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A Critical Evaluation of the Semiimplicit Runge-Kutta Methods for Stiff Systems

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Frequently we encounter systems of ordinary differential equations in which there exists a large spread in the magnitude of the governing time constants. Conventional methods such as the explicit Runge-Kutta methods are known to be unsuitable for the integration of these so called stiff systems. Severe step length restrictions are imposed by the requirements for numerical stability, and thus a prohibitively large number of steps is often required.

A number of researchers have been actively seeking new techniques for the solution of such systems. Some of the more recent methods which have been given considerable attention are improved semiimplicit Runge-Kutta (SIRK) methods (Michelsen, 1976, 1977; Villadsen and Michelsen, 1978), an extension of the work of Caillaud and Padmanabhan (1971) to include a suitable step size adjustment procedure.

Their general formulation for $\mathbf{y}' = \mathbf{f}(\mathbf{y})$ is

$$\mathbf{k}_i = (\underline{\mathbf{I}} - ah\underline{\mathbf{J}})^{-1} h\mathbf{f}\left(\mathbf{y}_n + \sum_{j=1}^{i-1} b_{ij}\mathbf{k}_j\right) \qquad i = 1, 2 \ldots N$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \sum_{i=1}^{N} R_i\mathbf{k}_i$$

where

$$\underline{\mathbf{J}} = (\partial \mathbf{f}_i/\partial \mathbf{y}_j)_{y_n}$$

N is the number of stages in the method. The constants a, b, and R are given by Michelsen (1977).

The Jacobian $\underline{\mathbf{J}}$ is evaluated once for each step, and the value of $\mathbf{f}$ at only one intermediate point is required. With LU decomposition of the matrix $(\underline{\mathbf{I}} - ah\underline{\mathbf{J}})$, the method requires only the solution of a set of linear equations equal in dimension to that of the system, with three different right-hand sides (for the third-order system). The solution process is then sequential in determining the $\mathbf{k}_i$.

A full step-half step technique is used for step size adjustment. At each selected step size, the problem is first integrated by using the full step size. The same integration is then performed in two steps, each of length one half the original step. A refined solution vector, where the dominant $0(h^4)$ error term cancels, is found, and the next step size is proposed based on an empirical procedure. The step size is adjusted to keep the local truncation error below some specified value.

This method is known to have the property of absolute stability (the stability region associated with the formulation contains the open left half plane) and has been successfully applied by Michelsen (1976, 1977) to a number of stiff systems. However, in most of the published results, comparisons are made with the fourth-order explicit Runge-Kutta method only (constant step size). In all cases, the semiimplicit methods have been shown to be superior. Although no data were presented, Michelsen (1977) claims that the third-order method yielded identical results as Gear's method (1971) using about the same amount of computation time.

In this work, we attempt to evaluate critically the SIRK methods by a direct comparison of the third-order method (Villadsen and Michelsen, 1978) with the code developed by Hindmarsh (1974), possibly the best all-purpose, optimized, stiff package available. It is hoped that by direct comparison with an established package for stiff systems some insight can be gained into the potential of the SIRK methods.

NUMERICAL RESULTS

The systems used in the comparison represent a large spectrum of problem types: linear, nonlinear, problems with real and complex eigenvalues, large and small stiff systems, and problems with various degrees of stiffness. We have considered eighteen different problems and have selected six to present as representative examples, the general trend of results being comparable to the others.

Problem 1: nonlinear system of reaction rate equations, Robertson (1967):

$$y_1' = -0.04y_1 + 10^4 y_2 y_3 \qquad \text{I.C. } y(0) = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2$$

$$y_3' = 3 \times 10^7 y_2^2 \qquad \text{Range} = (0, 10)$$

Problem 2: nonlinear example of Van der Pol's equation, Davis (1962):

$$y_1' = y_2 \qquad \text{I.C. } y(0) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$y_2' = 1\,000(1 - y_1^2)y_2 - y_1 \qquad \text{Range} = (0, 2)$$

Problem 3: nonlinear chemistry example, Gear (1969):

$$y_1' = -0.013y_1 - 1\,000y_1y_3 \qquad \text{I.C. } y(0) = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

