Time integration for coupled circuit-EM systems

Michael Matthes Sascha Baumanns

Mathematical Institute
University of Cologne

ICESTARS meeting in Hagenberg, Oct 9th 2009,
FH Oberösterreich, University of Applied Sciences,
Auditorium HS2

Outline

1. Part I - Public part
   - Coupled system
   - Space discretized system
   - Solving the DAE
   - Numerical Experiments
2. Part II - Internal part
   - MECS - Python Version
   - Example: Using the DAEn solver

PART I
–
Public part

Modified Nodal Analysis (MNA)

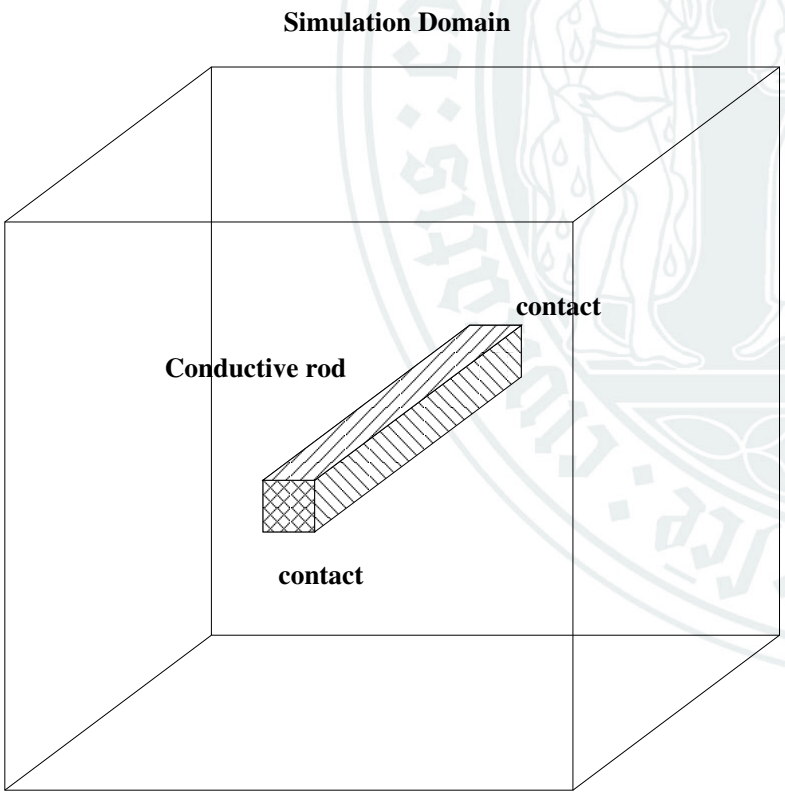
$$A_C \frac{\mathrm{d}q_C(A_C^T e, t)}{\mathrm{d}t} + A_R g(A_R^T e, t) + A_L j_L + A_V j_V + A_I i_s(t) = 0,$$

$$\frac{\mathrm{d}\phi(j_L, t)}{\mathrm{d}t} - A_L^T e = 0,$$

$$A_V^T e - v_s(t) = 0.$$

A_X	element-related (reduced) incidence matrices
$i_S(t)$ and $v_S(t)$	current and voltage sources
q_C, g and ϕ	physical relations given for conductance, charge and flux
$e(t)$	node potentials for $t \in \mathcal{I}$
$j_L(t)$	current through inductivities for $t \in \mathcal{I}$
$j_V(t)$	current through voltage sources for $t \in \mathcal{I}$

EM-Element



EM-Model Equations

$$-\nabla \cdot \sigma \left(\nabla \mathcal{V} + \Pi\right) - \nabla \cdot \varepsilon \left(\nabla \frac{\partial \mathcal{V}}{\partial t} + \frac{\partial \Pi}{\partial t}\right) = 0,$$

