Derivation of Third-Order Runge-Kutta Methods for Solving the Initial Value Problem $\frac{dx}{dt} = f(t,x)$ *with* $x(t_0) = x_0$

(I) $x_n = x_0 + h\sum_{k=0}^{n-1} c_k f(t_0 + \alpha_k h,\, x_k)$

where

(II) $x_k = x_0 + h\sum_{j=0}^{k-1} \beta_{kj} f(t_0 + \alpha_j h,\, x_j)$

} the Runge-Kutta Ansatz

In the following derivation, we will assume (at first) that f is a function of x only, $f = f(x)$. The Taylor Series for $x(t_0 + h)$, (the true solution at $t_0 + h$) about the point $t = t_0$, gives:

$$x(t_0 + h) = x_0 + hf(x_0) + \frac{h^2}{2!}\frac{df}{dt_0} + \frac{h^3}{3!}\frac{d^2 f}{dt_0^2} + O(h^4)$$

Now, since $\frac{df}{dt_0} = f_x f$ (note that we are using the abbreviation f_x for $\frac{\partial f}{\partial x}$)

and $\frac{d^2 f}{dt^2} = f_{xx} f^2 + f_x^2 f$, we have for the Taylor Series:

(III) $x(t_0 + h) = x(t_0) + hf + \frac{h^2}{2!} f_x f + \frac{h^3}{3!}(f_{xx} f^2 + f_x^2 f) + O(h^4)$

For our equation (I) we have:

(IV) $x_n = x_0 + h\sum_{k=0}^{n-1} c_k f(x_k)$ where for $f(x_k)$ we have (using the Taylor Series for f as a function of x):

$$f(x_k) = f(x_0) + (x_k - x_0) f_x + \frac{1}{2!}(x_k - x_0)^2 f_{xx} + O(h^3)$$

and $x_k - x_0 = h\sum_{j=0}^{k-1} \beta_{kj} f(x_j)$ from (II) and similarly

$$f(x_j) = f(x_0) + (x_j - x_0) f_x + \frac{1}{2!}(x_j - x_0)^2 f_{xx} + O(h^3)$$

(Note: All f, f_x, f_{xx}, etc. are evaluated at x_0 unless otherwise indicated)

So (IV) becomes:

$$x_n = x_0 + h\sum_{k=0}^{n-1} c_k \left\{ f + hf_x \sum_{j=0}^{k-1}\beta_{kj} f(x_j) + \frac{1}{2}\left(h\sum_{j=0}^{k-1}\beta_{kj} f(x_j)\right)^2 f_{xx} \right\} + O(h^4)$$

$$= x_0 + hf\sum_{k=0}^{n-1} c_k \; + h^2 f_x \sum_{k=1}^{n-1} c_k \sum_{j=0}^{k-1}\beta_{kj} f(x_j) + \frac{1}{2}h^3 f_{xx}\sum_{k=1}^{n-1} c_k \left(\sum_{j=0}^{k-1}\beta_{kj} f(x_j)\right)^2 + O(h^4)$$

$$= x_0 + hf\sum_{k=0}^{n-1} c_k \; + h^2 f_x \sum_{k=1}^{n-1} c_k \sum_{j=0}^{k-1}\beta_{kj}\left[f + h\sum_{i=0}^{j-1}\beta_{ji} f(x_0) f_x + \dots \right]$$

$$+ \; \frac{1}{2}h^3 f_{xx} f^2 \sum_{k=1}^{n-1} c_k \left(\sum_{j=0}^{k-1}\beta_{kj}\right)^2 + O(h^4)$$

(V) $$x_n = x_0 + hf\sum_{k=0}^{n-1} c_k \; + h^2 f_x f \sum_{k=1}^{n-1} c_k \, \alpha_k + h^3 f_x^2 f \sum_{k=2}^{n-1} c_k \sum_{j=1}^{k-1}\beta_{kj}\left(\sum_{i=0}^{j-1}\beta_{ji}\right)$$

$$+ \frac{1}{2}h^3 f_{xx} f^2 \sum_{k=1}^{n-1} c_k \, \alpha_k^2 \; + O(h^4)$$

So for the respective orders (comparing V and III), we obtain:

1	hf :	$\sum_{k=1}^{n-1} c_k = 1$	1[st] order (1); 2[nd] order (1–2); 3[rd] order (1–4)
2	$h^2 f_x f$:	$\sum_{k=1}^{n-1} c_k \alpha_k = \frac{1}{2}$	
3)	$h^3 f_x^2 f$:	$\sum_{k=2}^{n-1} c_k \sum_{j=1}^{k-1}\beta_{kj}\alpha_j = \frac{1}{6}$	
4)	$\frac{1}{2}h^3 f_{xx} f^2$:	$\sum_{k=1}^{n-1} c_k \alpha_k^2 = \frac{1}{3}$	

The number of stages, n, is the number of times the derivative function, f(t,x), is evaluated during each step. The minimum number of stages possible for a third-order Runge-Kutta method is 3. When n is 3, then the equations of condition become:

1) $c_0 + c_1 + c_2 = 1$

2) $c_1\alpha_1 + c_2\alpha_2 = \frac{1}{2}$

3) $c_2\beta_{21}\alpha_1 = \frac{1}{6}$

4) $c_1\alpha_1^2 + c_2\alpha_2^2 = \frac{1}{3}$

It should be noted that these equations are four ***nonlinear*** algebraic equations in the six unknown coefficients: $\{\alpha_1, \alpha_2, \beta_{21}, c_0, c_1, \text{ and } c_2\}$. These can be solved using the following hints:

> Guess values for α_1 and α_2 such that $\alpha_1 \neq \alpha_2$ and $\alpha_1 \neq 0$ and $\alpha_2 \neq 0$. Choose simple fractions, if you like. Then, solve equations 2) and 4) for c_1 and c_2. Then solve 1) for c_0, and 3) for β_{21}. Use $\alpha_1 \equiv \beta_{10}$ and $\alpha_2 \equiv \beta_{20} + \beta_{21}$ to get β_{10} and β_{20}.

Once you have values for the coefficients, you can construct your program. The equations II and I will be used to obtain values for x_1, x_2, and x_3 at each step. Once you have a value for x_3, you can advance the numerical integration to the next step (by updating the values of x_0 and t_0).