



OctConf 2017

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CERN, Geneva, Switzerland



GSoC 16 - ode15{i,s}

Francesco Faccio
francesco.faccio.93@gmail.com
Mentors: CdF, JackC

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

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

The Mathematical problem

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Initial value

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

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

$y, \dot{y}, F \in \mathbb{R}^N$, $\dot{y} = dy/dt$, y_0 and \dot{y}_0 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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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
- ▶ At each step we solve the nonlinear algebraic system
$$G(y_n) \equiv F(t_n, y_n, h_n^{-1} \sum_{t=0}^q \alpha_{n,i} y_{n-i}) = 0$$
- ▶ We use a Newton method to solve the system

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The solvers: ode15i

$[t, y] = \text{ode15i}(\text{odefun}, \text{tspan}, y0, yp0, \text{opt})$

- ▶ odefun $f(t, y, yp)$

The solvers: `ode15i`

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- ▶ `odefun` $f(t, y, y_p)$
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- ▶ `odefun` $f(t, y, yp)$
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- ▶ `y0` ColumnVector

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The solvers: `ode15i`

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- ▶ `odefun` $f(t, y, y_p)$
- ▶ `tspan` $[t_{\text{init}} \ t_{\text{final}}]$
- ▶ `y0` ColumnVector
- ▶ `yp0` ColumnVector
- ▶ `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`

$[t, y] = \text{ode15s}(\text{odefun}, \text{tspan}, y0, \text{opt})$

- ▶ `odefun` $f(t, y)$

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- ▶ `odefun` $f(t, y)$
- ▶ `tspan` $[t_{\text{init}} \ t_{\text{final}}]$
- ▶ `y0` ColumnVector
- ▶ `opt` `opt = odeset ('name', value, ...)`

Options

- ▶ NonNegative

Options

- ▶ NonNegative
- ▶ Mass

Options

- ▶ NonNegative
- ▶ Mass
- ▶ MStateDependence

Example

Van Der Pol equation

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

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Initial condition

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

Example

Van Der Pol equation

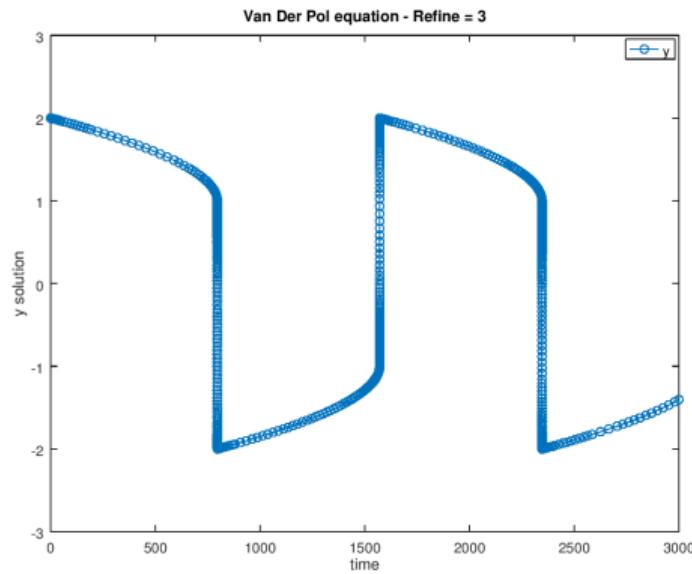
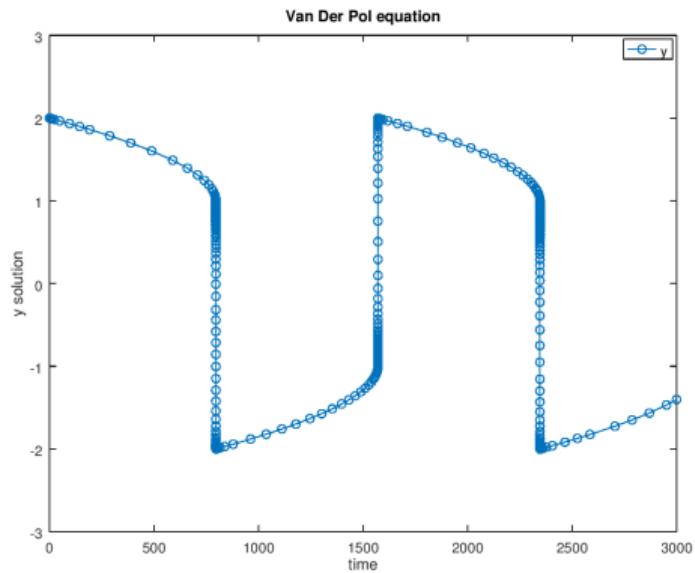
$$\begin{cases} y_1' = y_2 \\ y_2' = 1000(1 - y_1^2)y_2 - y_1 \end{cases}$$