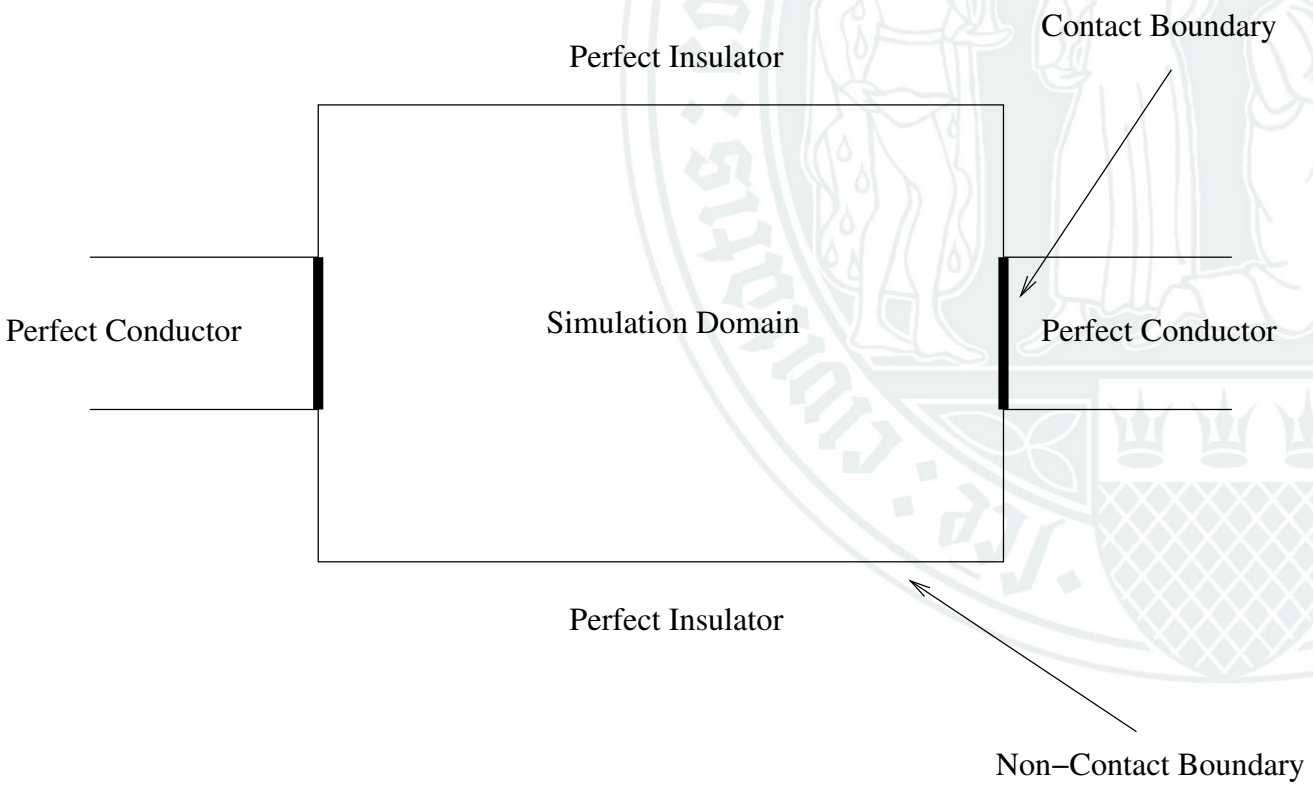
$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathcal{A}\right) - \frac{1}{\mu} \nabla \nabla \cdot \mathcal{A} + \sigma \left(\nabla \mathcal{V} + \frac{\partial \mathcal{A}}{\partial t}\right) + \varepsilon \left(\nabla \frac{\partial \mathcal{V}}{\partial t} + \frac{\partial \Pi}{\partial t}\right) = 0,$$

$$\Pi - \frac{\partial \mathcal{A}}{\partial t} = 0.$$

$\mathcal{V}$	scalar potential
$\mathcal{A}$	vector potential
Π	pseudo-canonical momentum $= \frac{\partial \mathcal{A}}{\partial t}$

Remark: There is some kind of freedom where to plug in Π.

