Numerical Methods for Differential Equation Solutions

Coupled Differential Equation solver

Under the marching forward techniques, there are various highly accurate explicit solution methods that apply step size adjustment in independent variables and computation of derivatives to march forward from one location to the next using Taylor's series expansion and partial derivatives of slopes with respect to independent and dependent variables. The most effective technique in this category is the fourth order Runge-Kutta (RK) method, which enhances the accuracy of the computation of derivatives to march forward from one location to the next. Equations for this robust technique including deductions where important are shown as follows. These equations shown for one independent and one dependent, variables can be extended for multiple input – multiple output (MIMO) system comprising coupled differential equations, where coefficients derived remain applicable for accurate solution of a large number of coupled differential equations.

Equation 1 shows the computation of dependent variable at the marched point location its value at present location and a weighted average of the slopes at these two consecutive locations.

$$y_{n+1} = y_n + h(ak_1 + bk_2)$$
 Equation 1

h is the adjusted step size, which will be discussed later, in this section. a and b are the weights of the two slopes, k_1 and k_2 , at two locations, n or present location and another between n and (n+1) (Equations 2-3). f is the function defining the slope.

$$k_1 = f(t_n, y_n)$$
 Equation 2

$$k_2 = f(t_n + ph, y_n + qhk_1)$$
 Equation 3

p and q are the constants that are optimal fractions for the most efficient march between n and (n+1) locations.

Equation 4 applies Taylor's series to include first partial derivatives in the expansion of k_2 .

$$k_2 = f(t_n, y_n) + \frac{\partial f(t_n, y_n)}{\partial t} ph + \frac{\partial f(t_n, y_n)}{\partial y} qhk_1 + O(h^2)$$
 Equation 4

Equations 2 and 4 are substituted in Equation 1 to obtain Equation 5.

$$y_{n+1} = y_n + haf(t_n, y_n) + hbf(t_n, y_n) + h^2bp\frac{\partial f}{\partial t} + h^2bqf(t_n, y_n)\frac{\partial f}{\partial y} + O(h^3)$$

Equation 5

A Taylor's expansion of y_{n+1} with respect to y_n can be written as in Equation 6.

$$y_{n+1} = y_n + hf(t_n, y_n) + \frac{h^2}{2!}f'(t_n, y_n) + \frac{h^3}{3!}f''(t_{\varepsilon}, y_{\varepsilon})$$
 Equation 6

 $f'(t_n, y_n)$ is the total derivative of the function with respect to t, which can be expressed in terms of partial derivative, as shown in Equation 7.

$$f'(t_n, y_n) = \left[\frac{df}{dt}\right]_n = \left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} \times \frac{dy}{dt}\right]_n = \left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f(t_n, y_n)\right]_n$$
 Equation 7

Substituting Equation 6 in Equation 5 gives Equation 8.

$$y_{n+1} = y_n + hf(t_n, y_n) + \frac{h^2}{2!} \frac{\partial f}{\partial t} + \frac{h^2}{2!} f(t_n, y_n) \frac{\partial f}{\partial y} + \frac{h^3}{3!} f''(t_{\varepsilon}, y_{\varepsilon})$$
 Equation 8

Equation 5 and Equation 8, the expressions of the various parameters used, a, b, p, q are obtained as in Equation 9.

$$a+b=1 \qquad \textit{Coefficient of } f(t_n,y_n)$$

$$bp=\frac{1}{2} \qquad \textit{Coefficient of } \frac{\partial f(t_n,y_n)}{\partial t}$$

$$bq=\frac{1}{2} \qquad \textit{Coefficient of } f(t_n,y_n)\frac{\partial f(t_n,y_n)}{\partial t}$$
 Equation 9

As there are three expressions for four unknown parameters, a, b, p, q, several choices are proposed by Euler, Ralston, Heun, etc. (Equations 11-13).

