Stability of generalized Runge–Kutta methods for stiff kinetics coupled differential equations

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Abstract
A stability and efficiency improved class of generalized Runge–Kutta methods of order 4 are developed for the numerical solution of stiff system kinetics equations for linear and/or nonlinear coupled differential equations. The determination of the coefficients required by the method is precisely obtained from the so-called equations of condition which in turn are derived by an approach based on Butcher series. Since the equations of condition are fewer in number, free parameters can be chosen for optimizing any desired feature of the process. A further related coefficient set with different values of these parameters and the region of absolute stability of the method have been introduced. In addition, the $A(\alpha)$ stability properties of the method are investigated. Implementing the method in a personal computer estimated the accuracy and speed of calculations and verified the good performances of the proposed new schemes for several sample problems of the stiff system point kinetics equations with reactivity feedback.

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1. Introduction

Stiff differential equations frequently arise in physical kinetics equations due to the existence of greatly differing time constants, which almost refer to the rate of decay or change. Initial value problems with strongly decreasing and increasing solution components with the independent variable are called stiff problems. The system of the point kinetics equations possesses a stiff character which include equations that describe the neutron level, reactivity, an arbitrary number of delayed neutron groups and any thermodynamic variables that enter into the reactivity equation. Usual integration routines suffer from one or more disadvantages, because of the different growth of the solution components.

In recent decades, there has been a considerable amount of research on methods for numerical integration of the stiff system of ODEs, usually looking for better stability properties; such methods are nearly implicit in character. In 1972, Butcher [1] published a valuable article in which he analysed general Runge–Kutta methods on the basis of the algebra of rooted trees (ART). He showed that the Runge–Kutta methods form a group (which is called after that Butcher group) and developed explicit expressions for the inverse of a method or the product of two methods. He also gave an explicit perturbative solution of nonlinear differential equations, written as a series indexed by rooted trees (now called B-series). Important developments were then made by Hairer and Wanner in 1974 [2]. Since then, B-series have been used in the analysis of Runge–Kutta methods.

Implicit Runge–Kutta formulae [3–6] have been widely used because of their excellent stability properties (such as A-stability, $A(\alpha)$ stability, L-stability and B-stability), but the need for solving nonlinear algebraic equations at each step makes these formulae generally too costly when considering some huge systems of ODEs.

Many other attempts have been made in order to reduce the computation cost per step by considering linearly implicit methods, in this way eliminating the need for solving nonlinear systems which usually are solved by Newton-type iteration. Such formulae have the computational advantage that it is necessary to solve only linear system of algebraic equation at each step. An example of such a scheme is the generalized Runge–Kutta scheme (GRK) proceeded from Rosenbrock [7], i.e. a Runge–Kutta scheme where the Jacobian matrix is introduced directly into the coefficients of the Runge–Kutta formula. This scheme proposed a special class of the Jacobian matrix at each Runge–Kutta stage. Among the many different GRK-like methods of this type we have the modified Rosenbrock methods (ROW) [8–11]. However, these formulae that are widely used require the exact Jacobian at every step; therefore, the computation is costly and from a practical point of view, such formulae are unattractive. For this reason, extensions of Rosenbrock methods are fixed for some number of steps so that the computation is reduced [12–14]. Moreover, Rosenbrock-type methods in which the exact Jacobian is no longer needed have been considered. The generalized Runge–Kutta methods [9, 12, 15] fall into this class. For an excellent survey of some of these methods the reader may be referred to [16].

The point-kinetics equations are a system of differential equations for the neutron density and for the delayed neutron precursor concentrations (delayed neutron precursors are radioactive isotopes which are formed in the fission process and decay through neutron emission). The neutron density and delayed neutron precursor concentrations determine the time-dependent behaviour of the power level of a nuclear reactor and are influenced, for example, by controlling the rod position. Computational solutions of the point-kinetics equations provide insight into the dynamics of nuclear reactor operation and are useful, for example, in understanding the power fluctuations experienced during start-up or shut-down when the control rods are adjusted. Recently, a large number of kinetics studies have been reported [17–24], which modelled the time-dependent behaviour of a nuclear reactor using the point-kinetics equations.

In this paper, a generalization of the straightforward Runge–Kutta method of order 4 with different $A(\alpha)$ stabilities is developed and applied to integrate stiff ordinary differential equations. The equations of condition for this class of semi-implicit methods are resolved inside a wide range of interval taking into consideration that the free parameters (ε and γ) are specified at different points over a wide range of stability intervals using the idea of inner and outer iterations. For a specified value of ε, the inner iteration is carried out on γ for some stated interval whenever $A(\alpha)$ stability is studied. Repeating this process at different values

of ε produces the outer iteration. Furthermore, different stabilities are obtained where the equations of condition are resolved and applied to the coupled linear and/or nonlinear point kinetics equations with fuel feedback. The percentage error of the neutron density is estimated and reported.

This paper is organized as follows. In section 2, the generalized Runge–Kutta (GRK) method is introduced and modified where the equations of condition are resolved. For further generalization of the method, new sets of free parameters are introduced and implemented by embedding inner and outer iterations. The stability of the modified Rosenbrock (ROW) methods is developed. In section 3, the GRK method with stability group constants is applied to the linear and/or nonlinear coupled system of the point kinetics equations. Finally in section 4, to verify the validity and efficiency of the developed method, comparisons are carried out on the numerical experiments between different analogous methods for step, ramp, oscillatory reactivity as well as the case in which the feedback reactivity is a function of neutron density.

2. Generalized Runge–Kutta method (GRK)

A generalized Runge–Kutta (GRK) method for the numerical solution of the autonomous initial value problem

$$y'(x) = f[y(x)], \qquad y(x_0) = y_0, \tag{1}$$

where y, y_0 and f in general are vectors in n-dimensional real space, is sought by integrating from x_0 to $(x_0 + h)$, in the form

$$y_{i+1} = y_i + \int_{x_0}^{x_0+h} f[y(x)]\, \mathrm{d}x$$

or, in the equivalent form

$$y_{i+1} = y_i + \sum_{j=1}^{s} C_j K_j, \tag{2}$$

where the vector K_j is determined by solving the s linear equations [7]

$$[I - \gamma h f'(y_0)]K_i = h f \left[y_i + \sum_{j=1}^{i-1} \alpha_{ij} K_j \right] + h f'(y_0) \sum_{j=1}^{i-1} \gamma_{ij} K_j \qquad i = 1, \ldots, s. \tag{3}$$

Method (3) is called the modified Rosenbrock method, short ROW method [7]; this method coincides with the corresponding Runge–Kutta method when $\gamma_{ij} = 0$. The method used a variable step size, which is estimated by computing the solution y_{i+1} given by equation (2), and a lower order estimate $\bar{y}_{i+1}$ with different coefficients $\bar{C}_i (\hat{s} \prec s)$ and the same K_i. Analogous to the approach followed in the Runge–Kutta Fehlberg methods for nonstiff systems, the third-order method is combined with a fourth-order method using the same time step size h to obtain an estimate of the truncation error, which in turn utilized to estimate the next step control. To compute the vector K_i $(i = 1, \ldots, s)$ given by equation (3), a linear system of order

n for four right-hand sides must be solved:

$$
\left.
\begin{aligned}
K_1 &= hBf(y_0) \\
K_2 + \left(\frac{\gamma_{21}}{\gamma}\right) K_1 &= B\left[hf(y_0 + \alpha_{21}K_1) + \left(\frac{\gamma_{21}}{\gamma}\right)K_1\right] \\
K_3 + \left(\frac{1}{\gamma}\right)\sum_{\ell=1}^{2}\gamma_{3\ell}K_\ell &= B\left[hf\left(y_0 + \sum_{\ell=1}^{2}\alpha_{3\ell}K_\ell\right) + \left(\frac{1}{\gamma}\right)\sum_{\ell=1}^{2}\gamma_{3\ell}K_\ell\right] \\
K_4 + \left(\frac{1}{\gamma}\right)\sum_{\ell=1}^{3}\gamma_{4\ell}K_\ell &= B\left[hf\left(y_0 + \sum_{\ell=1}^{3}\alpha_{4\ell}K_\ell\right) + \left(\frac{1}{\gamma}\right)\sum_{\ell=1}^{3}\gamma_{4\ell}K_\ell\right]
\end{aligned}
\right\}
\tag{4}
$$
$$
B = [I - h\gamma f'(y_0)]^{-1},
$$

where y_i is the approximate solution at x_i, h denotes the step size, $f'(y_0)$ is the Jacobian, $\mathbf{I}$ is the $(n \times n)$ identity matrix and s is the number of stages. The coefficients γ, C_i, α_{ij} and γ_{ij} are real numbers and fixed constants independent of the problem.