EM-Model Boundary Conditions - I



EM-Model Boundary Conditions - II

contact boundary:

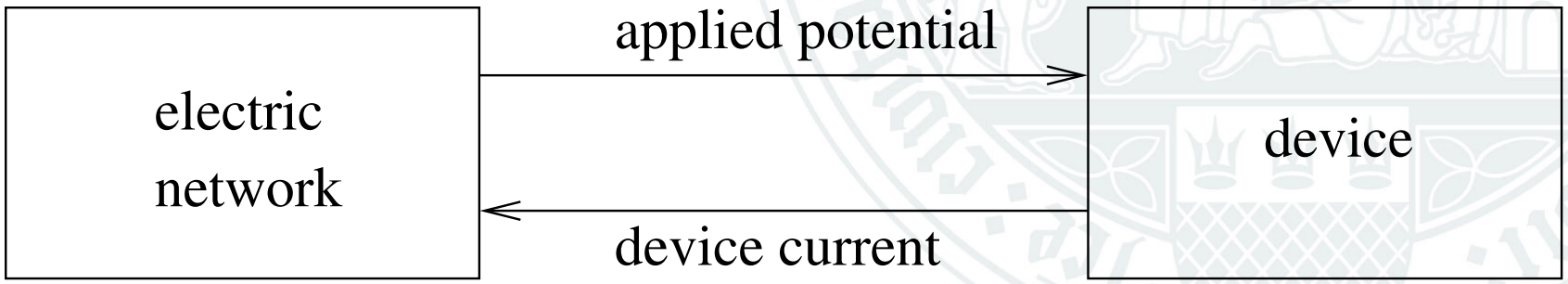
$$\mathcal{V} = f(x,t), \quad \mathcal{A} \cdot \tau = 0, \quad \frac{\partial (\mathcal{A} \cdot \nu)}{\partial \nu} = 0.$$

non-contact boundary:

$$\left(\nabla \mathcal{V} + \frac{\partial \mathcal{A}}{\partial t} \right) \cdot \nu = 0, \quad \mathcal{A} \cdot \tau = 0, \quad \frac{\partial (\mathcal{A} \cdot \nu)}{\partial \nu} = 0.$$

Coupling Conditions

Coupling via boundary conditions and current equation.



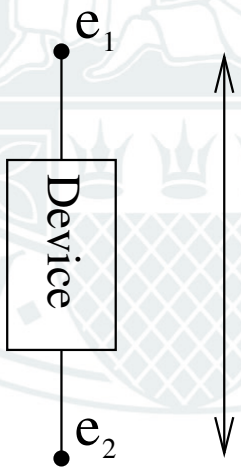
Remark: EM-model is charge conserving.

Coupling Conditions: MNA to EM-Model

- A_M describes the circuit topology of the device.
- $A_M^T e$ denotes the applied node potential.

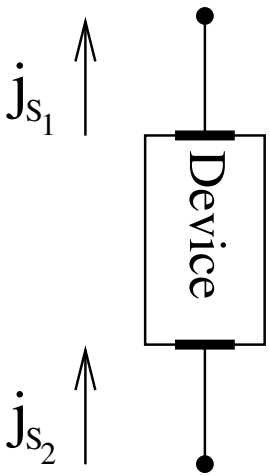
Dirichlet boundary condition for $\mathcal{V}$:

$$\mathcal{V} = \mathcal{V}_{bi}(x) + \mathcal{V}_{ext}\left(x, A_M^T e\right)$$



Coupling Conditions: EM-Model to MNA

- Γ_k k-th contact.