Combining Equations 1-3, Equation 10 is obtained.
$$y_{n+1} = y_n + ahf(t_n, y_n) + bhf(t_n + ph, y_n + qhy_n') + O(h^3)$$
 Equation 10

$$y'_n = slope \ at \ n = f(t_n, y_n)$$

Euler:
$$a = b = \frac{1}{2}$$
; $p = q = 1$

$$y_{n+1} = y_n + h\left[\frac{1}{2}f(t_n, y_n) + \frac{1}{2}f(t_n + h, y_n + hy_n')\right] + O(h^3)$$
 Equation 11

Ralston:
$$a = \frac{1}{3}$$
; $b = \frac{2}{3}$; $p = q = \frac{3}{4}$

$$y_{n+1} = y_n + h\left[\frac{1}{3}f(t_n, y_n) + \frac{2}{3}f\left(t_n + \frac{3h}{4}, y_n + \frac{3h}{4}y_n'\right)\right] + O(h^3)$$
 Equation 12

Heun:
$$a = \frac{1}{4}$$
; $b = \frac{3}{4}$; $p = q = \frac{2}{3}$

$$y_{n+1} = y_n + h\left[\frac{1}{4}f(t_n, y_n) + \frac{3}{4}f\left(t_n + \frac{2h}{3}, y_n + \frac{2h}{3}y_n'\right)\right] + O(h^3)$$
 Equation 13

The extension to higher order solutions, such as, the 4th order RK technique, is similar, based on Equation 14.

$$y_{n+1} = y_n + h(ak_1 + bk_2 + ck_3 + dk_4)$$
 Equation 14

$$k_1 = f(t_n, y_n) = y_n'$$

$$k_2 = f(t_n + ph, y_n + qhk_1)$$

$$k_3 = f(t_n + rh, y_n + shk_1 + uhk_2)$$

$$k_4 = f(t_n + vh, y_n + whk_2 + xhk_3)$$

$$y_{n+1} = y_n + h(af(t_n, y_n) + bf(t_n + ph, y_n + qhk_1) + cf(t_n + rh, y_n + shk_1 + uhk_2) + df(t_n + vh, y_n + whk_2 + xhk_3)) + O(h^3)$$

$$a+b+c+d=1$$

$$bp + cr + dv = bq + c(s + u) + d(w + x) = \frac{1}{2}$$

There are 3 equations and 12 variables, leaving 9 degrees of freedom, which are suggested as follows by the RK-Gill technique (Equation 15).

$$a = d = \frac{1}{6}$$
; $b = \frac{1 - \frac{\sqrt{2}}{2}}{3}$; $c = \frac{1 + \frac{\sqrt{2}}{2}}{3}$;

$$p = \frac{1}{2}; r = \frac{1}{2}; v = 1;$$

$$q = \frac{1}{2}; s = \left(\frac{\sqrt{2}}{2} - \frac{1}{2}\right); u = \left(1 - \frac{\sqrt{2}}{2}\right); w = -\frac{\sqrt{2}}{2}; x = 1 + \frac{\sqrt{2}}{2}$$
Equation 15

Equation 14 allows generic representation of the RK solution technique in Equation 16 and the values by the RK-Gill technique presented in matrix form in Equation 17.

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^o w_i \, \mathbf{k}_i$$

$$\mathbf{k}_i = f(\mathbf{t}_n + b_i h, \mathbf{y}_n + \sum_{j=1}^{i-1} a_{i,j} h \mathbf{k}_j)$$
 Equation 16

i and j are the indices for the order (o) of the solution technique. w_i is the weighting factor of the slopes (\mathbf{k}_i) at the various locations, such that $\sum_{i=1}^o w_i = 1$. b_i is a fraction to adjust the step size for the order i, such that $\sum_{i=2}^o w_i b_i = \frac{1}{2}$. $a_{i,j}$ is the coefficient to adjust the product of the slope and the step size in the intermediate locations, such that $\sum_{i=2}^o b_i (\sum_{j=1}^{i-1} a_{i,j}) = \frac{1}{2}$. Thus, there will be 3 equations, (4o-4) number of parameters and (4o-7) degrees of freedom. Symbols written in bold and non-Italics indicate vector or a MIMO system.

