Pure Modelica Unit Testing: From Mathematical Algorithms to Physical Modeling

OpenModelica Annual Workshop 2019

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Outline

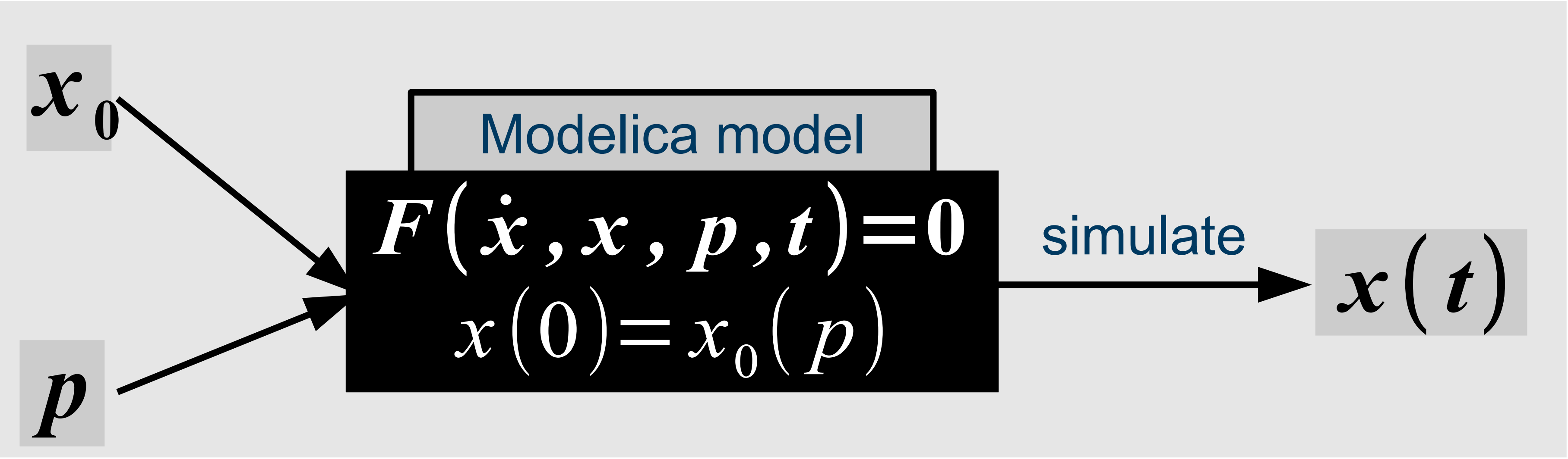
- First testing experiences
  - Mathematical algorithms in Modelica
- Unit testing in Modelica
  - existing technologies
- A bit more “formal” Unit testing
  - Upgrading to Physical Modeling

Motivation

Wiechert, W., Noack, S., and Elsheikh, A. (2010). Modeling languages for biochemical network simulation: Reaction vs equation based approaches. Advances in Biochemical Engineering / Biotechnology

“Simulation tools not only perform numerical solutions based on the system equations but also assist the modeler in systems analysis. Doubtlessly the most important systems analysis tool is Sensitivity Analysis ...

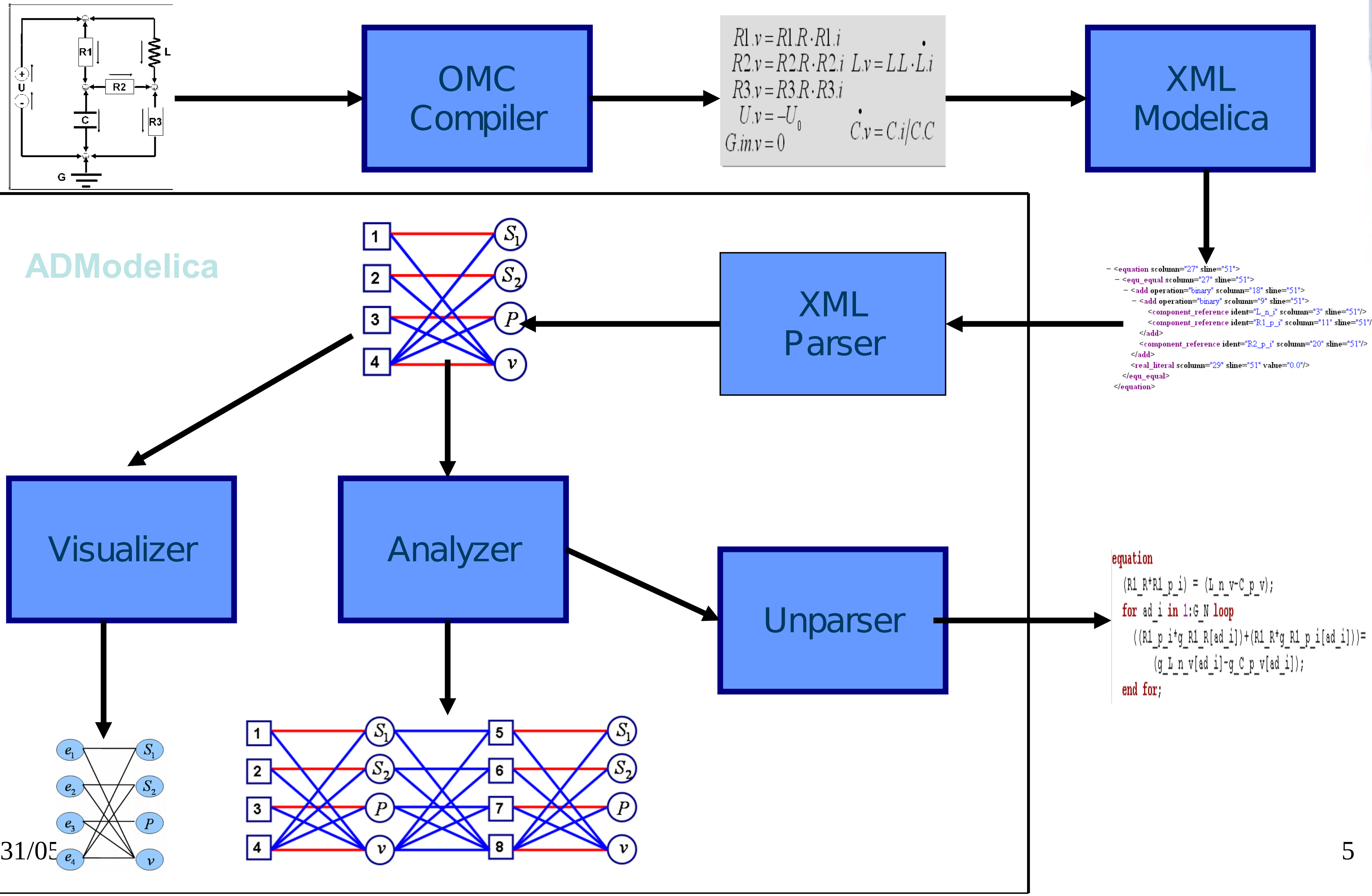
SA of Modelica Models



Dynamic Parameter Sensitivities (DPS)

$$\frac{\partial x}{\partial p}(t) \qquad \frac{\partial x}{\partial x_0}(t)$$

ADModelica (2007)



