Notes on Implementing MC's Method

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I. EXPLICIT RUNGE-KUTTA SCHEME

To integrate the ODE

$$\frac{dy}{dt} = f(y, t), \tag{1}$$

we start from the fundamental theorem of calculus

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(y(\tau), \tau)d\tau = y(t_n) + h \int_0^1 f(y(t_n + h\tau), t_n + h\tau)d\tau. \tag{2}$$

We can replace the integral with a quadrature approximation

$$y_{n+1} = y_n + h\Sigma_{i=1}^s b_i f(y(t_n + c_i h), t_n + c_i h), \tag{3}$$

where we have to construct an approximation, denoted by $Y_i \simeq y(t_n + c_i h)$. With explicit Runge-Kutta method we construct Y_i using

$$y_n, \quad f(Y_1, t_n + hc_1), \quad f(Y_2, t_n + hc_2), \quad ..., \quad f(Y_{i-1}, t_n + hc_{i-1}). \tag{4}$$

Then the explicit Runge-Kutta method can be sum up as the following,

$$Y_s = y_n + h\Sigma_{i=1}^{s-1} a_{si} f(Y_i, t_n + hc_i), \tag{5}$$
$$y_{n+1} = y_n + h\Sigma_{i=1}^s b_i f(Y_i, t_n + hc_i). \tag{6}$$

Further more for the chain rule,

$$y' = f(y, t) \tag{7}$$

$$y'' = \frac{d}{dt}y' = \left(\frac{\partial}{\partial t} + f\frac{\partial}{\partial y}\right)f = \frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y} \tag{8}$$

$$y''' = \frac{d}{dt}y'' = \left(\frac{\partial}{\partial t} + f\frac{\partial}{\partial y}\right)\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)$$

$$= \frac{\partial^2 f}{\partial t^2} + f\frac{\partial^2 f}{\partial t\partial y} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial y} + f\frac{\partial^2 f}{\partial y\partial t} + f\frac{\partial f}{\partial y}\frac{\partial f}{\partial y} + f^2\frac{\partial^2 f}{\partial y^2}$$

$$= \frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\partial y} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial y} + f^2\frac{\partial^2 f}{\partial y^2} + f\left(\frac{\partial f}{\partial y}\right)^2 \tag{9}$$

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Consider the case $t_n = 0$, $y(t) = t \Rightarrow y(0) = 0, y' = 1$, for the first order accuracy, the above scheme need to obtain the exact solution of $y(t) = t$.

$$Y_i = y_n + h\Sigma_{j=1}^{i-1}a_{ij} \simeq y(t_n + c_ih) = y_n + hc_i, \tag{10}$$

$$y_{n+1} = y_n + h\Sigma_{i=1}^{s}b_i = y_n + h. \tag{11}$$

$$\Rightarrow \begin{cases} \Sigma_{j=1}^{i-1}a_{ij} = c_i, \\ \Sigma_{i=1}^{s}b_i = 1, \end{cases} \tag{12}$$

$a_{21} = c_2$ for example.

For up to the 3-order conditions, it sufices to study the case of **autonomous** differential equations, $y' = f(y)$, where the chain rule become

$$y' = f, \tag{13}$$

$$y'' = (f\frac{\partial}{\partial y})f = ff_y, \tag{14}$$

$$y''' = (f\frac{\partial}{\partial y})(ff_y) = ff_y^2 + f^2f_{yy} \tag{15}$$

A. Dense Output

Following the convention of Mongwane, we define

$$k_i := hf(Y_i, t_n + hc_i), \tag{16}$$

then the dense output formula are

$$y(t_n + \theta h) = y_n + \Sigma_{i=1}^{4}b_i(\theta)k_i + \mathcal{O}(h^4), \tag{17}$$

$$\frac{d^{(m)}}{dt^{(m)}}y(t_n + \theta h) = \frac{1}{h^m}\Sigma_{i=1}^{s}k_i\frac{d^{(m)}}{d\theta^{(m)}}b_i(\theta) + \mathcal{O}(h^{4-m}). \tag{18}$$

where

$$b_1(\theta) = \theta - \frac{3}{2}\theta^2 + \frac{2}{3}\theta^3, \tag{19}$$

$$b_2(\theta) = b_3(\theta) = \theta^2 - \frac{2}{3}\theta^3, \tag{20}$$

$$b_4(\theta) = -\frac{1}{2}\theta^2 + \frac{2}{3}\theta^3. \tag{21}$$

B. Taylor expansion of k_i for RK4 up to $\mathcal{O}(h^3)$

The taylor expansion of k_i around t_n are

$$k_1 = hy', \tag{22}$$

$$k_2 = hy' + \frac{h^2}{2}y'' + \frac{h^3}{8}(y''' - f_yy''), \tag{23}$$

$$k_3 = hy' + \frac{h^2}{2}y'' + \frac{h^3}{8}(y''' + f_yy''). \tag{24}$$

where $f_yy'' \equiv (y'')^2/y' = \frac{4(k_3^{(c)} - k_2^{(c)})}{h_{(c)}^3}$, and y', y'', y''' can be represented with $k_i^{(c)}$ of coarse grid using the dense output formula (17)-(18).

C.   Taylor expansion of Y_i for RK4 up to $\mathcal{O}(h^3)$

Similarly, we can also expand Y_i instead of k_i

$$Y_1 = y_n, \tag{25}$$

$$Y_2 = y_n + \frac{h}{2}y', \tag{26}$$

$$Y_3 = y_n + \frac{h}{2}y' + \frac{h^2}{4}y'' + \frac{h^3}{16}(y''' - f_y y'') \tag{27}$$

$$Y_4 = y_n + hy' + \frac{h^2}{2}y'' + \frac{h^3}{8}(y''' + f_y y'') \tag{28}$$

where $f_y y'' \equiv (y'')^2 / y' = \frac{4(k_3^{(c)} - k_2^{(c)})}{h_{(c)}^3}$, and y', y'', y''' can be represented with $k_i^{(c)}$ of coarse grid using the dense output formula (17)-(18).

1.   Pseudocode of MC's method

1. Integrate coarse grid from t_n to $t_n + h^{(c)}$ and store $k_i^{(c)}$ somewhere.

2. Interpolate in time for y, y', y'', y''' using (17)-(18) with stored $k_i^{(c)}$

   (a) at $\theta = 0.0$ for the first fine step,
   (b) at $\theta = 0.5$ for the second fine step.

3. Calculate Y_i for the first and second fine steps using (25)-(28).

4. Interpolate in space to fill Y_i in the fine ghost points.

5. Repeat.