$a_{i,j}$	b_i	j = 1	j = 2	j = 3	j = 4
i = 1	0				
i = 2	$\frac{1}{2}$	$\frac{1}{2}$			
i = 3	$\frac{1}{2}$	$\left(\frac{\sqrt{2}}{2} - \frac{1}{2}\right)$	$\left(1-\frac{\sqrt{2}}{2}\right)$		
i = 4	1		$-\frac{\sqrt{2}}{2}$	$1 + \frac{\sqrt{2}}{2}$	
w _j		$\frac{1}{6}$	$\frac{1-\frac{\sqrt{2}}{2}}{3}$	$\frac{1+\frac{\sqrt{2}}{2}}{3}$	$\frac{1}{6}$

Equation 17

The matrix in Equation 17 is known as Butcher Tableau. Further, RK 4th order and its 3/8-rule has the following Butcher Tableau (Equations 18-19).

$a_{i,j}$	b_i	j = 1	j = 2	j = 3	j = 4
i = 1	0				
i = 2	$\frac{1}{2}$	$\frac{1}{2}$			
i = 3	$\frac{1}{2}$	0	$\frac{1}{2}$		
i = 4	1	0	0	1	
w_j		$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

Equation 18

$a_{i,j}$	b_i	j = 1	j = 2	j = 3	j = 4
i = 1	0				
i = 2	<u>1</u>	<u>1</u>			
	3	3			

i = 3	$\frac{2}{3}$	$-\frac{1}{3}$	1		
i = 4	1	1	-1	1	
w _i		1	3	3	1
,		8	8	8	8

Equation 19

The RK-Fehlberg technique using 6^{th} order is known to be more effective in terms of step size control discussed further following Equation 20. The technique gives \mathbf{y}_{n+1} and $\bar{\mathbf{y}}_{n+1}$ based on the values shown in the form of matrix in Equation 20 in the common generic form in Equation 16.

$a_{i,j}$	b_i	<i>j</i> = 1	j = 2	j = 3	j = 4	<i>j</i> = 5	<i>j</i> = 6
i = 1	0						
i = 2	1	1					
	$\frac{\overline{4}}{4}$	$\frac{\overline{4}}{4}$					
i = 3	3	3	9				
	8	32	32				
i = 4	12	1932	7200	7296			
	13	${2197}$	$-{2197}$	2197			
i = 5	1	439	-8	3680	845		
		$\overline{216}$		513	$-{4104}$		
i = 6	1	216 8	2	3544	1859	11	
	$\frac{\overline{2}}{2}$	$-{27}$		$-{2565}$	$\frac{1}{4104}$	$-\frac{1}{40}$	
w_i for		25		1408	2197	1	
\mathbf{y}_{n+1}		216		2565	4104	_ _ 5	
w_j for		16		6656	28561	9	2
$\overline{\mathbf{y}}_{n+1}$		135		12825	56430	$-{50}$	55

Equation 20

Equation 22

The RK-Fehlberg technique proposes an acceptable step size for consecutive location as shown in Equation 21. It allows to accept the minimum step size between the two options.

$$\mathbf{h}_{n+1} = \mathit{Min}\{0.84\mathbf{h}_n \left[\frac{\varepsilon \mathbf{h}_n}{|\bar{\mathbf{y}}_{n+1} - \mathbf{y}_{n+1}|}\right]^{0.25}, 4\mathbf{h}_n\}$$
 Equation 21

 ε is the tolerance. The term 0.84 gives an additional safety factor. A jump of a maximum of four times \mathbf{h}_n is allowed if the error is within the given tolerance. This step size adjustment criterion can be introduced in the RK or RK-Fehlberg solution techniques for coupled ODE system.