Sample of generated code (I/II)

- Declaration part

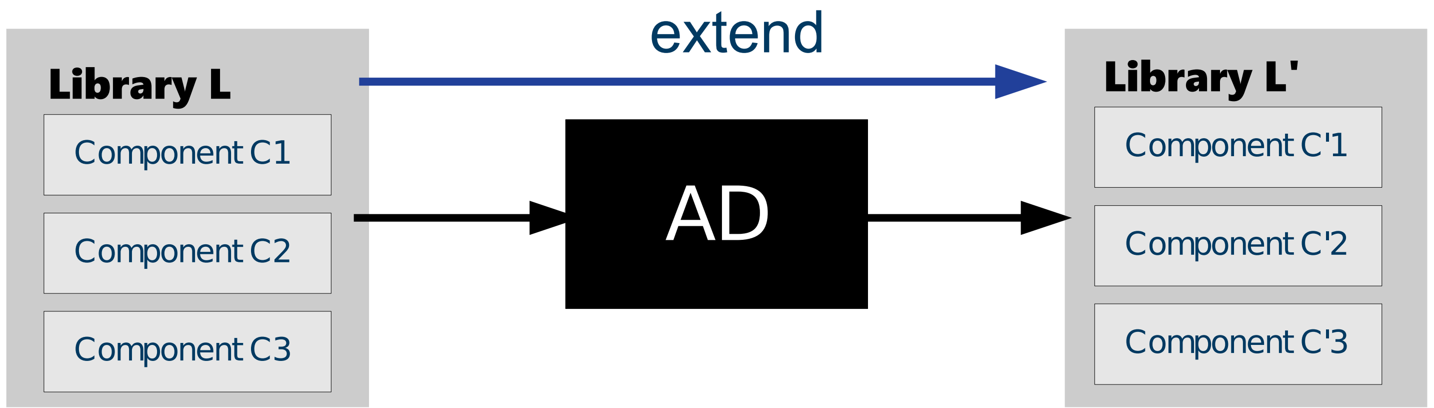
```
model ADSimpleReaction
  Real S(start=1);
  Real P(start=0);
  Real v;
  Real[3] g_S, g_P, g_v;
  parameter Real vmax=1;
  constant Real[3] g_vmax={1,0,0};
  parameter Real k=1;
  constant Real[3] g_k={0,1,0};
  parameter Real Ik=1;
  constant Real[3] g_Ik={0,0,1};
protected
  Real loc01,loc02,loc03,loc04,loc05;
  Real g_loc01,g_loc02,g_loc03,g_loc04,g_loc05;
```

Sample of generated code (II/II)

- Equation part

```
equation
  der(S)=-v;
  der(P)=v;
  //v = vmax * (S/(S+k)) * (Ik/(P+Ik));
algorithm
  loc01  := vmax*S;
  loc02  := S+k;
  loc03  := loc01/loc02;
  loc04  := P+Ik;
  loc05  := Ik/loc04;
  v      := loc03*loc05;
//Derivatives:
equation
  for i in 1:3 loop
    der(g_S[i])=-g_v[i];
    der(g_P[i])=g_v[i];
  end for;
algorithm
  for i in 1:3 loop
    g_loc01  := g_vmax[i]*S+vmax*g_S[i];
    g_loc02  := g_S[i]+g_k[i];
    g_loc03  := (g_loc01*loc02-loc01*g_loc02)/(loc02^2);
    g_loc04  := g_P[i]+g_Ik[i];
    g_loc05  := (g_Ik[i]*loc04-Ik*g_loc04)/(loc04^2);
    g_v[i]   := g_loc03*loc05+loc03*g_loc05;
  end for;
end ADSimpleReaction;
```

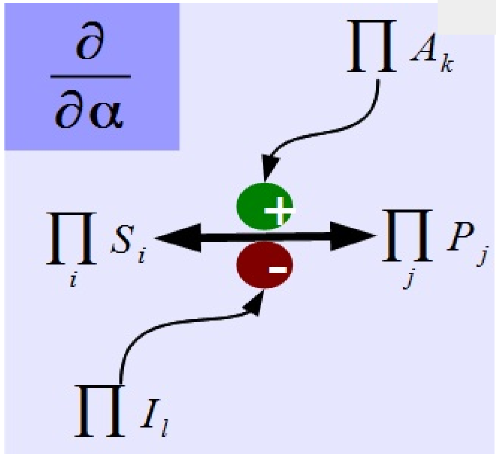
Algorithmic Differentiation (AD) of Modelica libraries (2011)



Algorithmic differentiation Modelica Libraries

The ADGenKinetics Library

2011

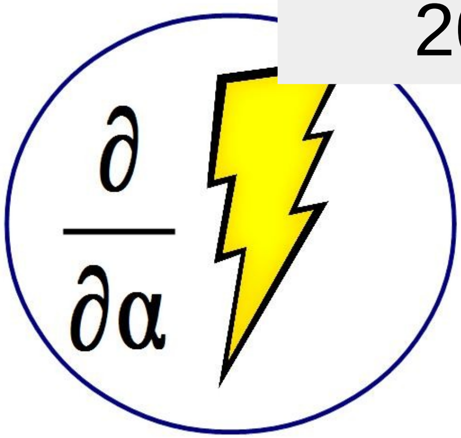


Algorithmically differentiated Modelica library for biochmeical reaction networks