In 1979, Kaps and Rentrop [9] suggested two different sets of coefficients, which have slightly different properties. The number of stages s is equal to the order of the method. The Jacobian $f'(y_0)$ is computed by difference approximation and should be replaced by an analytic version for very sensitive problems.

On the same line, two such cases for the stages s are considered here with $s = 3$ and $s = 4$ (i.e. third-order and fourth-order methods). Fourth- and third-order approximations denoted by y_{i+1} and $\bar{y}_{i+1}$, respectively are introduced according to the following formulae. The ROW method of order 4 given by

$$
y_{i+1} = y_i + \sum_{i=1}^{s} C_i K_i \qquad \text{for} \quad (s = 4)
\tag{5a}
$$

and the ROW method of order 3 given by

$$
\bar{y}_{i+1} = \bar{y}_i + \sum_{i=1}^{s} \bar{C}_i K_i \qquad \text{for} \quad (s = 3)
\tag{5b}
$$

are combined, where the coefficients γ, α_{ij} and γ_{ij} $(i = 1, \ldots, s: j = 1, \ldots, i-1)$. Therefore, K_i is the same for both formulae (5a) and (5b). The results of the fourth-order method are taken as initial guess for the next step. These two methods coincide with the corresponding conventional Runge–Kutta method when γ_{ij} equal zero.

2.1. Equations of condition

The determination of the coefficients required by the GRK method is fairly involved [9]. It can be said that they are obtained from the so-called equations of condition which in turn are derived by an approach similar to that followed in the usual Runge–Kutta method, except that the Butcher series [2] are used instead of the Taylor series. Since the equations of condition are fewer in number than the unknown, several of these can be chosen as free parameters in order to determine a complete set of constants. The previous calculations utilized only one free parameter, while in the present study, new set of parameters (ε and γ) are introduced for generalizing the method over a large interval. Each particular choice of these parameters leads to a method whose region of absolute stability can be analytically delimited. Furthermore, the validity of these parameters enables solving the equations of condition for third and fourth orders of stability intervals.

The determination of the coefficients γ, C_i, α_{ij} and γ_{ij} required by the method is obtained by solving equations of condition which are derived in [10] and by applying the theory of

Butcher series, the equations up to order 5 for y_{i+1} are calculated and listed in the following table:

Order 1		Order 5 (for truncation error investigations)	
$\sum C_i = 1$	(6)	$\sum C_i \alpha_i^4 = \frac{1}{5}$	(14)
Order 2		$\sum C_i \alpha_i^2 \alpha_{ik}\beta_k = \frac{1}{10} - \frac{1}{4}\gamma = p_{10}(\gamma)$	(15)
$\sum C_i \beta_i = \frac{1}{2} - \gamma = p_2(\gamma)$	(7)	$\sum C_i \alpha_{ik}\beta_k\alpha_{il}\beta_l = \frac{1}{20} - \frac{1}{4}\gamma + \frac{1}{3}\gamma^2 = p_{11}(\gamma)$	(16)
Order 3		$\sum C_i \alpha_i \alpha_{ik}\alpha_k^2 = \frac{1}{15}$	(17)
$\sum C_i \alpha_i^2 = \frac{1}{3}$	(8)	$\sum C_i \alpha_i \alpha_{ik}\beta_{kl}\beta_l = \frac{1}{30} - \frac{1}{4}\gamma + \frac{1}{3}\gamma^2 = p_{13}(\gamma)$	(18)
$\sum C_i \beta_{ij}\beta_j = \frac{1}{6} - \gamma + \gamma^2 = p_4(\gamma)$	(9)	$\sum C_i \beta_{ik}\alpha_k^3 = \frac{1}{20} - \frac{1}{4}\gamma = p_{14}(\gamma)$	(19)
Order 4		$\sum C_i \beta_{ik}\alpha_k\alpha_{kl}\beta_l = \frac{1}{40} - \frac{5}{24}\gamma + \frac{1}{3}\gamma^2 = p_{15}(\gamma)$	(20)
$\sum C_i \alpha_i^3 = \frac{1}{4}$	(10)	$\sum C_i \beta_{ik}\beta_{kl}\alpha_l^2 = \frac{1}{60} - \frac{1}{6}\gamma + \frac{1}{3}\gamma^2 = p_{16}(\gamma)$	(21)
$\sum C_i \alpha_i \alpha_{ik}\beta_k = \frac{1}{8} - \frac{1}{3}\gamma = p_6(\gamma)$	(11)	$\sum C_i \beta_{ik}\beta_{kl}\beta_{lm}\beta_m = \frac{1}{120} - \frac{1}{6}\gamma + \gamma^2 - 2\gamma^3 + \gamma^4$	
$\sum C_i \beta_{ik}\alpha_k^2 = \frac{1}{12} - \frac{1}{3}\gamma = p_7(\gamma)$	(12)	$= p_{17}(\gamma)$	(22)
$\sum C_i \beta_{ik}\beta_{kl}\beta_l = \frac{1}{24} - \frac{1}{2}\gamma + \frac{3}{2}\gamma^2 - \gamma^3 = p_8(\gamma)$	(13)		

where the summation indices $i, j, k, l, m = 1, \ldots, s$, and the following abbreviations are used:

$$\left. \begin{array}{ll} \alpha_i = \Sigma\alpha_{ij}, & \beta_{ij} = \alpha_{ij} + \gamma_{ij}, \\ \beta_i = \Sigma\beta_{ij}, & \alpha_{ij} = \gamma_{ij} = 0, \qquad \text{for } i \leqslant j \end{array} \right\}. \tag{23}$$

The equations of condition for a third order (i.e. equation (5b)) for $\bar{y}_{i+1}$ are obtained by replacing C_i by $\bar{C}_i$ and s by $\bar{s}$ in the above equations. In order to derive the system of equations of order 4, inserting relations (23) into equations of condition ((6)–(22)) with $s = 3$ and $s = 4$. The system of equations are obtained and listed in the following table.