Current through the k-th contact of the device:

$$j_{s_k} = \int_{\Gamma_K} -\sigma\left(\nabla\mathcal{V} + \Pi\right) - \varepsilon\frac{\partial}{\partial t}\left(\nabla\mathcal{V} + \Pi\right)\cdot\nu ds$$

General Coupling

$$
\begin{aligned}
A_C \frac{\mathrm{d}q_C(A_C^T e, t)}{\mathrm{d}t} + A_R g(A_R^T e, t) + A_L j_L + A_V j_V + A_I i_s(t) + A_M j_M &= 0, \\
\frac{\mathrm{d}\phi(j_L, t)}{\mathrm{d}t} - A_L^T e &= 0, \\
A_V^T e - v_s(t) &= 0, \\
j_M - g(\mathcal{V}, \Pi, A_M^T e) &= 0, \\
h(\mathcal{V}, \mathcal{A}, \Pi, A_M^T e) &= 0
\end{aligned}
$$

with g being the function representing the current through the EM device and h being the EM-operator.

Space Discretized System

Linear circuit with one EM-element (non-semiconductor material):

$$\begin{bmatrix} A_C C A_C^T & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & L & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{SE} H A_M^T & 0 & 0 & 0 & A_{SV} & 0 & A_{S\Pi} \\ A_{GE} H A_M^T & 0 & 0 & 0 & A_{GV} & 0 & A_{G\Pi} \\ A_{ME} H A_M^T & 0 & 0 & 0 & A_{MV} & A_{MA} & A_{M\Pi} \\ 0 & 0 & 0 & 0 & 0 & -I & 0 \end{bmatrix} \begin{pmatrix} e \\ j_L \\ j_V \\ j_M \\ V \\ A \\ \Pi \end{pmatrix}'$$

$$+ \begin{bmatrix} A_R G A_R^T & A_L & A_V & A_M & 0 & 0 & 0 \\ -A_L^T & 0 & 0 & 0 & 0 & 0 & 0 \\ A_V^T & 0 & 0 & 0 & 0 & 0 & 0 \\ B_{SE} H A_M^T & 0 & 0 & 1 & B_{SV} & 0 & B_{S\Pi} \\ B_{GE} H A_M^T & 0 & 0 & 0 & B_{GV} & 0 & B_{G\Pi} \\ B_{ME} H A_M^T & 0 & 0 & 0 & B_{MV} & B_{MA} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{pmatrix} e \\ j_L \\ j_V \\ j_M \\ V \\ A \\ \Pi \end{pmatrix} = \begin{bmatrix} -A_I i_s(t) \\ 0 \\ v_s(t) \\ r_S \\ r_G \\ r_M \\ 0 \end{bmatrix}$$

Remark: $A_{M\Pi}$, B_{GV} and B_{MA} non-singular.

Remarks

- Linear DAE of the form $Ay' + By + q = 0$.
- Index: No result yet but we think that it depends on the underlying device geometry and circuit topology. This would be different to the results obtained from the coupling to the DD-model.
- For the index investigation a deep understanding of the underlying matrices A_{XY} and B_{XY} is needed.

Solving the DAE

The time discretization is done with one of the following DAE solvers:

- DAEn - BDF solver, can handle DAEs of the form $M(t)y' + f(y,t) = 0$,
- GLIMDA - GLM solver, can handle DAEs of the form $Md(y,t)' + b(y,t) = 0$,
- own BDF solver - can handle DAEs of the form $f(d(y,t)', y, t) = 0$.

We implemented them all in Python.

Remark: The index of a DAE is very important for the efficiency and feasibility for the solver.

Numerical experiments - Oscillator

Oscillator vcoBi from D5.2:

Goal: Simulate the coupled inductors by the EM.