The stiffness in the solution is another area, where alternative solutions such as Gear's method, may be more effective. At any location, y_n can be represented in terms of eigen values (γ) of matrix **A** (Equation 22).

$$(\mathbf{A} - \gamma \mathbf{I})\mathbf{y} = 0$$

$$\mathbf{y}_n = \sum C_{ni} e^{\gamma_{ni}t_n} + Constant$$

For real $|Re \gamma_{ni}|$, for larger values, the first term will have a fast transient, while for smaller values, the fast term will have a slow transient, with increasing t_n . This helps to define the stiffness ratio as the ratio between the maximum and the minimum absolute eigen values at a given location (Equation 23).

$$stiffness\ ratio = \frac{|Re\ \overline{\gamma_{ni}}|}{|Re\ \gamma_{ni}|}$$
 Equation 23

When there is a large difference between the maximum and the minimum absolute eigen values, stiffness is likelihood to occur.

Stiff Coupled Differential Equation and Differential Algebraic Equation (DAE) solver

The Gear's technique is more effective for the solution of coupled ODEs with stiffness. The matrix for the predictor and the corrector equations correspond to the exact solution at any location. Equation 24 shows the coefficients in the 6^{th} order (k=6) Gear's Predictor and Corrector equations.

Coefficients	i = 1	i = 2	i = 3	i = 4	i = 5	i = 6	Constant
\mathbf{y}_{n+1}	360	450	400	225	72	10	60
	$\overline{147}$	$-{147}$	$\overline{147}$	$-{147}$	$\overline{147}$	$-\frac{147}{147}$	$\overline{147}$
$\bar{\mathbf{y}}_{n+1}$	77	150	100	50	15	2	60
	$-\frac{10}{10}$	10	$-\frac{10}{10}$	$\overline{10}$	$-\frac{10}{10}$	$\overline{10}$	$\overline{10}$

Corrector (implicit):
$$\mathbf{y}_{n+1} = (\sum_{i=1}^{n} Coefficient_i \mathbf{y}_{n-i+1}) + h \times Constant \times \mathbf{y'}_{n+1}$$

Predictor (explicit):
$$\overline{\mathbf{y}}_{n+1} = (\sum_{i=1}^{k} \overline{Coefficient}_{i} \mathbf{y}_{n-i+1}) + h \times \overline{Constant} \times \mathbf{y'}_{n}$$

Equation 24

Subtraction between the Corrector and the Predictor in Equation 24 is for the computation of \mathbf{y}_{n+1} using the 6^{th} order Gear's Predictor and Corrector method. Coefficients are represented by α and constants by β . All the steps are expanded under Equation 25.