$s = 3$		$s = 4$	
Order 1			
$\bar{C}_1 + \bar{C}_2 + \bar{C}_3 = 1$	(24)	$C_1 + C_2 + C_3 + C_4 = 1$	(35)
Order 2			
$\bar{C}_2\beta_{21} + \bar{C}_3(\beta_{31} + \beta_{32}) = p_2(\gamma)$	(25)	$C_2\beta_{21} + C_3(\beta_{31} + \beta_{32}) + C_4(\beta_{41} + \beta_{42} + \beta_{43}) = p_2(\gamma)$	(36)
Order 3			
$\bar{C}_2\alpha_{21}^2 + \bar{C}_3(\alpha_{31} + \alpha_{32})^2 = \frac{1}{3}$	(26)	$C_2\alpha_{21}^2 + C_3(\alpha_{31} + \alpha_{32})^2 + C_4(\alpha_{41} + \alpha_{42} + \alpha_{43})^2 = \frac{1}{3}$	(37)
$\bar{C}_3\beta_{32}\beta_{21} = p_4(\gamma)$	(27)	$C_3\beta_{32}\beta_{21} + C_4\beta_{42}\beta_{21} + C_4\beta_{43}(\beta_{31} + \beta_{32}) = p_4(\gamma)$	(38)
Order 4			
$\bar{C}_2\alpha_{21}^3 + \bar{C}_3(\alpha_{31} + \alpha_{32})^3 = \frac{1}{4}$	(28)	$C_2\alpha_{21}^3 + C_3(\alpha_{31} + \alpha_{32})^3 + C_4(\alpha_{41} + \alpha_{42} + \alpha_{43})^3 = \frac{1}{4}$	(39)
$\bar{C}_3(\alpha_{31} + \alpha_{32})\beta_{21}\alpha_{32} = p_6(\gamma)$	(29)	$C_3\alpha_{32}\beta_{21}(\alpha_{31} + \alpha_{32}) + C_4\alpha_{42}\beta_{21}(\alpha_{41} + \alpha_{42} + \alpha_{43})$	
$\bar{C}_3\beta_{32}\alpha_{21}^2 = p_7(\gamma)$	(30)	$\quad + C_4\alpha_{43}(\beta_{31} + \beta_{32})(\alpha_{41} + \alpha_{42} + \alpha_{43}) = p_6(\gamma)$	(40)
		$C_3\beta_{32}\alpha_{21}^2 + C_4\beta_{42}\alpha_{21}^2 + C_4\beta_{43}(\alpha_{31} + \alpha_{32})^2 = p_7(\gamma)$	(41)
		$C_4\beta_{43}\beta_{32}\beta_{21} = p_8(\gamma)$	(42)
Order 5			
$\bar{C}_2\alpha_{21}^4 + \bar{C}_3(\alpha_{31} + \alpha_{32})^4 = \frac{1}{5}$	(31)	$C_2\alpha_{21}^4 + C_3(\alpha_{31} + \alpha_{32})^4 + C_4(\alpha_{41} + \alpha_{42} + \alpha_{43})^4 = \frac{1}{5}$	(43)
		$C_3\alpha_{32}\beta_{21}(\alpha_{31} + \alpha_{32})^2$	
		$\quad + C_4\alpha_{43}(\beta_{31} + \beta_{32})(\alpha_{41} + \alpha_{42} + \alpha_{43})^2 = p_{10}(\gamma)$	(44)
$\bar{C}_3(\alpha_{31} + \alpha_{32})^2\alpha_{32}\beta_{21} = p_{10}(\gamma)$	(32)	$C_3\alpha_{32}^2\beta_{21}^2 + C_4\alpha_{42}^2\beta_{21}^2 + C_4\alpha_{42}\beta_{21}(\beta_{31} + \beta_{32})$	
		$\quad + C_4\alpha_{43}^2(\beta_{31} + \beta_{32})^2 = p_{11}(\gamma)$	(45)
		$C_3\alpha_{32}\alpha_{21}^2(\alpha_{31} + \alpha_{32}) + C_4\alpha_{42}\alpha_{21}^2(\alpha_{41} + \alpha_{42} + \alpha_{43})$	
		$\quad + C_4\alpha_{43}(\alpha_{31} + \alpha_{32})^2(\alpha_{41} + \alpha_{42} + \alpha_{43}) = \frac{1}{15}$	(46)
$\bar{C}_3\alpha_{32}^2\beta_{21}^2 = p_{11}(\gamma)$	(33)	$C_4\alpha_{43}\beta_{21}\beta_{32}(\alpha_{41} + \alpha_{42} + \alpha_{43}) = p_{13}(\gamma)$	(47)
		$C_3\alpha_{21}^3\beta_{32} + C_4\beta_{42}\alpha_{21}^3 + C_4\beta_{43}(\alpha_{31} + \alpha_{32})^3 = p_{14}(\gamma)$	(48)
$\bar{C}_3\alpha_{32}\alpha_{21}^2(\alpha_{31} + \alpha_{32}) = \frac{1}{15}$	(34)	$C_4\alpha_{32}\beta_{21}\beta_{43}(\alpha_{31} + \alpha_{32}) = p_{15}(\gamma)$	(49)
		$C_4\beta_{43}\beta_{32}\alpha_{21}^2 = p_{16}(\gamma)$	(50)

Applying condition (23) in the case of $s = 3$ equations (13), (18)–(22) are disappeared ($\beta_{ij} = 0$, for $i \leqslant j$), while in the case of $s = 4$ only equation (22) is disappeared, for the same reason, from the above system of conditions. The system of conditions (33) and (34) for $s = 3$ and the system of conditions (35)–(50) for $s = 4$ for the unknown constants can be solved, where equations (35), (37) and (39) are combined using relations (23) and converted to the matrix form as

$$
\begin{pmatrix} 1 & 1 & 1 \\ 0 & \alpha_2^2 & \alpha_3^2 \\ 0 & \alpha_2^3 & \alpha_3^3 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 + C_4 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{3} \\ \frac{1}{4} \end{pmatrix},
$$

where

$$
\alpha_2 = \alpha_{21}, \qquad \alpha_3 = \alpha_{31} + \alpha_{32} \qquad \text{and} \qquad \alpha_3 = \alpha_4.
$$

Solving this system of equations for the constants C_i ($i = 1, \ldots, 4$), we get

$$
\left.\begin{aligned}
C_1 &= 1 - \frac{(\alpha_3^3 - \alpha_2^3)}{3(\alpha_2\alpha_3)^2(\alpha_3 - \alpha_2)} + \frac{\alpha_3 + \alpha_2}{4(\alpha_2\alpha_3)^2} \\
C_2 &= \frac{4\alpha_3 - 3}{12\alpha_2^2(\alpha_3 - \alpha_2)} \\
C_3 + C_4 &= \frac{-4\alpha_2 + 3}{12\alpha_3^2(\alpha_3 - \alpha_2)}
\end{aligned}\right\}. \tag{51}
$$

Recalling equation (42)

$$
\beta_{32}\beta_2 = \frac{p_8}{C_4\beta_{43}} = u, \qquad \text{where} \quad \beta_2 = \beta_{21}. \tag{52}
$$

The constants $\bar{C}_1$, $\bar{C}_2$, $\bar{C}_3$ can be determined from equations (24), (26) and (27) which could be represented in the following matrix form:

$$
\begin{pmatrix} 1 & 1 & 1 \\ 0 & \alpha_2^2 & \alpha_3^2 \\ 0 & 0 & u \end{pmatrix} \begin{pmatrix} \bar{C}_1 \\ \bar{C}_2 \\ \bar{C}_3 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{3} \\ p_4(\gamma) \end{pmatrix}.
$$

Through solving this system for the constants ($i = 1, 2, 3$), we get

$$
\begin{aligned}
\bar{C}_1 &= 1 - \frac{1}{3\alpha_2^2} + \frac{\alpha_3^2 - \alpha_2^2}{\alpha_2^2 u} p_4(\gamma) \\
\bar{C}_2 &= \frac{1}{3\alpha_2^2} - \frac{\alpha_3^2}{\alpha_2^2 u} p_4(\gamma) \\
\bar{C}_3 &= \frac{p_4(\gamma)}{u}.
\end{aligned} \tag{53}
$$

Using equation (41) gives

$$
C_3\beta_{32} + C_4\beta_{42} = \left(p_7(\gamma) - C_4\beta_{43}\alpha_3^2\right)/\alpha_2^2 = v. \tag{54}
$$

