OctConf 2017

March 20-22
CERN, Geneva, Switzerland

GSoC 16 - ode15{i,s}

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March 21, 2017

Outline

1. The Mathematical and Numerical problem
2. The solvers
3. Building Octave with SUNDIALS
4. A case test
5. To do

Plan

1. The Mathematical and Numerical problem
2. The solvers
3. Building Octave with SUNDIALS
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The Mathematical problem

Problem

$$F(t, y, \dot{y}) = 0$$

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Initial value

$$y(t_0) = y_0 \qquad \dot{y}(t_0) = \dot{y}_0$$

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$$y, \dot{y}, F \in \Re^N, \quad \dot{y} = dy/dt, \quad y_0 \text{ and } \dot{y}_0 \text{ are given}$$

Numerical approach

- We use the variable-order, variable-step BDF $\sum_{t=0}^{q} \alpha_{n,i} y_{n-i} = h_n \dot{y}_n$

  where y_n and $\dot{y}_n$ are the computed approximations to $y(t_n)$ and $\dot{y}(t_n)$, $h_n = t_n - t_{n-1}$ is the step size and $\alpha_{n,i}$ depends on the order q and the history of the step size

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- At each step we solve the nonlinear algebraic system

  $$G(y_n) \equiv F(t_n, y_n, h_n^{-1} \sum_{t=0}^{q} \alpha_{n,i} y_{n-i}) = 0$$

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  $$G(y_n) \equiv F(t_n, y_n, h_n^{-1} \sum_{t=0}^{q} \alpha_{n,i} y_{n-i}) = 0$$
- We use a Newton method to solve the system

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The solvers: ode15i

$[t, y] = ode15i(odefun, tspan, y0, yp0, opt)$

- odefun $f(t, y, yp)$

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- odefun $f(t, y, yp)$
- tspan $[tinit \;\; tfinal]$
- y0 ColumnVector
- yp0 ColumnVector
- opt opt = odeset ('name', value, ...)

Options

- RelTol

Options

- RelTol
- AbsTol

Options

- RelTol
- AbsTol
- MaxStep

Options

- RelTol
- AbsTol
- MaxStep
- InitialStep

Options

- RelTol
- AbsTol
- MaxStep
- InitialStep
- InitialSlope

Options

- RelTol
- AbsTol
- MaxStep
- InitialStep
- InitialSlope
- MaxOrder

More options

- OutputFcn

More options

- OutputFcn
- OutputSel

More options

- OutputFcn
- OutputSel
- Refine

More options

- OutputFcn
- OutputSel
- Refine
- Stats

More options

- OutputFcn
- OutputSel
- Refine
- Stats
- Events

More options

- OutputFcn
- OutputSel
- Refine
- Stats
- Events
- Jacobian

The solvers: ode15s

$$[t, y] = ode15s(odefun, tspan, y0, opt)$$

- odefun $\quad f(t, y)$

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Options

- NonNegative

Options

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- Mass

Options

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- Mass
- MStateDependence

Van Der Pol equation

$$\begin{cases} y_1' = y_2 \\ y_2' = 1000(1 - y_1^2)y_2 - y_1 \end{cases}$$

Example

Van Der Pol equation

$$\begin{cases} y_1' = y_2 \\ y_2' = 1000(1 - y_1^2)y_2 - y_1 \end{cases}$$

Initial condition

$$y_1(0) = 2 \qquad y_2(0) = 0$$

Van Der Pol equation

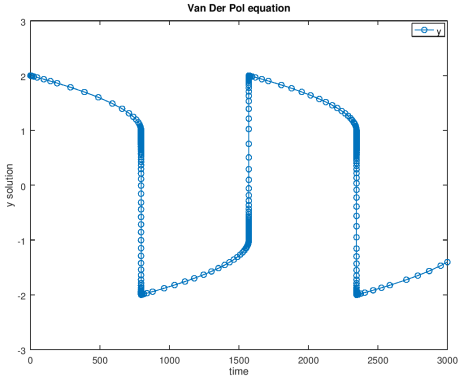
$$\begin{cases} y_1' = y_2 \\ y_2' = 1000(1 - y_1^2)y_2 - y_1 \end{cases}$$