$$\begin{aligned} \mathbf{y}_{n+1} &= \overline{\mathbf{y}}_{n+1} + \beta_o [h\mathbf{y'}_{n+1} - \left\{ \frac{\overline{\alpha}_1 - \alpha_1}{\beta_o} \mathbf{y}_n + \frac{\overline{\alpha}_2 - \alpha_2}{\beta_o} \mathbf{y}_{n-1} + \dots + \frac{\overline{\alpha}_k - \alpha_k}{\beta_o} \mathbf{y}_{n-k+1} + h \frac{\overline{\beta}_0}{\beta_o} \mathbf{y'}_n \right\}] \\ & \qquad \qquad \gamma_i = \frac{\overline{\alpha}_i - \alpha_i}{\beta_o}; \quad i = 1, 2, \dots, k \\ & \qquad \qquad \delta_0 = \frac{\overline{\beta}_0}{\beta_o} \\ & \qquad \qquad \mathbf{y}_{n+1} &= \overline{\mathbf{y}}_{n+1} + \beta_o [h\mathbf{y'}_{n+1} - \{\gamma_1 \mathbf{y}_n + \gamma_2 \mathbf{y}_{n-1} + \dots + \gamma_k \mathbf{y}_{n-k+1} + h \delta_0 \mathbf{y'}_n \}] \\ & \qquad \qquad h \overline{\mathbf{y}}_{n+1}' &= \{\gamma_1 \mathbf{y}_n + \gamma_2 \mathbf{y}_{n-1} + \dots + \gamma_k \mathbf{y}_{n-k+1} + h \delta_0 \mathbf{y'}_n \} \\ & \qquad \qquad \overline{\mathbf{y}}_{n+1} &= \overline{\alpha}_1 \mathbf{y}_n + \overline{\alpha}_2 \mathbf{y}_{n-1} + \dots + \overline{\alpha}_k \mathbf{y}_{n-k+1} + h \overline{\beta}_0 \mathbf{y'}_n \\ & \qquad \qquad \mathbf{y}_{n+1} &= \overline{\mathbf{y}}_{n+1} + \beta_o [h\mathbf{y'}_{n+1} - h \overline{\mathbf{y}}_{n+1}'] \\ & \qquad \qquad \mathbf{y}_{n+1} &= \overline{\mathbf{y}}_{n+1} + \beta_o [h\mathbf{f}(t_{n+1}, \overline{\mathbf{y}}_{n+1} + \beta_o b) - h \overline{\mathbf{y}}_{n+1}'] \\ & \qquad \qquad \mathbf{y}_{n+1} &= \overline{\mathbf{y}}_{n+1} + \beta_o b \end{aligned}$$

$$\mathsf{Where}, b = [h\mathbf{f}(t_{n+1}, \overline{\mathbf{y}}_{n+1} + \beta_o b) - h \overline{\mathbf{y}}_{n+1}']$$

Thus, the matrix in Equation 24 is updated for the computation of y_{n+1} .

Coefficients	i = 1	i = 2	i = 3	i = 4	i = 5	<i>i</i> = 6	Constant
$\bar{\alpha}_i$	-7.7	15	-10	5	-1.5	0.2	6
γ_i	-24.865	44.25	-31.1667	16	-4.875	0.656667	14.7

The Backward Differentiation Formula (BDF) method uses the coefficients for the Gear's Corrector method to compute \mathbf{y}_{n+1} implicitly. Depending on the order of the method, from 1 to 6, \mathbf{y}_{n+1} will depend on \mathbf{y}_n and \mathbf{y}'_{n+1} ; \mathbf{y}_n , \mathbf{y}_{n-1} and \mathbf{y}'_{n+1} ; \mathbf{y}_n , \mathbf{y}_{n-1} , \mathbf{y}_{n-2} and \mathbf{y}'_{n+1} ; \mathbf{y}_n , \mathbf{y}_{n-1} , \mathbf{y}_{n-2} , \mathbf{y}_{n-3} , \mathbf{y}_{n-4} , and \mathbf{y}'_{n+1} ; \mathbf{y}_n , \mathbf{y}_{n-1} , \mathbf{y}_{n-2} , \mathbf{y}_{n-3} , \mathbf{y}_{n-4} , \mathbf{y}_{n-5} and \mathbf{y}'_{n+1} ; respectively, by the matrix in Equation 26 with the coefficients for the Gear's Corrector method.

Order	α_1	α_2	α_3	α_4	α_5	α_6	β_o		
1	1						1		\mathbf{y}_n
2	4	1					2		\mathbf{y}_{n-1}
	3	3					3		
3	18	9	2				6		y_{n-2}
	<u>11</u>	$-\frac{1}{11}$	<u>11</u>				<u>11</u>	×	
4	48	36	16	3			12		y_{n-3}
	$\overline{25}$	$-{25}$	$\overline{25}$	$-{25}$			$\overline{25}$		
5	300	300	200	75	12		60		\mathbf{y}_{n-4}
	$\overline{137}$	$-{137}$	$\frac{137}{137}$	$-{137}$	$\frac{137}{137}$		$\frac{137}{137}$		
6	360	450	400	225	72	10	60		y_{n-5}
	$\overline{147}$	$-{147}$	$\overline{147}$	$-\frac{147}{147}$	$\overline{147}$	$-\frac{147}{147}$	$\overline{147}$		2 0
									y'_{n+1}