Similarly, equations (25), (38) and (54) can be rewritten in the following matrix form:

$$
\begin{pmatrix} v & C_4\beta_{43} \\ \bar{C}_2 & \bar{C}_3 \end{pmatrix} \begin{pmatrix} \beta_2 \\ \beta_3 \end{pmatrix} = \begin{pmatrix} p_4(\gamma) \\ p_2(\gamma) \end{pmatrix}
$$

and by solving this system for the constants β_i ($i = 1, 2$), we get

$$
\beta_2 = \frac{\bar{C}_3}{\Omega} p_4 - \frac{C_4\beta_{43}}{\Omega} p_2(\gamma), \tag{55a}
$$

$$\beta_3 = -\frac{\bar{C}_2}{\Omega} p_4(\gamma) - \frac{v}{\Omega} p_2(\gamma), \tag{55b}$$

where

$$\Omega = v\bar{C}_3 - \bar{C}_2 C_4 \beta_{43}. \tag{55c}$$

Also, by converting equations (40) and (41) to the matrix form

$$\begin{pmatrix} \beta_2 & 0 \\ C_3 & C_4 \end{pmatrix} \begin{pmatrix} \beta_{32} \\ \beta_{42} \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix}$$

and then solving this system for the constants β_{32} and β_{42}, we get

$$\beta_{32} = \frac{u}{\beta_2} \tag{56a}$$

$$\beta_{42} = \frac{-uC_3}{C_4\beta_2} + \frac{v}{C_4}. \tag{56b}$$

By inserting $\alpha_{43} = 0$ and $\alpha_{42} = \alpha_{32}$ into equations (36) and (40), the following equations are obtained:

$$\beta_4 = \frac{p_2(\gamma) - C_2\beta_2 - C_3\beta_3}{C_4} \tag{57a}$$

$$\alpha_{32} = \frac{p_6(\gamma)}{(C_3 + C_4)\alpha_3\beta_2}. \tag{57b}$$

The remaining free parameters, except γ, can be chosen so that several equations of condition of order 5, e.g. equation (48), are satisfied. Accordingly, equations (37), (39), (41) and (48) could be written in the matrix form as

$$\begin{pmatrix} \alpha_2^2 & \alpha_3^2 & \alpha_3^2 & 0 \\ \alpha_2^3 & \alpha_3^3 & \alpha_3^3 & 0 \\ 0 & \beta_{32}\alpha_2^2 & \beta_{42}\alpha_2^2 & \beta_{43}\alpha_3^2 \\ 0 & \beta_{32}\alpha_2^3 & \beta_{42}\alpha_2^3 & \beta_{43}\alpha_3^3 \end{pmatrix} \begin{pmatrix} C_2 \\ C_3 \\ C_4 \\ C_4 \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{1}{4} \\ p_7(\gamma) \\ p_{14}(\gamma) \end{pmatrix},$$

since

$$\det \begin{pmatrix} \alpha_2^2 & \alpha_3^2 & \alpha_3^2 & 0 \\ \alpha_2^3 & \alpha_3^3 & \alpha_3^3 & 0 \\ 0 & \beta_{32}\alpha_2^2 & \beta_{42}\alpha_2^2 & \beta_{43}\alpha_3^2 \\ 0 & \beta_{32}\alpha_2^3 & \beta_{42}\alpha_2^3 & \beta_{43}\alpha_3^3 \end{pmatrix} = 0.$$

The last system is singular except when $C_3 = 0$. On the other hand, C_4 has no influence on the truncation error; its value can also be chosen so that $C_3 = 0$. Then equations (37), (39), (41) and (48) can be rewritten in the matrix form where the values of C_2, C_4, $C_4\beta_{42}$ and $C_4\beta_{43}$ are solutions of the linear system:

$$\begin{pmatrix} \alpha_2^2 & \alpha_3^2 \\ \alpha_2^3 & \alpha_3^3 \end{pmatrix} \begin{pmatrix} C_2 & C_4\beta_{42} \\ C_4 & C_4\beta_{43} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} & p_7(\gamma) \\ \frac{1}{4} & p_{14}(\gamma) \end{pmatrix}.$$

By solving this system for the constants β_{32}, β_{42}, C_2 and C_4, we get

$$C_2 = \frac{4\alpha_3 - 3}{12\alpha_2^2(\alpha_3 - \alpha_2)} \tag{58a}$$

$$C_4 = \frac{-4\alpha_3 + 3}{12\alpha_3^2(\alpha_3 - \alpha_2)} \tag{58b}$$

$$\beta_{42} = \frac{\alpha_3 p_7(\gamma) - p_{14}(\gamma)}{C_4\alpha_2^2(\alpha_3 - \alpha_2)} \tag{59a}$$

$$\beta_{43} = \frac{-\alpha_2 p_7(\gamma) - p_{14}(\gamma)}{C_4\alpha_3^2(\alpha_3 - \alpha_2)}. \tag{59b}$$

Depending on the free parameters α_2 and α_3 and by substituting $C_4\beta_{43}$, from equation (59b) into equations (52), (54) and (55c), the values of the constants u, v and Ω were obtained.

Also, by using the value $C_4\beta_{42}$ from equation (59a) and the value β_{32} from equation (56a) the values of C_3 and C_4 can be separately obtained by substituting into equation (54):

$$C_3 = \frac{v - C_4\beta_{42}}{\beta_{32}}.$$

By applying a back substitution the values of β_2 and β_3 are obtained from equations (55a) and (55b). The value of α_{32} from equation (57b) gives $\alpha_{31} = \alpha_3 - \alpha_{32}$. Similarly, from equations (55b) and (56a) the value of $\beta_{31} = \beta_3 - \beta_{32}$ is obtained.

On the other hand, the value of β_{41} is obtained from equations (57a), (56b) and (59b) where

$$\beta_{41} = \beta_4 - \beta_{42} - \beta_{43}.$$

Since $\beta_{ij} = \alpha_{ij} + \gamma_{ij}$ the values of the following constants are easily obtained:

$$\gamma_{21} = \beta_{21} - \alpha_{21}, \qquad \gamma_{31} = \beta_{31} - \alpha_{31}, \qquad \gamma_{32} = \beta_{32} - \alpha_{32}, \qquad \gamma_{41} = \beta_{41} - \alpha_{41}$$
$$\gamma_{42} = \beta_{42} - \alpha_{42}, \qquad \gamma_{43} = \beta_{43} \qquad \text{and} \qquad \alpha_{43} = 0.$$

The remaining free parameters, except γ, can be chosen so that again several equations of condition of order 5, here equation (43), are satisfied.

For $\alpha_2 \neq \alpha_3$ equations (35), (37), (39) and (43) possessed a solution, iff

$$\det \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & \alpha_2^2 & \alpha_3^2 & \frac{1}{3} \\ 0 & \alpha_2^3 & \alpha_3^3 & \frac{1}{4} \\ 0 & \alpha_2^4 & \alpha_3^4 & \frac{1}{5} \end{pmatrix} = 0.$$

Therefore,

$$\alpha_3 = \frac{\frac{1}{5} - \frac{1}{4}\alpha_2}{\frac{1}{4} - \frac{1}{3}\alpha_2}. \tag{60}$$

The choice of α_2 for most of the popular previous Rosenbrock methods has one degree of freedom, i.e. one free parameter. In the present study, further free parameters can be determined so that several orders of conditions of order 5 (e.g. equations (43) and (48)) are satisfied. The remaining free parameters are chosen so that it has two degrees of freedom; to do this let $\alpha_2 = \varepsilon\gamma$, where ε and γ are constants that essentially determine the stability properties.

2.2. Inner and outer iterations

In the previous section, the free parameters α_2, ε and γ are chosen under the condition

$$0 \leqslant \alpha_i \leqslant 1, \qquad i = 2, \ldots, s. \tag{61}$$

This restriction is merely required for the evaluation of the right-hand side of the differential equation in the integration interval, which represented a good restriction for the free parameters α_2 and α_3, i.e.

$$0 \leqslant \alpha_2 \leqslant 1, \qquad 0 \leqslant \alpha_3 \leqslant 1. \tag{62}$$

The present study on the free parameter γ shows that the value of $\gamma \in [0.376, 0.399]$ gives $\alpha_3 < 0$ which contradicted with the above restriction, while the value of $\gamma \in [0.0, 0.374] \cup [0.401, 1.5[$ satisfied the restriction (61) and good results are obtained with different $A(\alpha)$ stabilities.