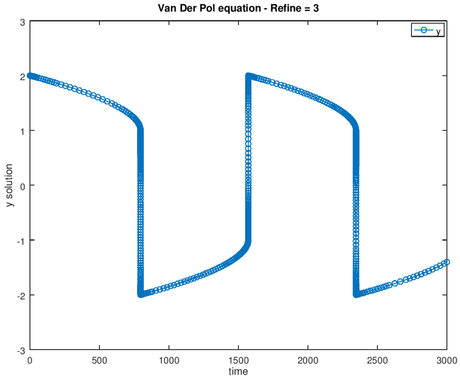
Initial condition

$$y_1(0) = 2 \qquad y_2(0) = 0$$

```
[t,y] = ode15s(@vdp,[0 3000],[2 0]);
```

Refining the grid





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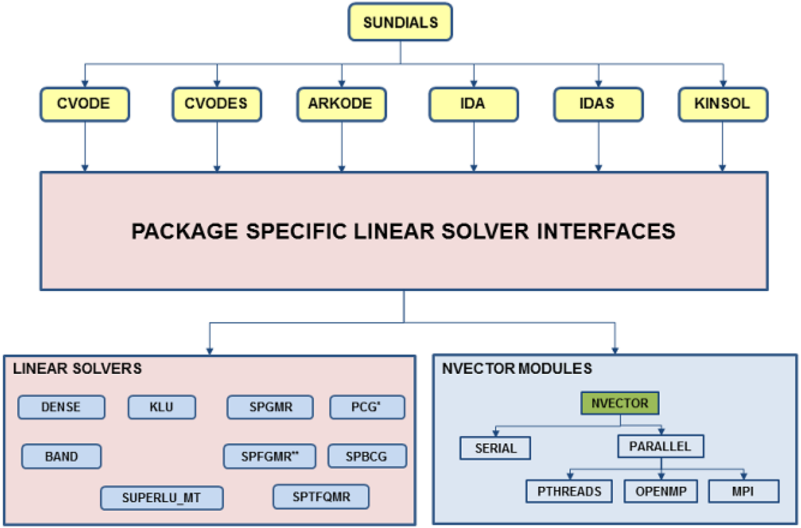
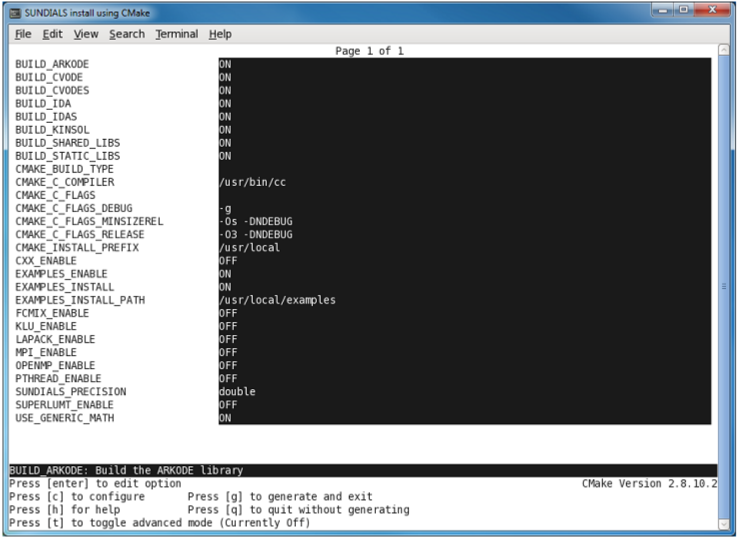
IDA organization

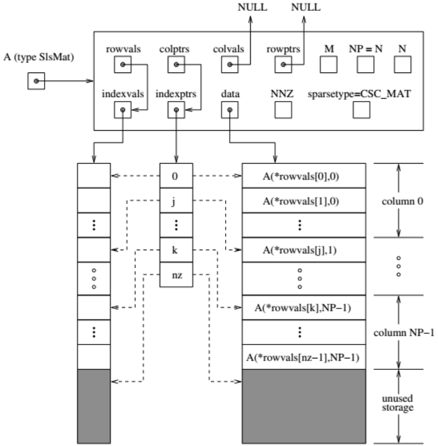


Configuring SUNDIALS



Nice Data Structures

Sparse matrices stored in CSC format



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A case test

FitzHugh-Nagumo equations

$$\begin{cases} \partial u/\partial t = k_1 u - k_2 u^2 - u^3 - v + D\Delta u \quad in \;\; \Omega \\ \partial v/\partial t = \epsilon(k_3 u - a_1 v - a_0) + \delta D \Delta v \\ +Initial \;\; Conditions \\ +Boundary \;\; Conditions \end{cases}$$

A case test

Video simulation

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To do

- decic
- complex values
- improve methods
- improve tests

Thank you for your attention!