Table 1. Numerical Results of Six Stiff Problems

Problem	Method	Steps	Decompositions	CPU time (s) CDC/6400	Relative accumulated error
					for $y_2(10)$
		197	197	2.23	$<1 \times 10^{-7}$
	SIRK	48	48	0.58	1.5×10^{-6}
1		15	15	0.19	3.6×10^{-5}
		123	20	0.46	$<1 \times 10^{-7}$
	Gear	46	11	0.18	6.7×10^{-6}
		39	11	0.14	1×10^{-4}
					for $y_2(1.22)$
		2 640	2 640	17.36	$<1 \times 10^{-5}$
	SIRK	464	464	3.24	4×10^{-4}
2		152	152	1.08	2.7×10^{-2}
		3 089	174	11.02	$<1 \times 10^{-5}$
	Gear	1 472	94	4.2	1.3×10^{-4}
		225	34	1.22	3.8×10^{-2}
					for $y_3(50)$
		150	150	1.70	$<1 \times 10^{-7}$
	SIRK	36	36	0.47	1.2×10^{-6}
3		18	18	0.22	1.6×10^{-5}
		73	14	0.29	$<1 \times 10^{-7}$
	Gear	34	9	0.15	2.1×10^{-6}
		20	6	0.08	9.1×10^{-5}
					for $y_3(100)$
		1 627	1 627	20.88	$<1 \times 10^{-6}$
	SIRK	187	187	2.46	3.4×10^{-5}
4		108	108	1.53	2.1×10^{-4}
		2 863	199	14.15	$<1 \times 10^{-6}$
	Gear	999	93	4.02	2×10^{-4}
		542	62	2.49	1.5×10^{-3}
					for $y_4(10)$
		3 236	3 236	113.83	$<1 \times 10^{-7}$
	SIRK	1 094	1 094	43.27	4×10^{-7}
5		91	91	3.25	1.2×10^{-3}
		1 536	90	8.97	$<1 \times 10^{-7}$
	Gear	787	54	6.30	1×10^{-6}
		537	40	3.22	1×10^{-5}
					for $y_1(5)$
		4 726	4 726	103.20	3.2×10^{-5}
6	SIRK	1 535	1 535	28.49	1.5×10^{-3}
		567	567	10.5	0.15
		247	247	4.49	14.6
	Gear	98	18	.63	1.5×10^{-5}

$$y_2' = -2\,500 y_2 y_3 \qquad \text{Range} = (0, 50)$$

$$y_3' = -0.013 y_1 - 1\,000 y_1 y_3 - 2\,500 y_2 y_3$$

Problem 4: nonlinear example of an oscillating chemical system, Field and Noyes (1974):

$$y_1' = 77.27(y_2 - y_1 y_2 + y_1 - 8.375 \times 10^{-6} y_1^2) \qquad \text{I.C. } y(0) = \begin{bmatrix} 4 \\ 1.1 \\ 4 \end{bmatrix}$$

$$y_2' = (-y_2 - y_1 y_2 + y_3)/77.27 \qquad \text{Range} = (0, 300)$$

$$y_3' = 0.161(y_1 - y_3)$$

Problem 5: linear, moderately stiff, complex eigenvalue problem, Johnson and Barney (1976):

$$y_1' = -1\,000 y_1 + y_2 + 988 e^{-y_5}$$

$$y_2' = -1\,001 y_2 + 1\,000 e^{-y_5} \qquad \text{I.C. } y(0) = \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 0 \end{bmatrix}$$

$$y_3' = -y_3 + y_4 - e^{-y_5}$$

$$y_4' = -y_3 - y_4 + e^{-y_5} \qquad \text{Range} = (0, 100)$$

$$y_5' = 1$$

Problem 6: nonlinear, parasitic solution example, Hornbeck (1975):

$$y_1' = 5(y_1 - y_2^2) \qquad \text{I.C. } y(0) = \begin{pmatrix} 0.08 \\ 0 \end{pmatrix}$$

$$y_2' = 1 \qquad \text{Range} = (0, 5)$$

The numerical results appear in Table 1, where a number of runs for each problem and method are presented.