To generalize and check the stability of the method at different points along the interval $[0, 1]$ different methods with the value of α_2 are proposed.

Substituting equation (60) into equation (61) gives

$$0 \leqslant \frac{\frac{1}{5} - \frac{1}{4}\alpha_2}{\frac{1}{4} - \frac{1}{3}\alpha_2} \leqslant 1.$$

The last inequality determines the range of α_2 so that

$$\alpha_2 \in [0, 0.6] \cup [0.8, 1[\, . \tag{63}$$

The new parameter ε is introduced so that outer iteration is performed and then the stability and truncation error are estimated; consequently outer iteration on γ is carried out. The parameter α_2 satisfying (63) in terms of the arbitrary constant ε resulted in

$$\varepsilon \in \left[0, \tfrac{0.6}{\gamma}\right] \cup \left[\tfrac{0.8}{\gamma}, \tfrac{1}{\gamma}\right[. \tag{64}$$

These new parameters ε, γ and α_2 enable choosing and optimizing some features of the process, e.g. stability, accuracy and efficiency.

2.3. Stability of the GRK (ROW) method

Stability properties of the ROW method of order $\geqslant s$ have been studied [9] and we now quote the obtained results which have been modified slightly in order that it can be applicable to a wide range of interval. Some care must be taken when selecting a value of γ or ε which is at the boundary of $A(\alpha)$ stability domain, since a small change in γ or ε can cause change in α and less stability is obtained.

To compute the stability function $R(z)$ for generalized Runge–Kutta schemes, consider Dahlquist's test equation

$$y' = \lambda y, \qquad y(x_0) = y_0, \qquad \lambda \in C, \qquad y_0 \in C, \qquad y : \Re \to C$$

that is a set of independent equations each of the form $z_i' = \lambda_i z_i$. In a general nonlinear equation, λ_i is identified with the eigenvalues of the Jacobian $\dfrac{\partial y'}{\partial y}$. These values determine the local behaviour of the system to a first approximation. The eigenvalues λ_i may of course be complex.

Since $f'(y) = \lambda$, it holds $K_i = R_i(z)y_0$, $z = \lambda h$, where $R_i(z)$ are rational functions with a denominator $(1 - \gamma z)^i$ and a degree of numerator $\leqslant i$; thus the numerical solution y_h from equation (2) is

$$y_h = R(z)y_0 \tag{65}$$

Table 1. $A(\alpha)$ stable and the coefficient set for different values of γ.

γ	0.2	0.21	0.22	0.23	0.24	0.25
α ($s = 4$)	$A(0)$	$89.32°$	$89.55°$	$89.39°$	$88.82°$	$86.53°$
Coefficients						
γ_{21}	$-0.259\,999\,99$	$-0.267\,210\,78$	$-0.271\,247\,06$	$-0.270\,954\,88$	$-0.264\,685\,69$	$-0.249\,999\,94$
γ_{31}	$-0.695\,085\,35$	$-0.246\,340\,63$	$0.061\,981\,38$	$0.291\,297\,44$	$0.473\,747\,79$	$0.630\,000\,59$
γ_{32}	$0.879\,633\,19$	$0.469\,196\,80$	$0.203\,011\,75$	$0.023\,020\,21$	$-0.099\,298\,78$	$-0.180\,000\,42$
γ_{41}	$0.703\,998\,21$	$0.574\,987\,59$	$0.440\,136\,64$	$0.297\,613\,14$	$0.143\,565\,55$	$-0.030\,000\,32$
γ_{42}	$-0.837\,151\,05$	$-0.715\,094\,21$	$-0.592\,296\,54$	$-0.470\,087\,89$	$-0.350\,074\,29$	$-0.233\,999\,79$
γ_{43}	$-0.057\,142\,85$	$-0.073\,636\,35$	$-0.090\,967\,71$	$-0.109\,310\,36$	$-0.128\,888\,88$	$-0.149\,999\,99$
α_{21}	$0.400\,000\,00$	$0.419\,999\,99$	$0.440\,000\,00$	$0.460\,000\,00$	$0.479\,999\,99$	$0.500\,000\,00$
α_{31}	$-0.542\,273\,82$	$-0.390\,184\,40$	$-0.241\,187\,75$	$-0.095\,863\,94$	$0.044\,874\,49$	$0.180\,000\,25$
α_{32}	$1.399\,416\,69$	$1.253\,820\,78$	$1.112\,155\,56$	$0.975\,174\,25$	$0.844\,014\,35$	$0.719\,999\,73$
β_{43}	$0.000\,000\,00$	$0.000\,000\,00$	$0.000\,000\,00$	$0.000\,000\,00$	$0.000\,000\,00$	$0.000\,000\,00$
C_1	$0.164\,352\,18$	$0.183\,539\,39$	$0.200\,644\,25$	$0.216\,031\,55$	$0.229\,998\,71$	$0.242\,798\,45$
C_2	$0.488\,281\,25$	$0.484\,027\,92$	$0.483\,279\,50$	$0.485\,803\,54$	$0.491\,426\,23$	$0.499\,999\,94$
C_3	$0.000\,000\,00$	$0.000\,000\,00$	$-0.000\,000\,01$	$0.000\,000\,00$	$0.000\,000\,00$	$0.000\,000\,00$
C_4	$0.347\,366\,90$	$0.332\,432\,66$	$0.316\,075\,92$	$0.298\,165\,14$	$0.278\,575\,15$	$0.257\,201\,67$
$\bar{C}_1$	$-1.008\,284\,45$	$-0.880\,243\,30$	$-0.786\,632\,42$	$-0.722\,037\,55$	$-0.685\,127\,38$	$-0.679\,012\,66$
$\bar{C}_2$	$1.987\,390\,16$	$1.877\,331\,02$	$1.808\,860\,78$	$1.777\,327\,06$	$1.783\,247\,23$	$1.833\,333\,73$
$\bar{C}_3$	$0.020\,894\,27$	$0.002\,912\,26$	$-0.022\,228\,37$	$-0.055\,289\,46$	$-0.098\,119\,92$	$-0.154\,321\,12$

with the stability function

$$R(z) = 1 + \sum_{i=1}^{s} C_i R_i(z) = \frac{P(z)}{Q(z)}.$$

For a rational approximation in equation (65) of order p, the stability function of a ROW method with order $p \geqslant s$ is given by

$$\left.\begin{aligned}
R(z) &= \frac{\sum_{i=0}^{s} L_i^{(s-i)}\left(\frac{1}{\gamma}\right)(-\gamma z)^i}{(1 - \gamma z)^s}, \\
\text{where} \quad L_i^j(z) &= \sum_{n=0}^{i} (-1)^n \binom{i+j}{i-n} \frac{z^n}{n!}
\end{aligned}\right\} \tag{66}$$

which stands for the generalized Laguerre polynomials [25]. $R(z)$ was a rational approximation to e^z of order $\geqslant s$. By means of the stability function, some stability properties could be characterized very conveniently.

One has stability at infinity, iff $\lim_{z\to\infty} |R(z)| = \left|L_s\left(\frac{1}{\gamma}\right)\right| \leqslant 1$, where $L_s = L_s^{(0)}$.

For $\gamma > 0$, a method (3) will be A-stable, iff $|R(\mathrm{i}y)| \leqslant 1$ for $y \in \Re$ and method (3) will be $A(\alpha)$-stable iff $|R(z)| \prec 1 \; \forall \alpha \in \left(0, \frac{\pi}{2}\right)$, for $z \in S(\alpha)$, where $S(\alpha) = \{z \in C, \mathrm{Re}(z) \prec 0 \; \wp \; 0 \leqslant |\arg(-z)| \prec \alpha\}$. The method is $A(0)$-stable if there exists an $\alpha \in \left(0, \frac{\pi}{2}\right)$ such that $R(z)$ is $A(\alpha)$-stable.

