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 \[ \{ \text{the Runge-Kutta Ansatz} \} \]

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

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:

\[
x(t_0 + h) = x_0 + h f(x_0) + \frac{h^2}{2!} df \bigg|_{t_0} + \frac{h^3}{3!} d^2 f \bigg|_{t_0} + O(h^4)
\]

Now, since \( \frac{df}{dt} = f_x f \) (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) \[ x(t_0 + h) = x(t_0) + h f_x + \frac{h^2}{2!} f_{xx} f^2 + \frac{h^3}{3!} (f_{xx} f^2 + f_x^2 f) + O(h^4) \]

For our equation (I) we have:

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

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

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:

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

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

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

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

(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. \( hf \); \( \sum_{k=1}^{n-1} c_k = 1 \) \( \quad \text{1st order} \)
2. \( h^2 f_x f \); \( \sum_{k=1}^{n-1} c_k \alpha_k = \frac{1}{2} \) \( \quad \text{2nd order} \)
3. \( h^3 f_x^2 f \); \( \sum_{k=2}^{n-1} c_k \sum_{j=1}^{k-1} \beta_{kj} \alpha_j = \frac{1}{6} \) \( \quad \text{3rd order} \)
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 \( \alpha_1 \) and \( \alpha_2 \) 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 \( \beta_{21} \). Use \( \alpha_1 = \beta_{10} \) and \( \alpha_2 = \beta_{20} + \beta_{21} \) to get \( \beta_{10} \) and \( \beta_{20} \).

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 \( t_0 \)).