MATLAB®:

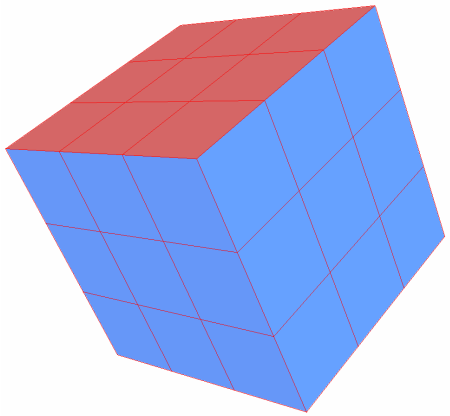
- Simulation done with equivalent circuits for MOSFETs
- Simulation done with drift-diffusion model for MOSFETs

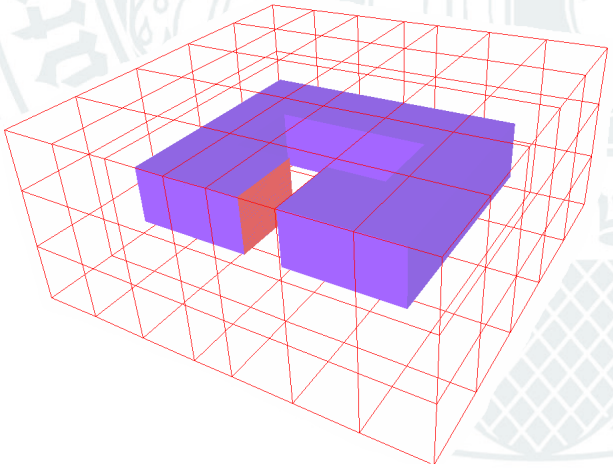
Python:

- equivalent circuit in progress.
- drift-diffusion model not implemented so far.
- BSIM not coupled to the network equations so far (for reference purposes).

Numerical experiments - Simple circuits with EM - I

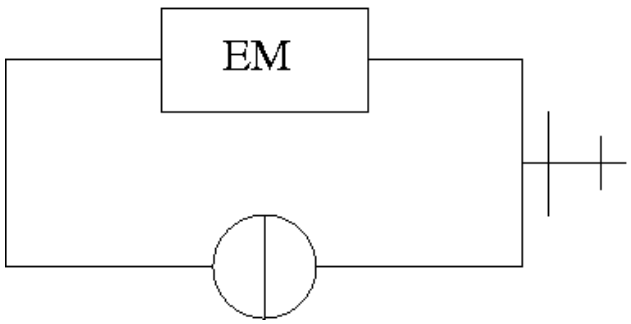
We tested different EM-elements in different circuit configurations.
Index does not exceed 2 for simple grids (given by MAGWEL).

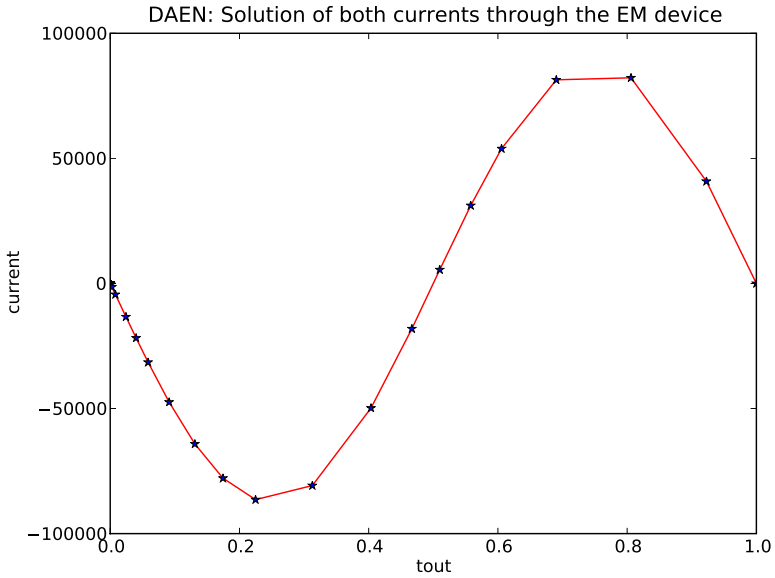




Numerical experiments - Simple circuits with EM - II

Simple circuit with sinusoidal voltage source and simple EM-element.