Table 1 shows the stability of third- and fourth-order methods within the interval (0.2, 0.25). For $\gamma \in (0.2, 0.25)$, $L_3\left(\frac{1}{\gamma}\right)$ is small, and the stability region of the third- and fourth-order methods is very large, table 1, see also figure 1 for Laguerre polynomials. A coefficient set is also listed in table 1 for different values of γ. For choosing γ and/or ε besides stability consideration the truncation error is taken into account in the inner and outer iterations which is important for a valuable application.
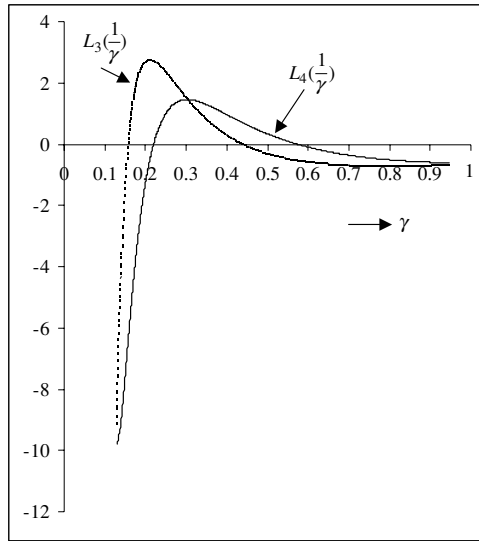
Figure 1. Laguerre polynomials.

3. Point reactor kinetics equations

The point reactor kinetics equations for the six group of delayed neutrons with feedback are written as

$$\frac{dN(t)}{dt} = \frac{\rho(N, t) - \beta}{\Lambda} N(t) + \sum_{i=1}^{\ell} \lambda_i C_i(t) \tag{67}$$

$$\frac{dC_i(t)}{dt} = \frac{\beta_i}{\lambda} N(t) - \lambda_i C_i(t), \qquad i = 1, 2, \ldots, \ell \tag{68}$$

$$\frac{d\theta}{dt} = 1.0, \tag{69}$$

where the notations are usual [17–20], $\rho(N, t)$ is in general a function of time and neutron density or fuel temperature in feedback problems. The quantities $N(t)$ and $C_i(t)$ are, in general, functions of time t, and λ_i, β_i and Λ are assumed constants. The dependent variable θ has been appended to the system of the point kinetics equations to convert the system to autonomous one, so the system dimension of the method will be $n \times n$ matrix.

Let y^k denote the kth component of a vector y; then the following correspondence is established:

$$y^1 = N(t), \qquad y^k = C_{k-1}, \qquad k = 2, \ldots, (\ell + 1), \qquad y^{(\ell+2)} = \theta.$$

With these, the vector $f(y)$ from equations (67)–(69) will be

$$f(y) = \begin{pmatrix} \frac{\rho(y^1, y^{(\ell+2)}) - \beta}{\Lambda} y^1 + \sum_{i=1}^{\ell} \lambda_i y^{i+1} \\ \frac{\beta_1}{\Lambda} y^1 - \lambda_1 y^2 \\ \vdots \\ \frac{\beta_\ell}{\Lambda} y^1 - \lambda_\ell y^{(\ell+1)} \\ 1 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{(\ell+1)} \\ f_{(\ell+2)} \end{pmatrix}$$

and the Jacobian matrix will take the form

$$
f'(y) = \begin{bmatrix}
\frac{1}{\Lambda}[\rho(y^1, y^{(\ell+2)}) - \beta] & \lambda_1 & \lambda_2 & \cdots & \lambda_\ell & \frac{y^1}{\Lambda}\frac{\partial\rho}{\partial y^{(\ell+2)}} \\
\frac{\beta_1}{\Lambda} & -\lambda_1 & 0 & \cdots & 0 & 0 \\
\frac{\beta_2}{\Lambda} & 0 & -\lambda_2 & \cdots & 0 & 0 \\
\vdots & & & \ddots & & \\
\frac{\beta_\ell}{\Lambda} & 0 & 0 & & -\lambda_\ell & 0 \\
0 & 0 & 0 & \cdots & 0 & 0
\end{bmatrix}.
$$

By denoting the matrix $[\mathbf{I} - h\gamma\ f'(y_0)]$ by $\mathbf{A}$, we get

$$
A = \begin{bmatrix}
1 - \frac{p}{\Lambda}[\rho(y^1, y^{(\ell+2)}) - \beta] & -p\lambda_1 & -p\lambda_2 & \cdots & -p\lambda_\ell & \frac{-p}{\Lambda}y^1\frac{\partial\rho}{\partial y^{(\ell+2)}} \\
\frac{-p\beta_1}{\Lambda} & 1 + p\lambda_1 & 0 & \cdots & 0 & 0 \\
\frac{-p\beta_2}{\Lambda} & 0 & 1 + p\lambda_2 & \cdots & 0 & 0 \\
\vdots & & & \ddots & & \\
\frac{-p\beta_\ell}{\Lambda} & 0 & 0 & & 1 + p\lambda_\ell & 0 \\
0 & 0 & 0 & \cdots & 0 & 1
\end{bmatrix},
$$

where we have made $p = h\gamma$.

The algorithm for calculating y_{i+1} given y_i consists in determining K_i using equations (4), evaluating y_{i+1} and $\bar{y}_{i+1}$ by means of equations (5a) and (5b) with y^1 as the controlling variable. The algorithm is coded in Visual FORTRAN for a personal computer as shown in figure 2. To assess the method, a set of problems described in the published reference is used, this set included step, ramp, zigzag ramp input reactivity and compensated reactivity feedback to the six-delayed group equation.

4. Numerical examples and discussions

The new group of coefficients is coded and applied to the point kinetics equations for different types of reactivities. The accuracy of the neutron flux is tested using the new set of coefficients with two different types of iterations, inner and outer iterations, for the free parameters γ and/or ε and α_{21}. The first iteration on γ lies within the range of interval [0.20, 0.25], while the second one is chosen so that $\alpha_{21} \in [0, 0.6] \cup [0.8, 1]$; exact results are obtained at the end of the first interval when α_{21} is near 0.6. A new family of GRK groups (equations of condition) are calculated and applied to the point kinetics equations. The best value of the new set of coefficients is denoted by GRK4-H which corresponds to $\gamma = 0.25$ with the free parameter $\alpha_{21} = 0.56$. For $\gamma = 0.25$ the fourth-order method is A(86.53°).

The generalized Runge–Kutta technique with the new set of coefficients is tested for different types of problems and the results are compared against those obtained from the other methods. The problems include step reactivity insertion, ramp input, oscillatory reactivity and finally reactivity feedback for average one group and six groups of delayed neutrons. These problems will be discussed in the following sections.