https://github.com/modelica-3rdparty/ADGenKinetics

The ADMSL Library

2014



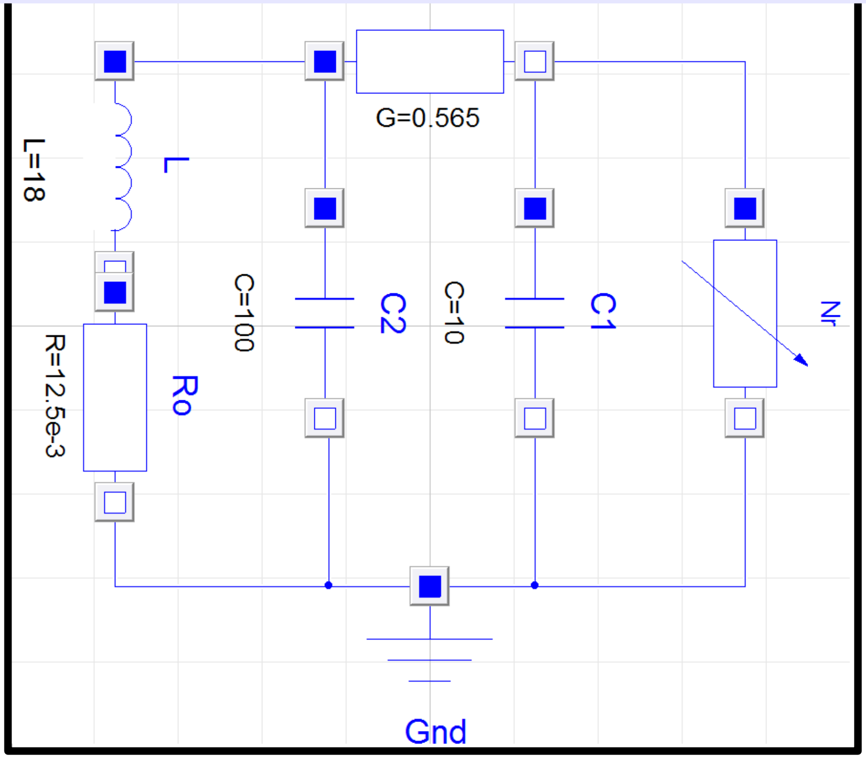
Serves as an example of algorithmically differentiated Modelica library

https://github.com/AIT-CES-LAB/ADMSL

Chua Circuit

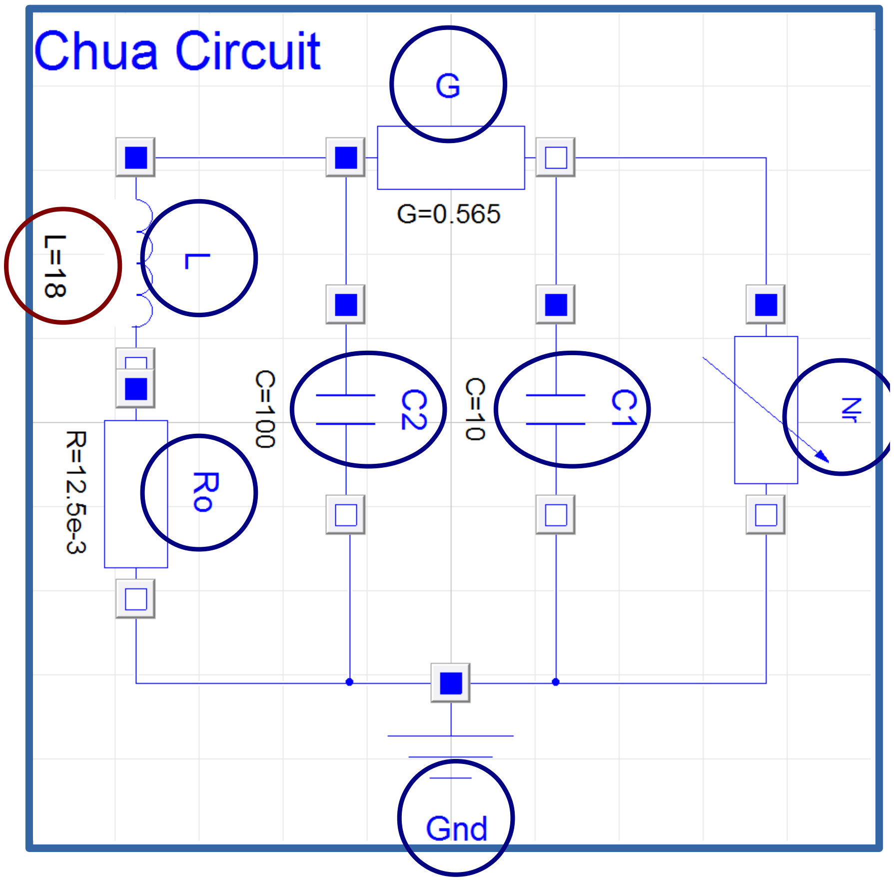
Standard Modelica model for an electrical circuit

Modelica.Electrical.Analog.Basic.Examples.ChuaCircuit



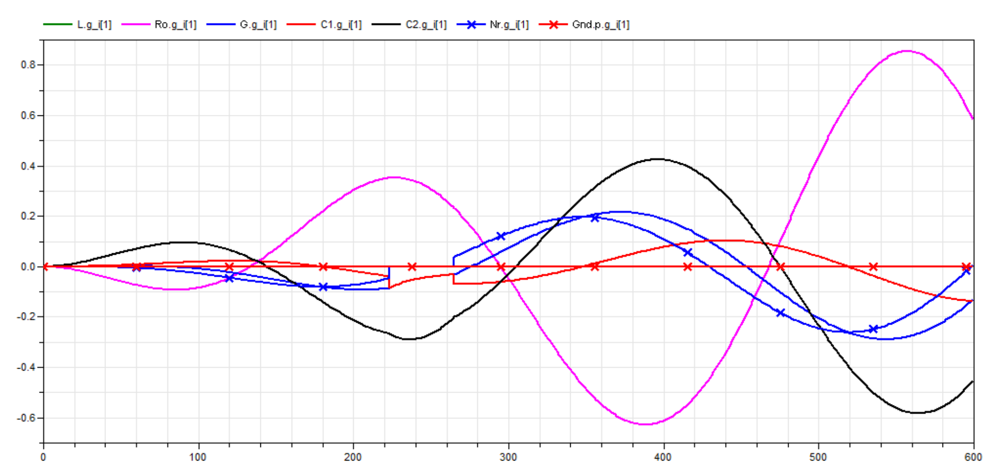
This examples simulates
the current and voltage
at all components

Chua Circuit importing ADMSL



The sensitivities of the current w.r.t. L

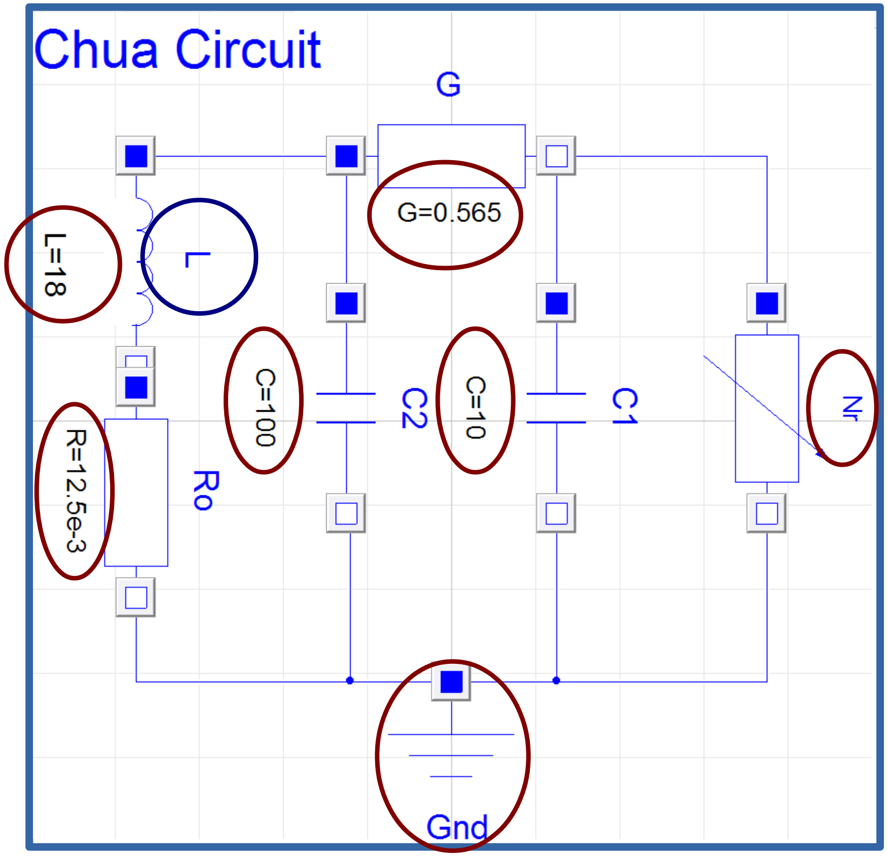
$$\frac{\partial\, X.i}{\partial\, L.L}$$