EM-element behaves like a resistor with a resistance of $8.74 * 10^{-4}$ Ohm.

PART II
–
Internal part
Background and Usage Cologne software

Why Python?

- easy to use, easy to program
- advanced numerical packages numpy and scipy
- easy to include modules written in other programming languages

Overview of MECS - I

MECS (Multiphysical Electric Circuit Simulator):

- developed and maintained by our research group.
- originally implemented in MATLAB®.
- using the drift-diffusion model for semiconductors.
- drift-diffusion model not available in the Python version so far.

Overview of MECS - II

MECS can generate DAEs of the type

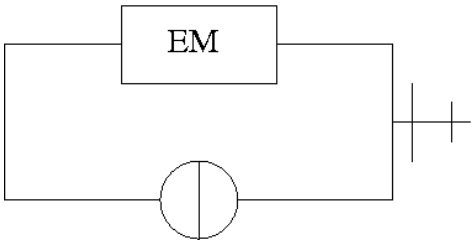
- $My' + b(y,t) = 0$ (standard) or
- $Md(y,t)' + b(y,t) = 0$ (proper).

In the following we concentrate on the standard case. We need evaluations of

- M, $b(y,t)$ and $\frac{\partial b(y,t)}{\partial y}$ (standard case).

Overview of MECS - III

- Input: netlist and options.
- MECS:
  1. Initialization of the circuit elements and setup of the DAE.
  2. Simulation of the circuit by evaluation of the elements element-wise ($R, C, \ldots$). (Control goes to a DAE solver)
- netlist: Mainly spice3 with little extensions. So far not all spice3 elements available.




```
* Simple Circuit with EM-Element
V1 0 1 sin(0 1 1 0 0)
$EM1 1 0 prototype_inductor 0
```

MECS Elements - I

MECS Elements:

- resistors, capacitors, inductors, voltage and current sources.
- external elements (include e.g. MAGWEL EM-element).

Recall: DAE has the form $My' + b(y, t) = 0$ with $y = (e, j, x)$.

- e: node potentials.
- j: internal variables (currents through inductors and capacitors) + current through external elements.
- x: external variables (e.g. pseudo-canonical momentum, scalar and vector potential).
- t: time.

MECS Elements - II

Elements:

- Initialization:
  - Input: type, parameter and names of all elements of the type, massnode, DAE formulation.
- Evaluation:
  - Input: flag, y, timestep.
  - Output: Corresponding part of M, $b(y,t)$ or $\frac{\partial b(y,t)}{\partial y}$.

MAGWEL EM-element in MECS

We can handle:

- insulating and conducting materials.
- mixture of both.
- two port elements.

Recall the EM equations

$$\begin{aligned} j_M - g(\mathcal{V}, \Pi, A_M^T e) &= 0 \\ h(\mathcal{V}, \mathcal{A}, \Pi, A_M^T e) &= 0 \end{aligned} \quad \Leftrightarrow \quad \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{pmatrix} x \\ A_M^T e \end{pmatrix} = \begin{pmatrix} 0 \\ j_M \end{pmatrix}$$

with $x = (\mathcal{V}, \mathcal{A}, \Pi)$.

EM-element in MECS: Communication MAGWEL/MECS

MAGWEL EM-element:

- Initialization:
  - Input: devicename, contact nodes, reference node
  - setup the coupling matrix A_M
  - call MAGWEL (once):
    - number of nodes and links
    - matrices A, B, C, D.
    - evaluate EM part of M and $\frac{\partial b(y,t)}{\partial y}$ (once).
- Evaluation:
  - Input: flag, y.
  - Output: Corresponding part of M, $b(y,t)$ or $\frac{\partial b(y,t)}{\partial y}$.