4.1. Step reactivity input

To check the accuracy of the algorithm, the code is applied to different points of step reactivity. This case corresponds to a negative step insertion of reactivity of 0.007$
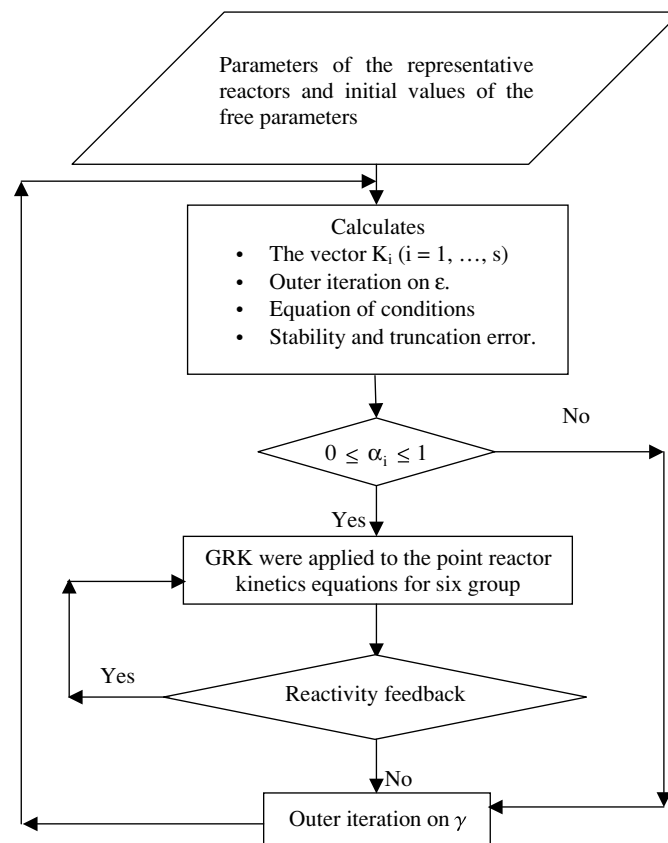
Figure 2. Block diagrams for the method of calculation.

in a thermal reactor [23]. The obtained results are shown in table 2. Calculations are made using the developed method of the new groups of coefficient sets GRK4-H. Comparison is made using the reactor kinetic data described as $\Lambda = 0.000\,02$ s, $\beta_{tot} = 0.007$, $\beta_i = (0.000\,266, 0.001\,491, 0.001\,316, 0.002\,849, 0.000\,896$ and $0.000\,182)$ and $\lambda_i = (0.0127, 0.0317, 0.115, 0.311, 1.40$ and $3.87)$ s^{-1}.

4.2. Ramp reactivity input

The reactivity case of a linear function of times (the so-called ramp input) is considered as an example of time-dependent reactivity. Comparisons are made with a ramp variation defined as $\rho = \rho_0 + \mu t$ for the different time-dependent reactivities. The values of the parameters used in this example were $\Lambda = 1.0 \times 10^{-4}$ s, $\beta_{tot} = 0.0064$, $\beta_i = (0.000\,211, 0.001\,402, 0.001\,254, 0.002\,528, 0.000\,736$ and $0.000\,269)$ and $\lambda_i = (0.0124, 0.0305, 0.115, 0.301, 1.138$ and $3.01)$ s^{-1}. The reference of $N(t)$ values is that reported in [26] with the exact value calculated at $t = 0.35$ s and the results are listed in table 2.

4.3. Oscillatory reactivity

In this case, the reactivity $\rho(t)$ is a function of time given as $\rho(\text{t}) = \xi \sin(t)$ which differentiated and inserted into the matrix $\mathbf{A} = \mathrm{I} - h\gamma f'(y)$. The parameter ξ is a positive number that

Table 2. Negative step insertion of reactivity of 0.007\$ for a thermal reactor [23].

γ Inner Iteration	α_{21} Outer Iteration	Step reactivity	Ramp reactivity	Oscillatory reactivity	Feedback reactivity
0.201	0.008	4.5083	$-2.124\,45 \times 10^{12}$	3.31	2.4214×10^{11}
	0.016	4.5087	$-2.073\,00 \times 10^{3}$	3.30	2.4211×10^{11}
	0.024	4.5087	1.000 235	3.30	2.4208×10^{11}
	0.032	4.5087	1.003 385	Exact	2.4206×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	0.376	Exact	Exact	Exact	2.4199×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	0.6	Exact	Exact	Exact	2.4198×10^{11}
	0.808	Exact	1.003 392	Exact	2.4201×10^{11}
	0.824	Exact	Exact	Exact	2.4199×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	1.0	Exact	Exact	Exact	2.4198×10^{11}
0.202	0.008	4.5083	-1.8328×10^{12}	3.31	2.4214×10^{11}
	0.016	4.5087	-1.7677×10^{3}	3.30	2.4211×10^{11}
	0.024	4.5088	1.000 758	3.30	2.4208×10^{11}
	0.032	Exact	1.003 385	Exact	2.4206×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	0.376	Exact	Exact	Exact	2.4199×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	0.6	Exact	Exact	Exact	2.4198×10^{11}
	0.808	Exact	1.003 392	Exact	2.4201×10^{11}
	0.84	Exact	Exact	Exact	2.4199×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	1.0	Exact	Exact	Exact	2.4198×10^{11}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
0.25	0.008	4.5083	$-5.584\,35 \times 10^{6}$	3.31	2.4213×10^{11}
	0.016	4.5087	1.002 304	3.30	2.4211×10^{11}
	0.024	4.5087	1.003 384	3.30	2.4208×10^{11}
	0.032	4.5088	1.003 386	Exact	2.4206×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	0.376	Exact	Exact	Exact	2.4199×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	0.6	Exact	Exact	Exact	2.4198×10^{11}
	0.808	Exact	Exact	Exact	2.4201×10^{11}
	0.84	Exact	Exact	Exact	2.4199×10^{11}
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	1.0	Exact	Exact	Exact	2.4198×10^{11}
PWS	–	4.5088	1.003 394	3.29	$2.214\,400 \times 10^{11}$
Exact	–	4.5088	1.003 394	3.29	$2.420\,364 \times 10^{11}$

Table 3. Compensated response to ramp function reactivity.

a	b	Method	First peak	Time to the first peak	Flux	TC
0.1	1×10^{-11}	PWS	$2.395\,7590 \times 10^{11}$	0.224 70	$1.006\,6510 \times 10^{10}$	3.02
		GRK4-A	$2.464\,9574 \times 10^{11}$	0.226 26	$1.006\,6499 \times 10^{10}$	4.33
		GRK4-T	$2.465\,2371 \times 10^{11}$	0.226 26	$1.006\,6500 \times 10^{10}$	4.33
		GRK4-H	$2.465\,4628 \times 10^{11}$	0.226 26	$1.006\,6501 \times 10^{10}$	4.33
					(at $t = 2.0727$)	
	1×10^{-13}	PWS	$2.866\,6680 \times 10^{13}$	0.235 80	$1.006\,6520 \times 10^{12}$	2.96
		GRK4-A	$2.958\,0990 \times 10^{13}$	0.240 66	$1.006\,6480 \times 10^{12}$	4.44
		GRK4-T	$2.958\,0157 \times 10^{13}$	0.240 66	$1.006\,6480 \times 10^{12}$	4.44
		GRK4-H	$2.957\,7276 \times 10^{13}$	0.240 66	$1.006\,6482 \times 10^{12}$	4.44
					(at $t = 2.0727$)	
0.01	1×10^{-11}	PWS	$2.006\,4920 \times 10^{10}$	1.106 10	$1.026\,3960 \times 10^{9}$	2.58
		GRK4-A	$2.023\,2131 \times 10^{10}$	1.107 36	$1.024\,6410 \times 10^{9}$	5.21
		GRK4-T	$2.023\,2020 \times 10^{10}$	1.107 36	$1.024\,6424 \times 10^{9}$	5.21
		GRK4-H	$2.023\,2065 \times 10^{10}$	1.107 36	$1.024\,6394 \times 10^{9}$	5.21
					(at $t = 2.0727$)	
	1×10^{-13}	PWS	$2.483\,1920 \times 10^{12}$	1.155 20	$9.670\,5500 \times 10^{10}$	2.74
		GRK4-A	$2.506\,1997 \times 10^{12}$	1.156 68	$9.637\,4374 \times 10^{10}$	4.44
		GRK4-T	$2.506\,1921 \times 10^{12}$	1.156 68	$9.637\,4817 \times 10^{10}$	4.44
		GRK4-H	$2.506\,1852 \times 10^{12}$	1.156 68	$9.637\,4301 \times 10^{10}$	4.44
					(at $t = 2.0727$)	
0.001	1×10^{-11}	PWS	$1.274\,0690 \times 10^{9}$	7.488 00	$1.921\,2660 \times 10^{8}$	9.06
		GRK4-A	$1.276\,0915 \times 10^{9}$	7.487 28	$1.920\,7147 \times 10^{8}$	4.66
		GRK4-T	$1.276\,1036 \times 10^{9}$	7.487 28	$1.920\,7122 \times 10^{8}$	4.39
		GRK4-H	$1.276\,0943 \times 10^{9}$	7.487 28	$1.920\,6984 \times 10^{8}$	4.39
					(at $t = 9.0$)	
	1×10^{-13}	PWS	$1.721\,0060 \times 10^{11}$	7.682 60	$2.004\,6470 \times 10^{10}$	9.11
		GRK4-A	$1.724\,5128 \times 10^{11}$	7.682 04	$2.004\,0163 \times 10^{10}$	4.61
		GRK4-T	$1.724\,5159 \times 10^{11}$	7.682 04	$2.004\,0077 \times 10^{10}$	4.61
		GRK4-H	$1.724\,5002 \times 10^{11}$	7.682 04	$2.003\,9905 \times 10^{10}$	4.61
					(at $t = 9.0$)	