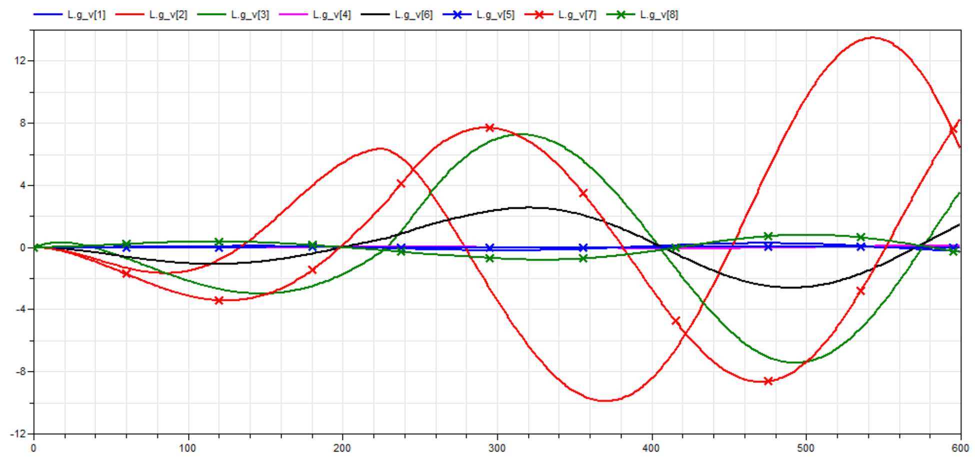


Chua Circuit importing ADMSL

The sensitivities of the voltage at L w.r.t. all parameters

$$\frac{\partial V_L}{\partial X.p}$$





Applications of DPS

1) Modeling-Orietned

Control Coefficients, Local SA, Parameter Sweeping Studies, Model Simplification, ...

2) Statistical

Regression Analysis, Global SA, Identifiability Analysis, ...

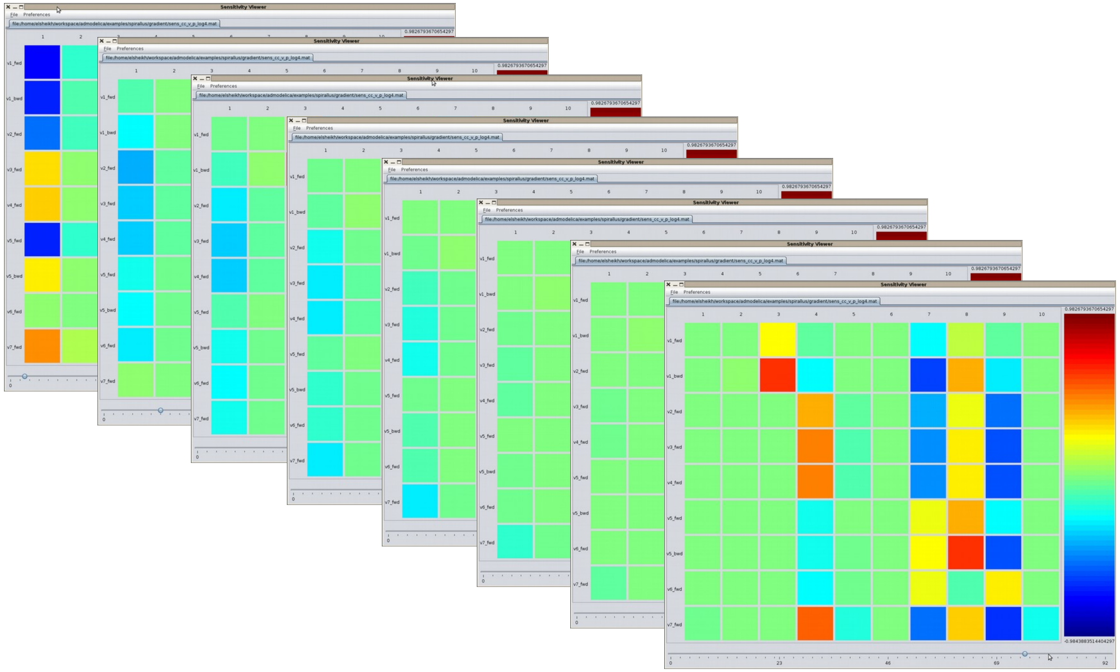
3) Optimization

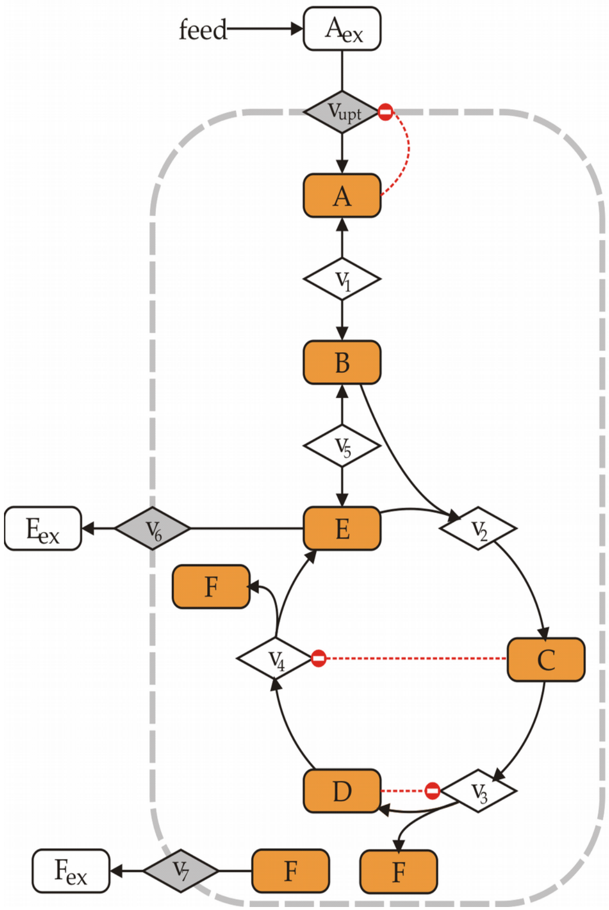
Cost-functions expressed in terms of DPS

