Simulation Tools

Structure of a Multistep Code

Claus Führer

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Iterations

Nonlinear System

$$y_n = h\beta_k f(y_n) + \text{old values}$$

Fixed point iteration (functional iteration, `CV_FUNCTIONAL`)

$$y_n(i+1) = h\beta_k f(y_n^{(i)}) + \text{old values}$$

Newton iteration (`CV_NEWTON`)

$$G'(y_n^{(i+1)})\Delta y = -G(y_n^{(i)})$$

with $G(y) = y - h\beta_k f(y) - \text{old values}$.

variable coefficient vs fixed leading coefficient

Coefficients depend on step size ratios:

$$r_i = \frac{h_{n-i}}{h_{n-i-1}}$$

$$\alpha_{k-i} = \alpha_{k-i}(r_0, r_1, \ldots, r_k) \quad \beta_{k-i} = \beta_{k-i}(r_0, r_1, \ldots, r_k)$$

In CVODE fixed leading coefficient,i.e.

$$\beta_k = \beta_k(r_0)$$

(saves Jacobian evaluations).

Tolerances and Norms

SUNDIALS uses weighted norms (state dependent weights)

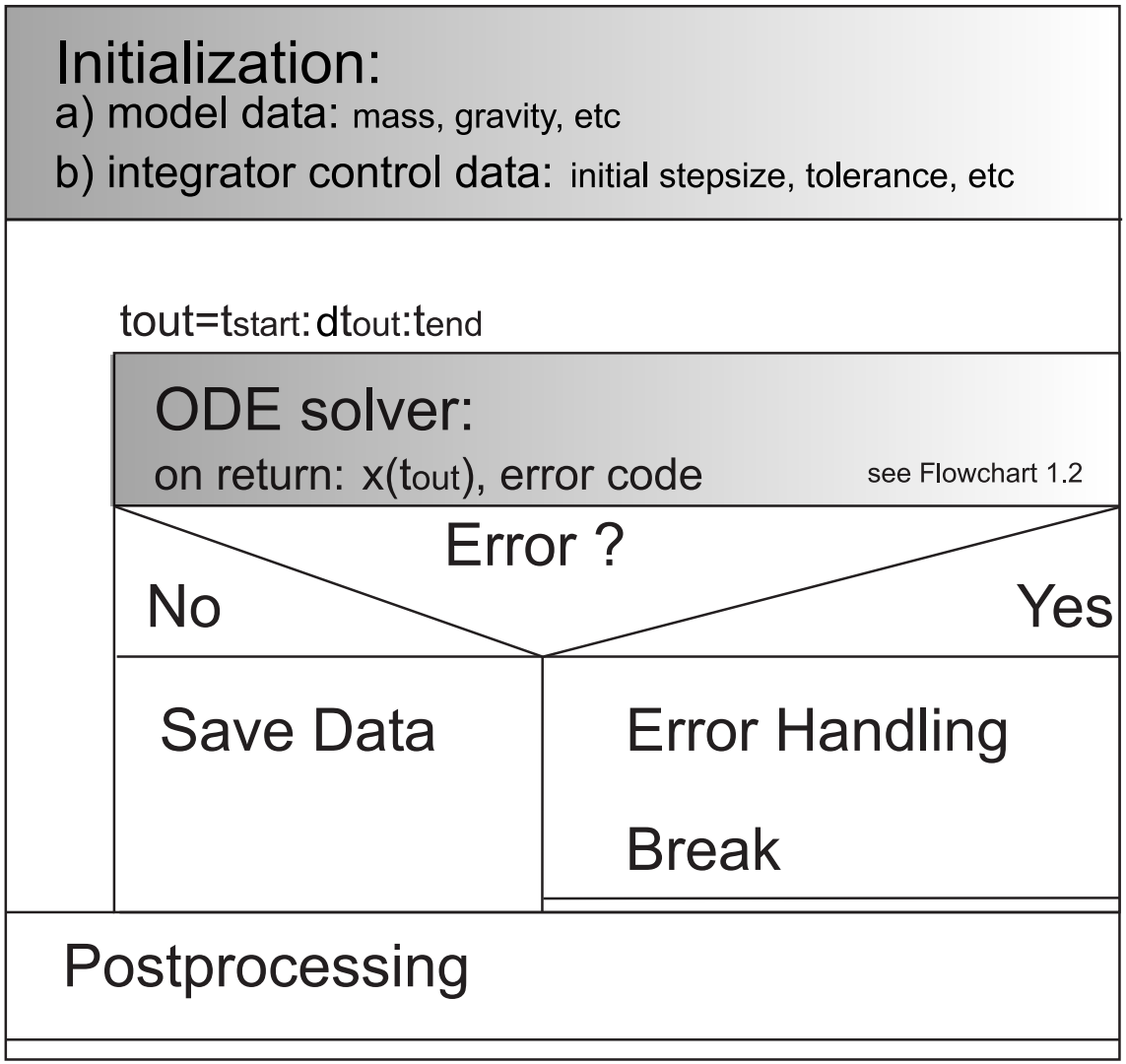
Weights

$$W_i = \mathrm{RTOL} \cdot |y_i| + \mathrm{ATOL}_i$$

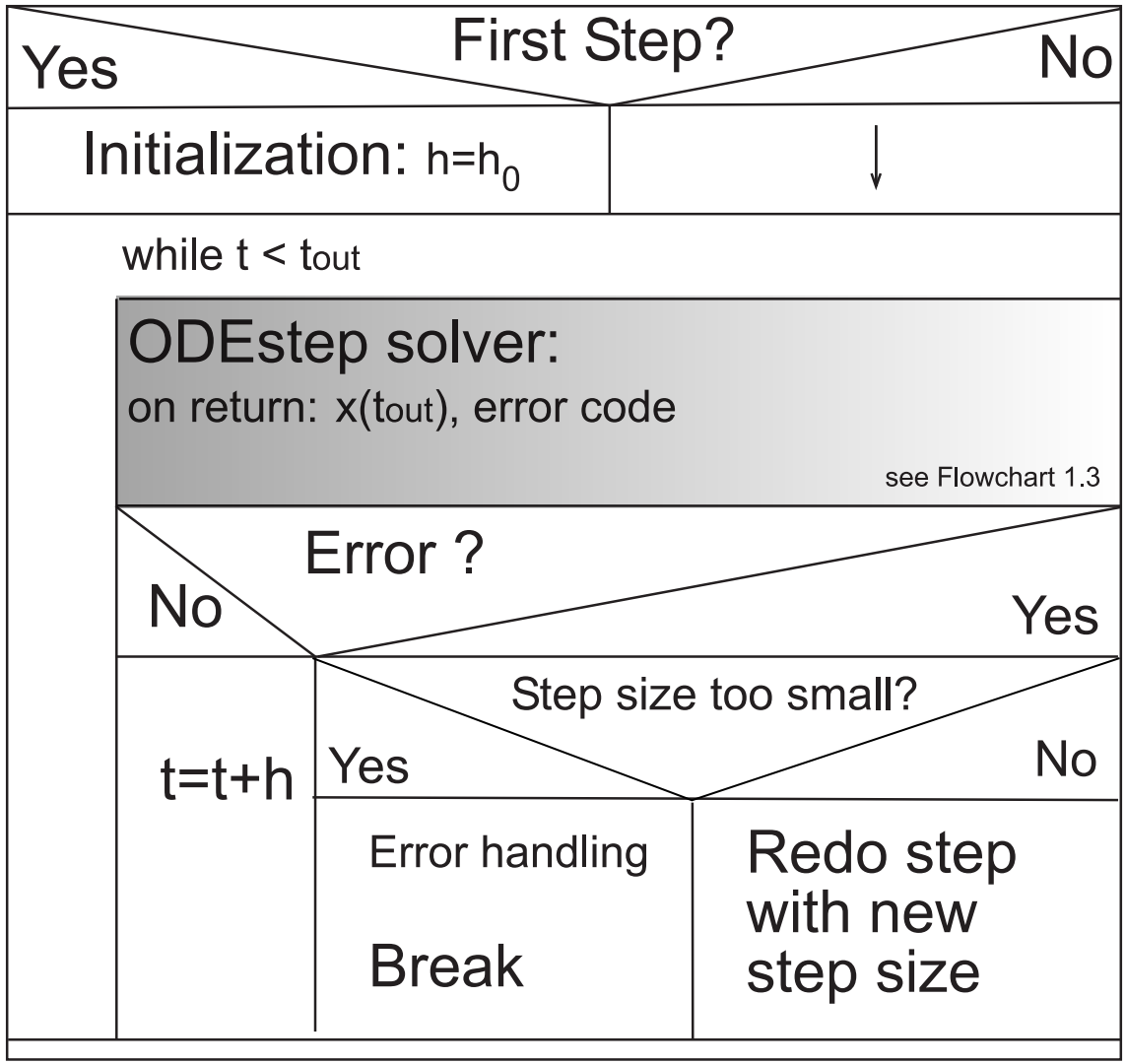
Weighted root mean square norm

$$\|v\| = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\frac{v_i}{W_i})^2}$$

Flowchart 1: Generic integrator call



Flowchart 1.2: Generic single step integrator call



Flowchart 1.3: Generic integrator organisation