Communication MAGWEL/MECS

up to now:

- Communication via files. We need just the matrix dump. Possible because we have linear systems.

future:

- Direct communication via pointers. (MECS part easy)

Example: Using the DAEn solver

- Originally implemented in MATLAB® by Michael Hanke.
- BDF solver using a combination of error estimation and order selection strategies.
- handles DAEs of the form $M(t)y' + f(y,t) = 0$ with $M(t)$ possibly singular.

Using DAEn - Example: Ringmodulator

- The Ringmodulator is represented by a stiff system of 15 nonlinear ordinary differential equations.
- It depends on a factor C_s.
- For $C_s = 0$ we have a DAE of index 2 with 11 differential and 4 algebraic equations.
- From the testset on http://pitagora.dm.uniba.it/~testset/problems/ringmod.php

Using DAEn - Example: Ringmodulator

We have five relevant Python files:

- **csparse.py** - (main sparse matrix format)
- **ringmodulator.py** - (equations for the ringmodulator)
- **funcDAE_standard.py** - (interface for DAEs of the form $My' + f = 0$, provides numerical jacobians)
- **daen.py** - (BDF-solver DAEn)
- **test_daen_ringmodulator.py** - (script for running the solver)

Using DAEn - Example: Ringmodulator

ringmodulator.py:

```
class Ringmodulator(object):

  def __init__(self,y0=zeros(15),timeinterval=(0,1e-3),Cs=2e-12):
    self.C = 1.6*1e-8
    ...

  def mass(self,y,t):
    return Csparse(diag([self.C,self.C,self.Cs,self.Cs,self.Cs,
                         self.Cs,self.Cp,self.Lh,self.Lh,self.Ls2,
                         self.Ls3,self.Ls2,self.Ls3,self.Ls1,self.Ls1]))

  def f(self,y,t):
    return array([-(y[7]-0.5*y[9]+0.5*y[10]+y[13]-1./self.R*y[0]),
                  -(y[8]-0.5*y[11]+0.5*y[12]+y[14]-1./self.R*y[1]),
                  ...
```