Atiyah Elsheikh and Sergei Kucherenko. (2019)
Dynamic parameter sensitivities: Summary of applications – version 1.0.
Technical Report, to appear

Scaled Parameter Sensitivities

$$CC_p^x = \frac{p}{x(t)} \frac{\partial x}{\partial p}(t)$$

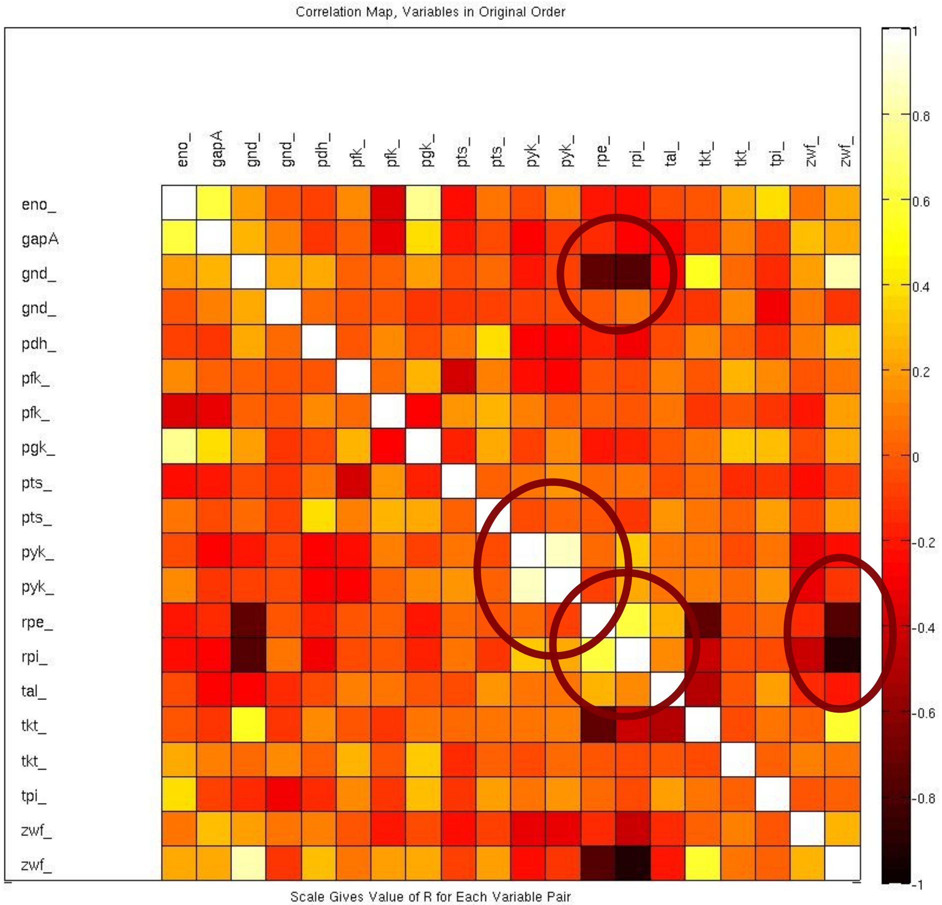




Several snapshots at different time points

Correlation among parameters

Correlation among parameters
Based on Fischer Information Matrices



Strongly Correlated Parameters

Testing AD

Finite Difference Methods

$$\frac{\partial x}{\partial p_j}(t, p) = \frac{x(t, p+e_j \delta_j) - x(t, p)}{\delta_j} + O(\delta_j)$$

$$\delta_j = \epsilon p_j$$

Adhoc Testing (2007-2014)

1)Evaluate DPS with FD

externally with Matlab

small models

2) Simulate AD models

3) Check if the curves behave similarly

Sometimes compute Relative errors

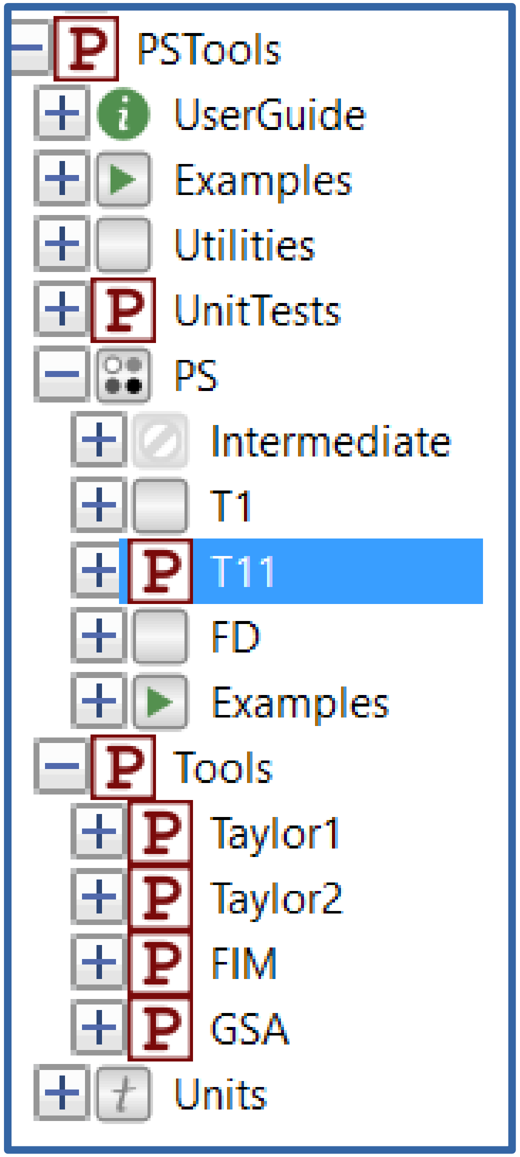
4)Investigate cause of errors, if any

Under Development (2019)
Highly Experimental

PSTools Library

- Promotes the usage of PS at Modelica level
- Serves as utility package for arbitrary Modelica libraries
- PS Package
  - Extensive set of examples for analytical derivatives
    - Including hybrid systems
  - Generic Models for advanced FD
  - Second-order DPS
- Tools Package
  - Taylor series approximation
  - Parameter Sweeping studies
  - Control Coefficients
  - ...

