 2$  SIRK, ESIRK methods 134

4.19 Normalized error constant  $\widehat{C}(r, c)$  of SIRK, ESIRK  $E_2 = (\frac{7-4\sqrt{2}}{3}, 1), E_2 = (\frac{1}{4}, 1)$  for  $s = 2 \dots\dots\dots 134$

4.20 ContourPlot of  $\frac{\partial^2}{\partial r^2} \widehat{C}(r, c_1, c_2)|_{r=1}, \widehat{C}(r)$  is the normalized error constant for  $s = 3$  ESIRK,  $y\text{-axis} : c_2, x\text{-axis} : c_1 \dots\dots\dots 135$

4.21  $s = 3$ , Normalized error constants  $\widehat{C}(r)$  of SIRK, ESIRK  $E_1 : (0, \frac{1}{2}, 1), E_2 : (0, \frac{1}{5}, 1), E_3 : (0, -\frac{1}{2}, 1), E_5 : (-\frac{3}{2}, -1, 1), E_4 : (-1, -\frac{9}{10}, 1) \dots\dots\dots 136$

4.22  $s = 4$ , Normalized error constants  $\widehat{C}(r)$  of SIRK, ESIRK  $E_1 : (0, \frac{1}{3}, \frac{2}{3}, 1), E_2 : (-1, -\frac{1}{2}, 0, 1), E_3 : (-1, -\frac{1}{2}, \frac{1}{2}, 1), E_4 : (-2, -1, 0, 1) \dots\dots\dots 139$

4.23 Normalized error constants  $\widehat{C}(r)$  of order-5 SIRK and ESIRK methods  $E_1 : (0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1), \text{ and } E_2 : (-1, -\frac{1}{2}, 0, \frac{1}{2}, 1), \text{ and } E_3 : (-2, -1, -\frac{1}{2}, 0, 1), \text{ and } E_4 : (-3, -2, -1, 0, 1) \dots\dots\dots 140$

4.24 Normalized error constants  $\widehat{C}(r)$  of order-6 SIRK and ESIRK methods  $E_1 : (0, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, 1), \text{ and } E_2 : (-1, -\frac{2}{3}, -\frac{1}{3}, \frac{1}{3}, \frac{2}{3}, 1), \text{ and } E_3 : (-2, -\frac{3}{2}, -1, -\frac{1}{2}, 0, 1), \text{ and } E_4 : (-4, -3, -2, -1, 0, 1) \dots\dots\dots 140$

4.25	Normalized error constants $\widehat{C}(r)$ of order-8 SIRK, ESIRK methods $E_1 : (0, \frac{1}{7}, \frac{2}{7}, \frac{3}{7}, \frac{4}{7}, \frac{5}{7}, \frac{6}{7}, 1)$ , $E_2 : (-1, -\frac{3}{4}, -\frac{2}{4}, -\frac{1}{4}, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1)$ , and $E_3 :$ $(-2, -\frac{5}{3}, -\frac{4}{3}, -\frac{2}{3}, -\frac{1}{3}, \frac{1}{3}, \frac{2}{3}, 1)$ , $E_4 : (-3, -\frac{5}{2}, -2, -\frac{3}{2}, -1, -\frac{1}{2}, 0, 1)$	141
4.26	Error estimation of order-2 ESIRK for the Kaps problem . . . . .	163
4.27	Work/Precision diagrams for order-4 ESIRK methods, A-stable: -, $A(\alpha = 1.56)$ -stable: -- . . . . .	179
4.28	Work/Precision diagrams for order-6 ESIRK methods, A-stable: -, $A(\alpha = 1.49)$ -stable: -- . . . . .	180
4.29	Work/Precision diagrams for order 4, 5, 6 ESIRK methods, order 4: +, order 5: o, order 6: x . . . . .	181
4.30	Work/precision diagram of ESIRK4 and <i>SDIRK4</i> . . . . .	182
4.31	Work/precision diagram of ESIRK5, <i>LSODE</i> and <i>RADAU5</i> . . . . .	183
4.32	Work/precision diagram of ESIRK5, <i>LSODE</i> and <i>RADAU5</i> . . . . .	184
4.33	Work/precision diagram of ESIRK5, <i>LSODE</i> and <i>RADAU5</i> . . . . .	185
5.1	Error vs. stepsize for order-2 singly-implicit methods with constant stepsize . . . . .	204
5.2	Flops vs. error for order-2 singly-implicit methods with constant stepsize . . . . .	204
5.3	Work/Precision diagram (flops/maximum error) for EDESI meth- ods solving the Kaps problem, $s = p + 1$ : --, $s = p + 2$ : - . . . . .	210
5.4	Work/precision diagrams of order-2 singly-implicit methods, SIRK: +, DESI: *, ESIRK: o, EDESI: x . . . . .	220
5.5	Work/precision diagrams of order-3 singly-implicit methods, SIRK: +, DESI: *, ESIRK: o, EDESI: x . . . . .	222
5.6	Work/precision diagrams of order-4 singly-implicit methods, SIRK: +, DESI: *, ESIRK: o, EDESI: x . . . . .	223

