Notes on dftatom

1 Radial grid

To allow general, nonuniform meshes, all methods first transform equations on general mesh $R(t)$, with $1 \le t \le N+1$, to equations on a uniform mesh t with step size $h = 1$. If the solution of a general mesh is $P(r)$ and the transformed solution on the uniform mesh is $u(t)$ then:

$$u(t) = P(R(t)) \tag{1}$$

$$u'(t) = \frac{\mathrm{d}u}{\mathrm{d}t} = \frac{\mathrm{d}P}{\mathrm{d}R} R'(t) \tag{2}$$

2 Runge-Kutta method (4th-order)

Assume an equation of the form $y = F(x, y)$ and step size $h = 1$:

$$y_{i+1} = y_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{3}$$

$$k_1 = F(x_i, y_i) \tag{4}$$

$$k_2 = F\left(x_{i+\frac{1}{2}}, y_i + \frac{1}{2}k_1\right) \tag{5}$$

$$k_3 = F\left(x_{i+\frac{1}{2}}, y_i + \frac{1}{2}k_2\right) \tag{6}$$

$$k_4 = F\left(x_{i+1}, y_i + k_3\right) \tag{7}$$