Initial condition

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

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

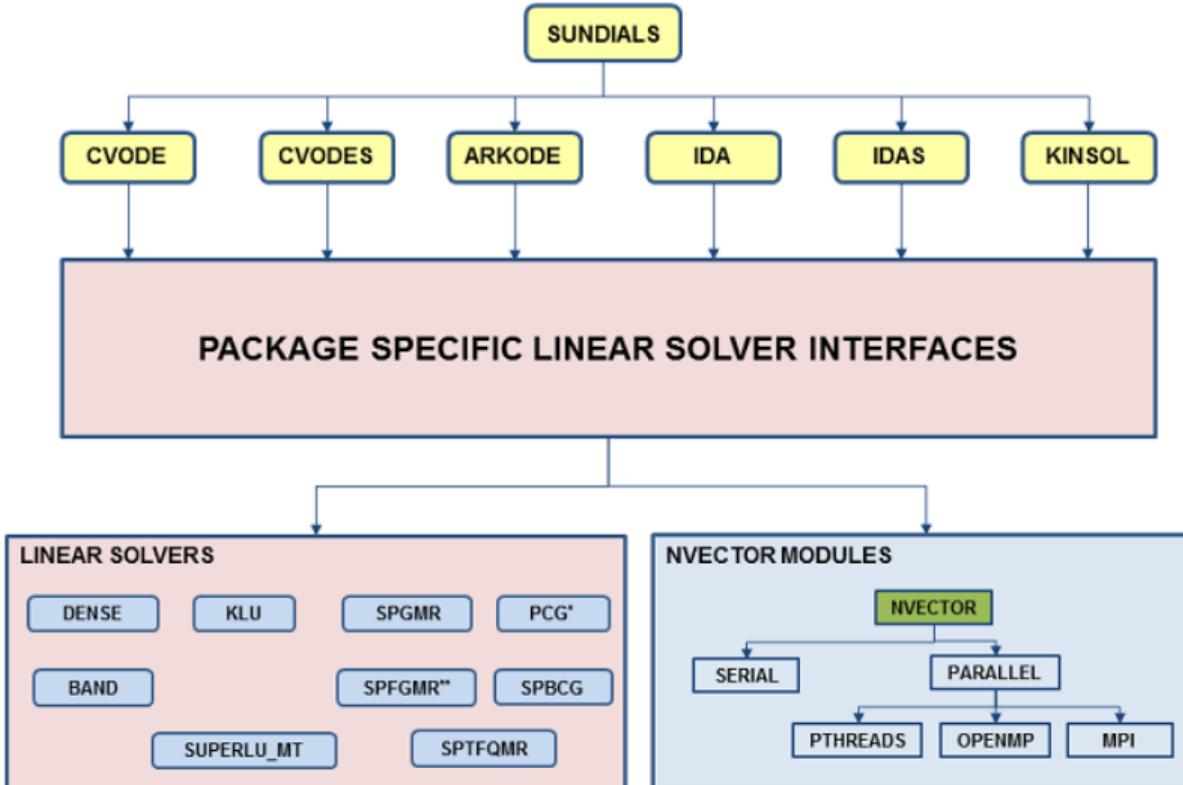
Refining the grid



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IDA organization



Configuring SUNDIALS

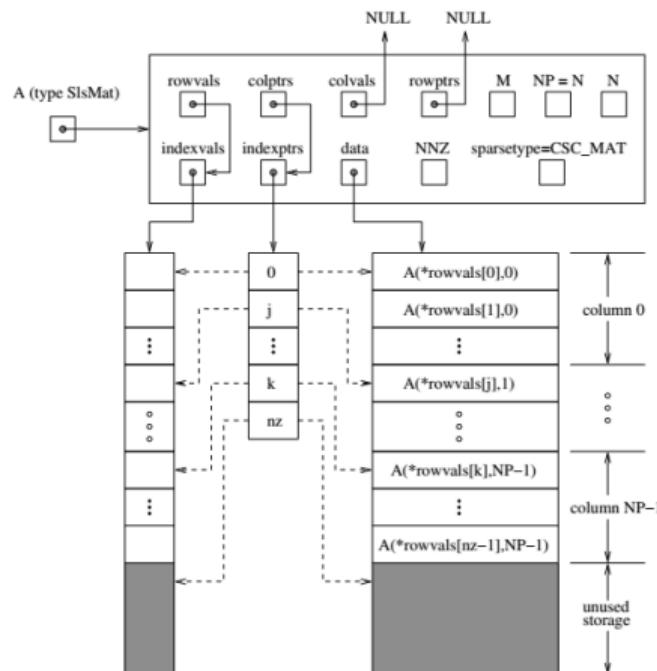
```
SUNDIALS install using CMake
File Edit View Search Terminal Help
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BUILD_ARKODE           ON
BUILD_CVODE             ON
BUILD_CVODES            ON
BUILD_IDA               ON
BUILD_IDAS              ON
BUILD_KINSOL             ON
BUILD_SHARED_LIBS        ON
BUILD_STATIC_LIBS        ON
CMAKE_BUILD_TYPE         CMAKE_BUILD_TYPE
CMAKE_C_COMPILER          /usr/bin/cc
CMAKE_C_FLAGS             -g
CMAKE_C_FLAGS_DEBUG       -Os -DNDEBUG
CMAKE_C_FLAGS_MINSIZEREL -O3 -DNDEBUG
CMAKE_C_FLAGS_RELEASE     /usr/local
CMAKE_INSTALL_PREFIX      OFF
CXX_ENABLE                ON
EXAMPLES_ENABLE           ON
EXAMPLES_INSTALL           ON
EXAMPLES_INSTALL_PATH     /usr/local/examples
FCMIX_ENABLE              OFF
KLU_ENABLE                 OFF
LAPACK_ENABLE              OFF
MPI_ENABLE                  OFF
OPENMP_ENABLE                OFF
PTHREAD_ENABLE              OFF
SUNDIALS_PRECISION         double
SUPERLUMT_ENABLE           OFF
USE_GENERIC_MATH           ON

BUILD_ARKODE: Build the ARKODE library
Press [enter] to edit option
Press [c] to configure      Press [g] to generate and exit
Press [h] for help           Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
CMake Version 2.8.10.2
```

Nice Data Structures

Sparse matrices stored in CSC format



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A case test

FitzHugh-Nagumo equations

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

A case test

Video simulation

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To do

- ▶ decic
- ▶ complex values
- ▶ improve methods
- ▶ improve tests

Thank you for your attention!