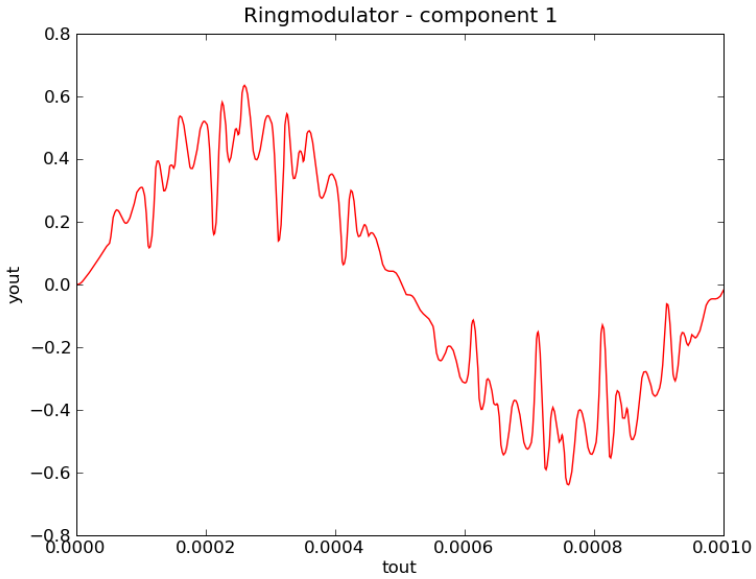
Using DAEn - Example: Ringmodulator

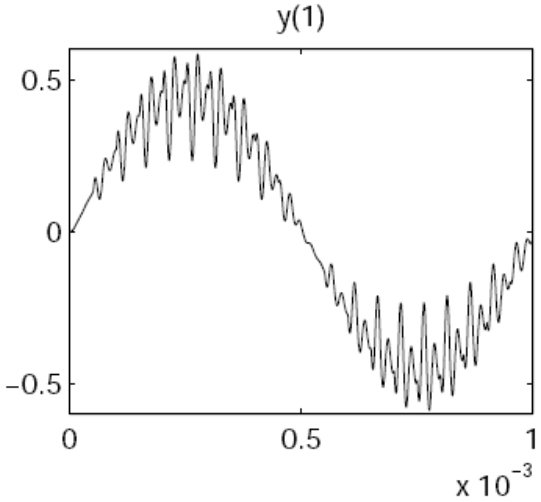
test_daen_ringmodulator.py:

```
ringmod = Ringmodulator(y0=zeros(15),timeinterval=(0,1e-3),Cs=2e-12)

dae=FuncDAE_standard(ringmod.mass,ringmod.f,y0,timeinterval)

options={'abstol':1e-4,
         'reltol':1e-4,
         'estrat':2,
         'ostrat':'Std',
         'scaling': 'on',
         'report': 'none'
        }

daesolver=DAEn(dae,options)
daesolver.run()

tout,yout = daesolver.get_solution()
```

Using DAEn - Example: Ringmodulator

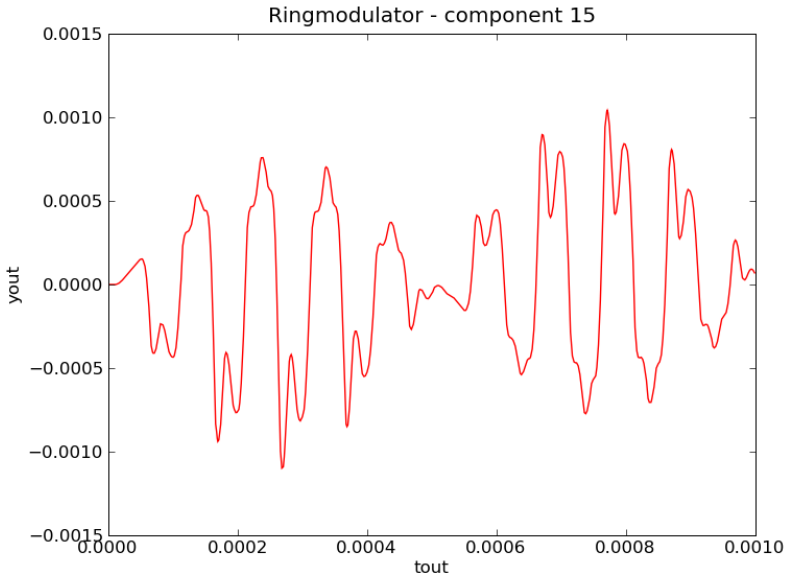
Comparison: low frequency input signal (component 1)

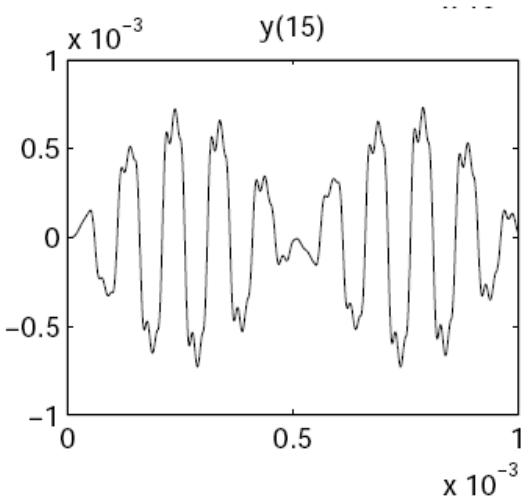




Using DAEn - Example: Ringmodulator

Comparison: resulting current (component 15)





Using the other solvers

Using the other solvers is done in a similar way. They just accept a different interface:

- GLIMDA - use FuncDAE_proper.py
- own BDF solver - use FuncDAE_fproper.py

The End

Thanks for your attention!