TC = Total calculation time (s).

represented the magnitude of the variable part of the excess reactivity in dollars. It should be assumed sufficiently small if compared to unity. The values of the parameters used in this example are $\Lambda = 1.0 \times 10^{-4}$ s, $\beta_{\text{tot}} = 0.006\,45$, $\mu = 0.6\$$, $\beta_i = (0.000\,21, 0.001\,41, 0.001\,27, 0.002\,55, 0.000\,74$ and $0.000\,27)$ and $\lambda_i = (0.0124, 0.0305, 0.111, 0.301, 1.13$ and $3.0)$ s^{-1}. The numerical results for this case are tabulated in table 2. A comparison is made at $t = 2.26$ s with the previously obtained results from other analytical methods.

4.4. Compensated reactivity

In this example, the transient with feedback for six delayed groups is coupled. The following case is chosen from the work conducted by Keepin and Cox [27]:

$$\rho(t) = 0.1t - 10^{-11} \int_0^t N(t')\,\mathrm{d}t'. \tag{70}$$

The delayed group parameters are $\beta_i = (0.000\,21, 0.001\,41, 0.001\,27, 0.002\,59, 0.000\,74$ and $0.000\,27)$, $\lambda_i = (0.0124, 0.0305, 0.111, 0.301, 1.13$ and $3.0)$ s^{-1} and the generation time is

$\Lambda = 5.0 \times 10^{-5}$ s. Then the new set of coefficients is applied to the point kinetics equations with feedback reactivity; the solution over a time interval is considered and constructed by making use of the solution at the end points of the time interval, so that the feedback reactivity would be easily computed via an iterative process. Results for this case are shown and compared in table 2. The developed new technique offers several values of the solutions at the same time t with error not exceeding 10^{-4}.

4.5. Comparisons of the numerical (GRK4-H) and the analytical (PWS) methods

The accuracy of the neutron flux is obtained with the adopted GRK4-H method and the power series (PWS) [19, 20] method. The following examples represent the point kinetics equation with different types of reactivity feedback.

Case I. In this example, the treatment of the GRK4-H method is established within the range of stability interval using the inner and outer iterations. This case is also chosen from the work of Keepin [27] as

$$\rho(t) = a(t) + b(t) \int_0^t N(t')\,dt', \tag{71}$$

where $a(t)$ represented the impressed reactivity variation (generally polynomial in t), and $b(t)$ is the 'shutdown coefficient' of the reactor system. It is usually taken as a negative constant of magnitude ranging from 10^{-13} cm^3 s^{-1} for slow system to 10^{-7} cm^3 s^{-1} for fast metal systems. The results of comparison for this case are shown in table 3.

Case II. In this case, prompt point reactor equations are solved for the ramp reactivity insertion with a linear temperature feedback and described in the following table.
   Mathematical treatments of the adiabatic model system without delayed neutrons.

System of equations	GRK solution
$\frac{dN(t)}{dt} = \rho(t)N(t)\big/\Lambda$ $\rho(t) = at + b\,[T(t) - T(0)]$ $\frac{dT(t)}{dt} = \frac{1}{C}N(t) = HN(t)$ $\frac{d\theta}{dt} = 1.0$	$y^1 = N(t),\ y^2 = T(t),\ y^3 = t$ $f(y) = \begin{pmatrix} \alpha(t)N(t) + \varepsilon N(t)T(t) \\ HN(t) \\ 1 \end{pmatrix}$
Rearrangement $\frac{dN(t)}{dt} = \alpha(t)N(t) + \varepsilon T(t)N(t),$ $\alpha(t) = \frac{at}{\Lambda} - \frac{bT(0)N(t)}{\Lambda},\ \varepsilon = \frac{b}{\Lambda}$ where b is the temperature coefficient of reactivity and $a = \rho(0)$, the initial conditions are given by $a = 10^{-2}, b = -10^{-4}\,\mathrm{K}^{-1},$ $T(0) = 300\,\mathrm{K},\ N(0) = 10^5$ $H = 10^{-14}\,\mathrm{K\,s}^{-1},\ \Lambda = 10^{-3}\,\mathrm{s}$	The Jacobian matrix takes the form $f'(y) = \begin{pmatrix} \alpha(t) + \varepsilon T(t) & \varepsilon N(t) & \frac{a}{\Lambda}N(t) \\ H & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$ The matrix $\mathbf{A} = \mathbf{I} - pf'(y)$ $\mathbf{A} = \begin{pmatrix} 1 - p(\alpha(t) + \varepsilon T(t)) & -p\varepsilon N(t) & \frac{-pa}{\Lambda}N(t) \\ -pH & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$ $p = h\gamma$ Using the system of equations (4) and substituting into equation (2), the neutron density is obtained.

Comparisons are made between four such cases, GRK4-A, GRK4-H, PWS methods and the exact values of the power density and the temperature at $t = 0.41$ s and $t = 0.82$ s. The results are listed in table 4.

Table 4. Results for a ramp reactivity insertion with a linear temperature feedback at $t = 0.41$ s. and $t = 0.82$ s [28].

Method	h	$t = 0.41$			$t = 0.82$		
		$N(t)$	$T(t)$	TC(s)	$N(t)$	$T(t)$	TC(s)
GRK4-A	1.64×10^{-6}	6484.7650	205.3327	1.59	10.025 53	409.4142	2.63
GRK4-H	1.64×10^{-6}	6484.752	205.3330	1.59	10.025 72	409.4140	2.63
P.W.S[a]	0.001	6484.5290	205.3443	0.1	9.999 55	409.8737	0.21
EXACT	...	6484.5723	205.3451	...	10.0	409.8754	...

[a] Here $N(t)$, $T(t)$ has been calculated with power series method.

5. Conclusions

A time-dependent reactivity inserted into a point reactor is coupled multiplicatively with the neutron density to form a set of linear and/or nonlinear systems of equations with time-dependent coefficients. In the present work, a new GRK method has been developed by introducing two free parameters which could be used to optimize any desired feature in the process. Inner and outer iterations are applied over a wide range of interval and the stability of the resulted parameters is tested to generate a new set of coefficients which, in turn, are applied to the point kinetics equations. The presented method has the ability to reproduce all features of the transients in the solutions. In addition, it is applied to several types of step, ramp input and periodical reactivity changes. The formalism is also well applicable to nonlinear problems, where the reactivity depends on the neutron density through temperature and thermal hydraulic reactivity feedback. For further validity and accuracy verification of the developed method, comparisons are made with a number of other accurate analytical and numerical methods.

The $A(\alpha)$ stability properties of the method are studied, which resulted in the development of the GRK4-H method with the free parameter $\gamma = 0.25$ which corresponding to A(86.53°) stability gives more accurate results for the point kinetics equation. It is applied to two cases of feedback problems and the results are comparable with those obtained by GRK4-A, PWS and exact solutions. Finally, it can be concluded that the new developed methods for the solution of the point kinetics equations are more elegant, more general and more powerful than other conventional methods.

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