Equation 26

The key differentiator between an explicit and implicit method is the computation of y'_{n+1} in the latter, which makes the algorithm slower, however, more effective for solving stiff equations. Eventually, the latter method is also applicable to differential algebraic equation (DAE) solutions. The predictor (explicit) \overline{y}_{n+1} can be easily calculated using Equation 24. The coefficients for the Gear's Predictor method to compute \overline{y}_{n+1} explicitly are shown in the matrix in Equation 27 that also includes the computation of \overline{y}_{n+1} .

Order	$\bar{\alpha}_1$	$\bar{\alpha}_2$	$\bar{\alpha}_3$	\bar{lpha}_4	$\bar{\alpha}_5$	$\bar{\alpha}_6$	$ar{eta_o}$		
1	1						1		\mathbf{y}_n
2	0	1					2		\mathbf{y}_{n-1}
3	_ 3	6	_ 1				<u>6</u>		y_{n-2}
	2	2	2				2		
4	10	18	6	1			12	×	y_{n-3}
	3	3	3	3			3		
5	65	120	60	20	3		60		\mathbf{y}_{n-4}
	$-\frac{1}{12}$	12	$-\frac{12}{12}$	$\overline{12}$	$-\frac{1}{12}$		$\overline{12}$		
6	77	150	100	50	15	2	60		y_{n-5}
	$-\frac{10}{10}$	10	$-{10}$	$\overline{10}$	$-\frac{10}{10}$	$\overline{10}$	$\overline{10}$		2 10 0
									$oldsymbol{y}_n'$

Predictor (explicit):
$$\overline{\mathbf{y}}_{n+1} = (\sum_{i=1}^k \overline{\alpha}_i \mathbf{y}_{n-i+1}) + h \times \overline{\beta}_o \times \mathbf{y'}_n$$

Equation 27

Then, b is solved iteratively within each step so that $b^{(q+1)} \approx b^{(q)}$ using Equation 28 or the Newton-Raphson technique in Equation 29. J_y is the Jacobian of the function f or y' i.e. partial derivative of f with respect to y.

$$hf(t_{n+1}, \overline{y}_{n+1} + \beta_o b) - (h\overline{y}'_{n+1} + b) = 0$$
 Equation 28

$$b^{(q+1)} = b^{(q)} - \frac{hf(t_{n+1}, \overline{y}_{n+1} + \beta_o b^{(q)}) - (h\overline{y}'_{n+1} + b^{(q)})}{h\beta_o J_y(t_{n+1}, \overline{y}_{n+1} + \beta_o b^{(q)}) - 1}$$
 Equation 29

Equation 30 computes \mathbf{y}_{n+1} from $\overline{\mathbf{y}}_{n+1}$ and b.

$$\mathbf{y}_{n+1} = \overline{\mathbf{y}}_{n+1} + \beta_o b$$
 Equation 30

For DAE, if function g(t, y, u) = 0 represents the set of algebraic equations, then Equation 28 is updated to compute iteratively, the two step sizes, b and d, using Equations 31-32. While the remaining Equations 26, 27 and 30 will be applied to move to the next feasible location.

$$hf(t_{n+1}, \overline{\mathbf{y}}_{n+1} + \beta_o b, \overline{\mathbf{u}}_{n+1} + \beta_o d) - (h\overline{\overline{\mathbf{y}}}'_{n+1} + b) = 0$$
 Equation 30

$$g(t_{n+1},\overline{\mathbf{y}}_{n+1}+\beta_o b,\overline{\mathbf{u}}_{n+1}+\beta_o d)=0$$
 Equation 31