Unit Testing is must

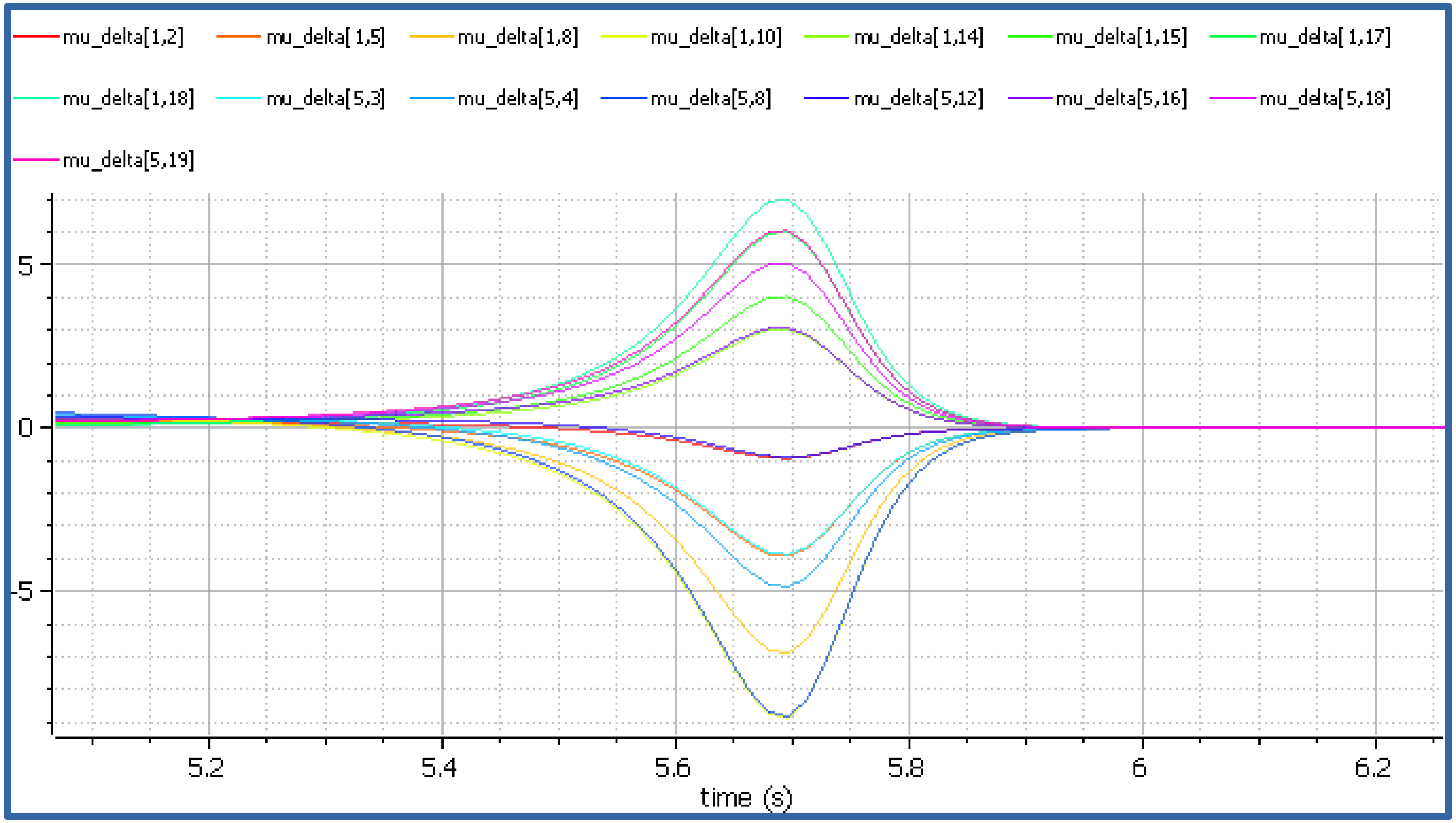


FD with PSTools

```
model ParM
  extends Utilities.Parameterized(
     NP = 2,
     _P = {0.4, 0.5},
     PNAME = {"p1", "p2"},
    NX = 2,
    _X = {_M.x1, _M.x2},
    XNAME = {"x1", "x2"}
 );
protected
    MyModel _M(
         p1 = _P[1],
         p2 = _P[2]);
end ParM;
```

```
model FDParM
  PSTools.PS.FD.CD2
  PS(redeclare replaceable
     Model  ParModel = ParM);
end FDParM;
```

Parameter Sweeping Studies



Unit Testing Technologies for Modelica

Marco Kessler, Testing Tutorial
Dassault Systems, Modelica 2017 Prague (Link)

- CSV Compare – ESI ITI
- BuildingPy – LBNL
- PySimulator – DLR
- test.openmodelica.org
- XogenyTest – Xogeny

- Model Management – Dymola
- Testing tool kits (many Companies)
- Testing Library -- Dymola

XogenyTest

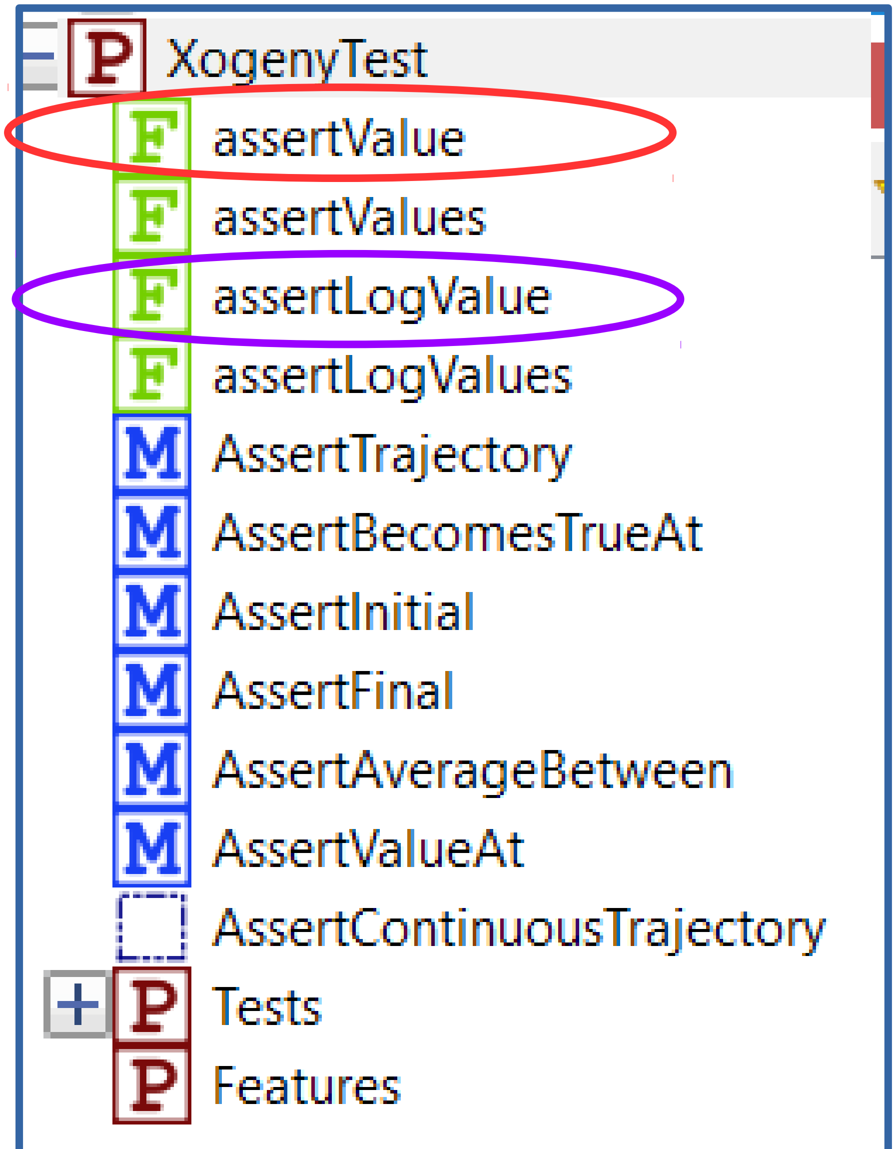
- Pure Modelica
- Minimal
  - external scripting
  - log files
- Easy to use
- No dependencies