Although it is difficult to draw any definite conclusions from these results, a general pattern is indicated. The Gear package appears to be more reliable and much more efficient when high accuracy is desired. On the problems tested, the Gear package has been found to be always more computationally efficient (as much as 100 times) than the third-order SIRK method in obtaining solutions accurate to six or seven figures.

For most cases, the semiimplicit algorithm will approach the Gear package in computational efficiency as the specified error tolerance requirement is lowered. In fact, the efficiency of Michelsen's algorithm (Villadsen and Michelsen, 1978) surpasses that of the Gear routine for problems 2 and 4, where significance of three and four figures, respectively, is desired.

Results of problem 6 deviate drastically from the general trend. The Gear package is unquestionably the better routine in obtaining the desired solution.

DISCUSSION

In analyzing the above results, we must keep in mind two important facts:

1. The SIRK methods require a triangular matrix decomposition at each step. This is not the case in considering the Gear package, for correction vectors are determined iteratively.
2. The SIRK methods are one-step methods; that is, the numerical technique utilized to calculate the approximation to the solution at t_{n+1} is based solely on the value at one previous step, namely t_n. In the Gear package, values of the dependent variable at a number of previous points (depending on the order of the method) are utilized to estimate the solution at t_n; hence the method is termed multistep.

It is clear from the first factor that for larger systems of equations, the SIRK methods will become less computationally efficient relative to the Gear package primarily on the basis of the increased size of the system which must be decomposed at each step.

The one-step characteristic of the SIRK methods permits them to have the property of absolute stability for higher order formulations. Absolute stability for the implicit multistep methods of Gear is limited to order two or less (Dalquist, 1963). From this, it would appear that the SIRK methods would have an advantage over Gear's method for problems in which very negative decay constants would force the order of the method to be reduced to two in order to ensure stability. Enright and Hull (1976), in a comparison of various numerical techniques for stiff systems, noted the difficulty encountered by various methods, based on the backward differentiation formulas (for example, Gear package), in integrating stiff problems which have eigenvalues of the Jacobian matrix close to the imaginary axis (near the boundary of Gear's stiffly stable region). The property of absolute stability for higher orders of the SIRK methods (Michelsen, 1976) is well recognized.

However, we must also consider the drawbacks of the one-step formulations. As pointed out by Carnahan et al. (1969), certain equations with specified initial conditions cannot be solved efficiently by one-step methods because of the parasitic nature of the solution. Problem 6 is an example of this type. This innocent appearing differential equation has been discussed by Hornbeck (1975). The exact solution is of the form

$$y_1 = Ae^{5t} + t^2 + 0.4t + 0.08$$

where the term Ae^{5t} is the homogeneous solution, and the remainder is the particular solution. For the initial condition of $y_1(0) = 0.08$, $A = 0$, and the exact solution is

$$y_1 = t^2 + 0.4t + 0.08$$

When such an equation is solved by using a one-step method, each new step may be viewed as the solution of a new initial value problem. Even if the initial condition is error free for the first step, the initial conditions for subsequent steps will inevitably contain errors introduced by truncation and roundoff in previous steps. For problem 6, the exponential term lurks in the background, ready to explode if the numerical solution strays even slightly from the exact solution. For this particular problem, a very tiny change in the initial condition (0.08000010) will give a result at $t = 5$ three orders of magnitude greater than the true solution.

One final consideration to note in the SIRK formulations is that the method has been constructed so that a certain number of terms fit the Taylor series exactly (Caillaud and Padmanabhan, 1971). This requires that the Jacobian $\underline{J}$ be evaluated accurately (for example, by analytical differentiation). Gear's method, based on purely implicit formulations, requires only an approximate Jacobian matrix. It is apparent that the SIRK methods are limited to problems in which the differentials are well defined and can be determined analytically, whereas the Gear package is capable of utilizing internally calculated Jacobians.

The poor results obtained by the SIRK methods in obtaining high accuracy may be directly related to the order of the method. A better approach may be to run a fourth-order method in conjunction with the third-order method. This would eliminate the use of the half step-full step technique to evaluate the local truncation error and may also increase the accuracy of the solution.

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