Simulation Tools Structure of a Multistep Code

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Spring 2020



1 Initial Value Problems

2 Methods



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 $G(y) = y - h\beta_k f(y)$ – old values.



variable coefficient vs fixed leading coefficient

Coefficients depend on step size ratios:

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

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

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

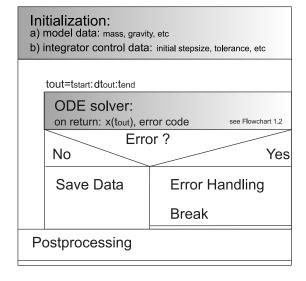
$$W_i = \text{RTOL} \cdot |y_i| + \text{ATOL}_i$$

Weighted root mean square norm

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

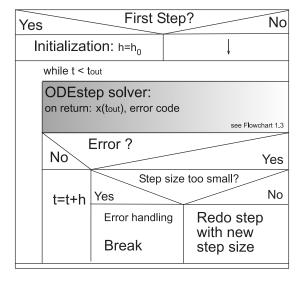


Flowchart 1: Generic integrator call





Flowchart 1.2: Generic single step integrator call





Flowchart 1.3: Generic integrator organisation

Predict			
Yes new Jacobian needed? No			
Compute Jacobian Jac _{new} = 1		Jac _{new} = 0	
Corrector iteration (Newton iteration) return: solution or error code Yes convergence ? No			
Estimate Error		Y Jac _{new} = 0 N	
YError	< Tol N	Redo the step	Redo the step
Accept step increase step size	Reject step decrease step size	with h=h/2 and require a new Jacobian	step size and require a new Jacobian