# List of Tables

2.1	Summary of the stability, stiff accuracy and orders of some A-stable one-step methods . . . . .	27
3.1	Total approximate number of operations for solving $N$ dimensional systems . . . . .	42
3.2	Total flops for solving the Kaps problem (3.9) . . . . .	44
3.3	$\lambda$ for L-stability with $s$ -stage SIRK methods . . . . .	47
3.4	Error constants of SIRK and DESI . . . . .	58
3.5	Numerical results for Kaps (3.9) using order-2 SIRK and DESI . .	60
4.1	$F(t)(y), \gamma(t), \alpha(t)$ for $\rho(t) \leq 4$ . . . . .	73
4.2	Number of order conditions for effective order $\geq s$ . . . . .	76
4.3	Absolute value of error constant for ESIRK methods . . . . .	107
4.4	The global error for the Kaps problem using $s = 2, 3$ SIRK and ESIRK methods with constant stepsize . . . . .	110
4.5	The average iteration number for the Kaps problem using $s = 2$ SIRK and ESIRK methods, $tol$ : tolerance for stopping the iteration.	111
4.6	The average iteration number for the Kaps problem using $s = 3$ SIRK and ESIRK methods, $tol$ : tolerance for stopping the iteration.	112

LIST OF TABLES

---

4.7	Order 2, 3 SIRK, ESIRK methods with stepsize changing pattern $h, rh, h, \dots$ . . . . .	130
4.8	$s = 2, 3$ , Normalized error ratio (ESIRK/SIRK) for solving the Kaps problem . . . . .	137
4.9	Normalized error ratio (ESIRK/SIRK) using order-3 methods for DETEST $A_1, D_1$ . . . . .	139
4.10	$r$ -intervals for A-stability for order 2, 3 ESIRK methods . . . . .	145
4.11	$r$ -intervals for A-stability for order 4, 5 ESIRK methods . . . . .	146
4.12	$r$ -intervals for A-stability for order 6, 8 ESIRK methods . . . . .	147
4.13	Proper abscissae for ESIRK methods . . . . .	149
4.14	Numerical results for stiff DETEST $A_1, A_2, A_3, D_1, D_2, D_3$ with order-2 SIRK, ESIRK methods . . . . .	151
4.15	Numerical results for A-group of stiff DETEST with order-3 SIRK, ESIRK methods . . . . .	152
4.16	Numerical results for B-group of stiff DETEST with order-3 SIRK, ESIRK methods . . . . .	153
4.17	Results for C-group of stiff DETEST with order-3 SIRK, ESIRK methods . . . . .	154
4.18	Numerical results for D-group of stiff DETEST with order-3 SIRK, ESIRK methods . . . . .	155
4.19	Numerical results for E-group of stiff DETEST with order-3 SIRK, ESIRK methods . . . . .	156
4.20	Results when using previous solution value (A), predictor (4.73) (B) and predictor (4.74) (C) with order-2 ESIRK method . . . . .	172
4.21	Results when using previous solution value (A), predictor (4.73) (B) and predictor (4.74) (C) with order-3 ESIRK method . . . . .	173

4.22	$\frac{1}{\lambda}$ of $A(\alpha)$ -stable ESIRK methods with $\alpha \geq 1.45$ , the value of $\alpha$ is given in parentheses . . . . .	177
4.23	Numerical results for Van der Pol (2.7) by testing order-4 L-stable, $A(\alpha)$ -stable ESIRKs and order-4 L-stable <i>SDIRK</i> . . . . .	186
4.24	Numerical results for Van der Pol (2.7) problem by testing <i>LSODE</i> , <i>RADAU5</i> and order-5 L-stable ESIRK . . . . .	187
4.25	Numerical results for Robertson problem (2.6) by testing <i>LSODE</i> , <i>RADAU5</i> and order-5 L-stable ESIRK . . . . .	188
4.26	Numerical results for Oregonator (4.77) by testing <i>LSODE</i> , <i>RADAU5</i> and order-5 L-stable ESIRK . . . . .	189
5.1	Numerical results for the Kaps problem using order 2 SIRK, DESI, ESIRK and EDESI ( $s = p + 1, s = p + 2$ ) with constant stepsize . . . . .	205
5.2	Results when using predictor (4.74) (A) and previous solution value (B) with order 2, 3 EDESI . . . . .	215
5.3	Efficiency measurement of some singly-implicit methods . . . . .	217
5.4	Summary of SIRK and DESI . . . . .	224
5.5	Summary of ESIRK and EDESI . . . . .	225
5.6	Numerical results for Curtis (5.23) by testing order-2 singly-implicit methods . . . . .	226
5.7	Numerical results for Prothero-Robinson (2.5) by testing order-2 singly-implicit methods . . . . .	227
5.8	Numerical results for Kaps (3.9) by testing order-2 singly-implicit methods . . . . .	228
5.9	Numerical results for Oregonator (4.77) by testing order-2 singly-implicit methods . . . . .	229
5.10	Numerical results for Robertson (2.6) by testing order-2 singly-implicit methods . . . . .	230

*LIST OF TABLES*

---

5.11 Numerical results for Van der Pol (2.7) by testing order-2 singly-implicit methods . . . . .	231
5.12 Numerical results for Prothero-Robinson by testing order-3 methods	232
5.13 Numerical results for Curtis problem by testing order-3 methods . . . . .	233
5.14 Numerical results for Kaps by testing order-3 methods . . . . .	234
5.15 Numerical results for Oregonator by testing order-3 methods . . . . .	235
5.16 Numerical results for Robertson by testing order-3 methods . . . . .	236
5.17 Numerical results for Van der Pol by testing order-3 methods . . . . .	237
5.18 Numerical results for Prothero-Robinson by testing order-4 methods	238
5.19 Numerical results for Curtis problem by testing order-4 methods . . . . .	239
5.20 Numerical results for Kaps by testing order-4 methods . . . . .	240
5.21 Numerical results for Oregonator by testing order-4 methods . . . . .	241
5.22 Numerical results for Robertson by testing order-4 methods . . . . .	242
5.23 Numerical results for Van der Pol by testing order-4 methods . . . . .	243