Not meant to be comprehensive but definitely an ideal getting start

Michael Tiller
https://github.com/xogeny/XogenyTest

Tiller, Michael M., and Burit Kittirungsi.
"UnitTesting: A Library for Modelica Unit Testing"
Modelica Conference Vienna, Austria, 2006

XogenyTest



Low level functions

asserting whether an expected value x lies within ϵ-neighbourhood of a reference value r (i.e. $N_\epsilon(r)$)

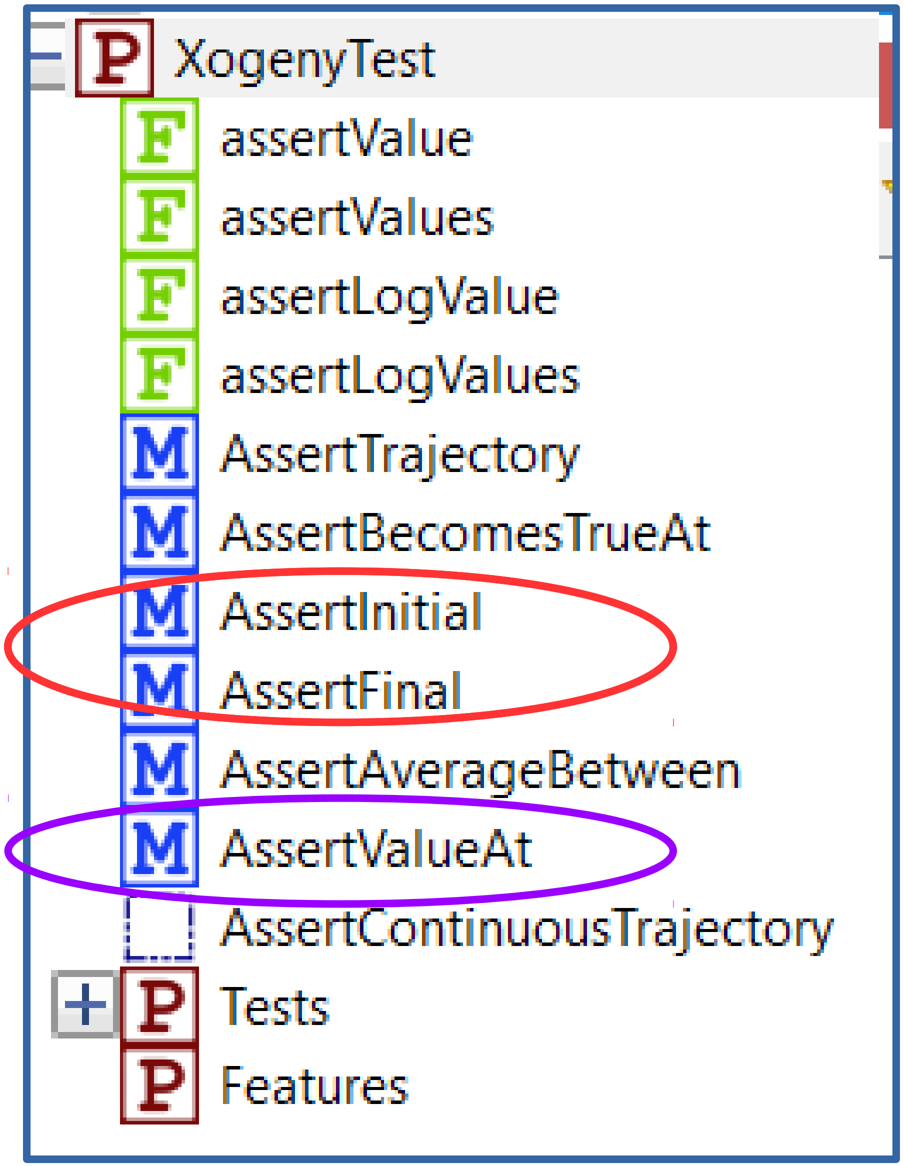
$$|x-r| < \epsilon$$

or

within the same order of magnitude

$$\left|\log\frac{x}{r}\right| < \epsilon$$

XogenyTest



Models

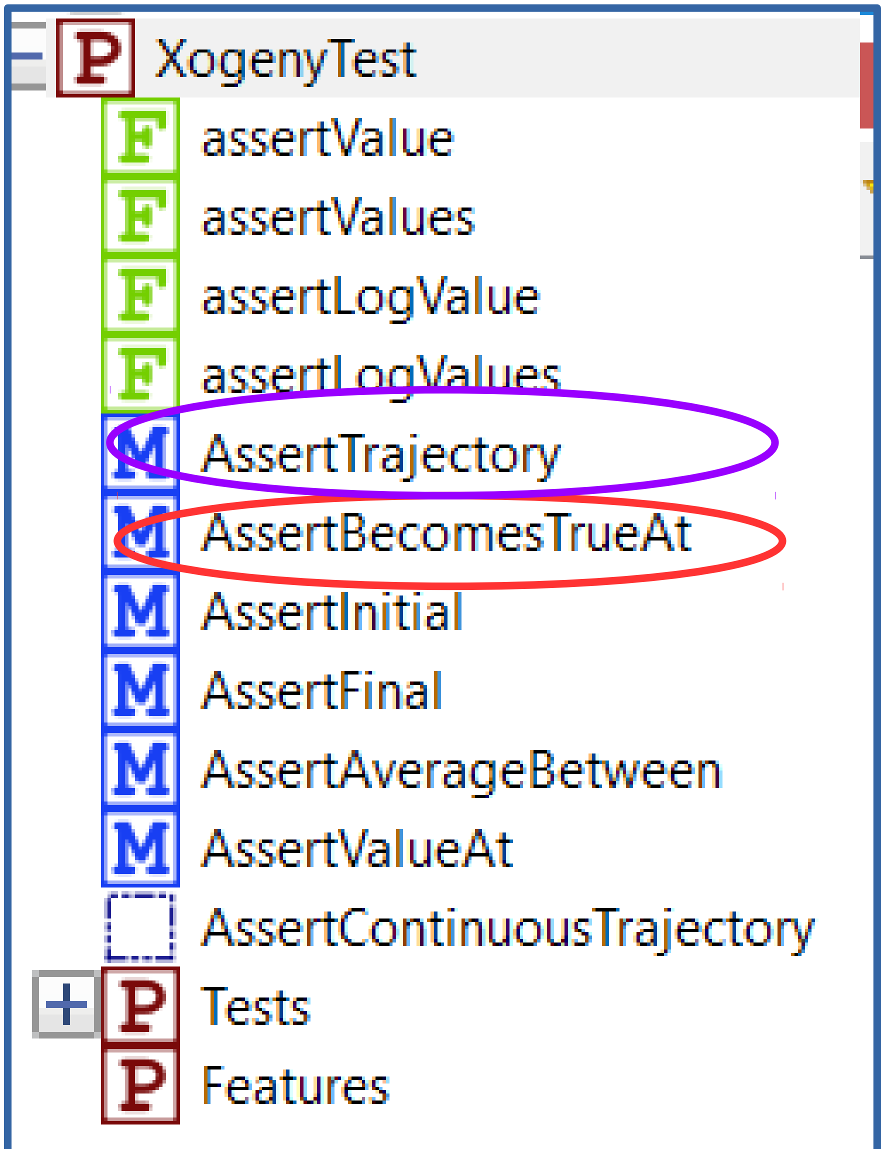
asserting an expected value x w.r.t. a reference value r at time $T \in \{t_0, t_f\}$

$$| x(T) - r | < \epsilon$$

or at time $t \in (t_0, t_f)$

$$| x(t) - r | < \epsilon$$

XogenyTest



<u>Models</u>

asserting an expected event $e(t)$ occurs at time T

$$e([T-\epsilon, T+\epsilon]) \rightarrow True$$

Asserting a trajectory $x(t)$ at discrete time points $\{t_1, t_2, \ldots, t_N\}$ w.r.t. reference values $r(t_i)$

$$|x(t_i) - r(t_i)| < \epsilon$$

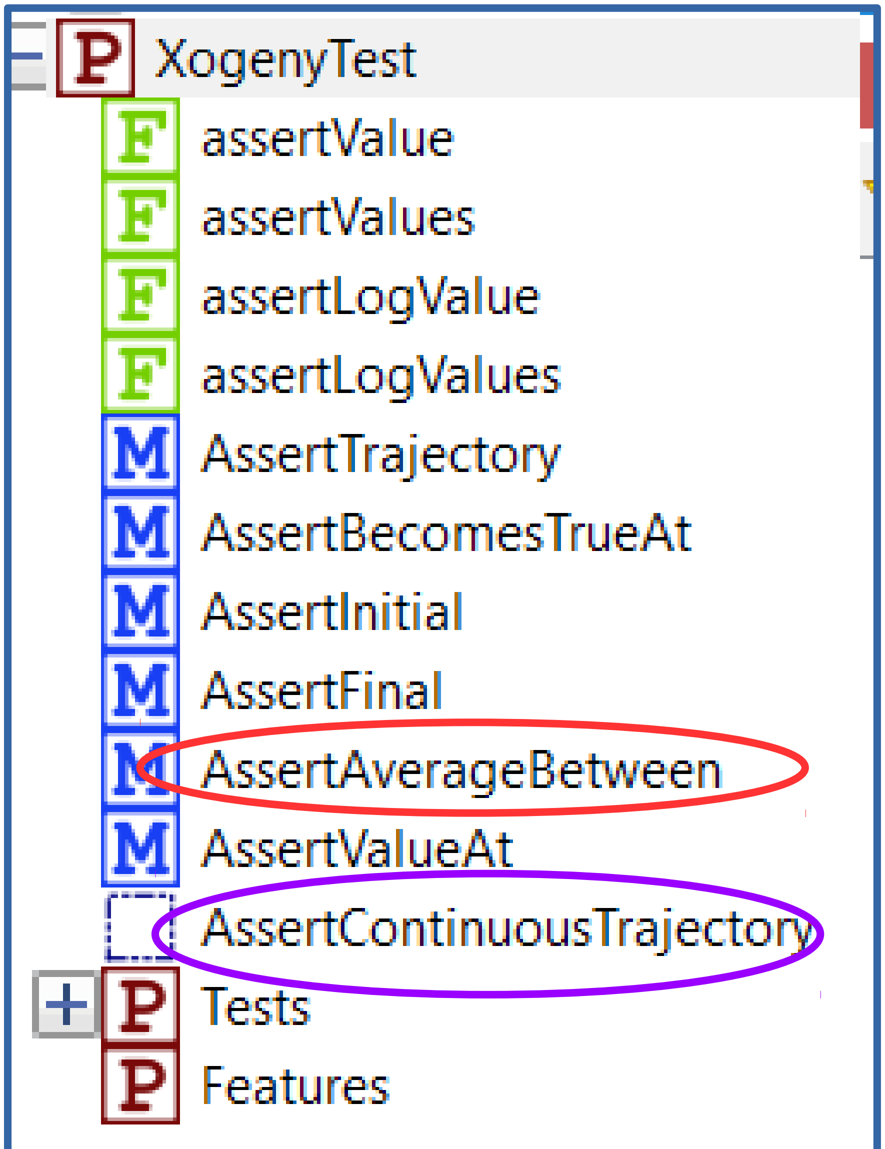
Examples (I/II)

```
model CheckSuccess

  Real x = time^2;

  AssertTrajectory check_x(
     actual=x,
     expected=[0,0; 1,1; 2,4; 3,9]);

  Annotation(
     TestCase(
          action="simulate",
          result="success"),
          experiment(StopTime=4));

end CheckSuccess;
```

Examples (II/II)

```
model CheckSuccess

  Real x = time;

  AssertBecomesTrueAt
        check_event(event=(x>2), at=2);

  Annotation(
     TestCase(
          action="simulate",
          result="success"),
          experiment(StopTime=4));

end CheckSuccess;
```

XogenyTest



Models

Assert thata signal $u(t)$
is of an average value a
over $[t_0, t_f]$

$$\frac{1}{t_f - t_0}\left|\int_{t0}^{t_f} u(t)\,dt\right| - a < \epsilon$$

Asset that difference between
trajectories $x_1(t)$ and $x_2(t)$
Is less than accu. error A_{err}

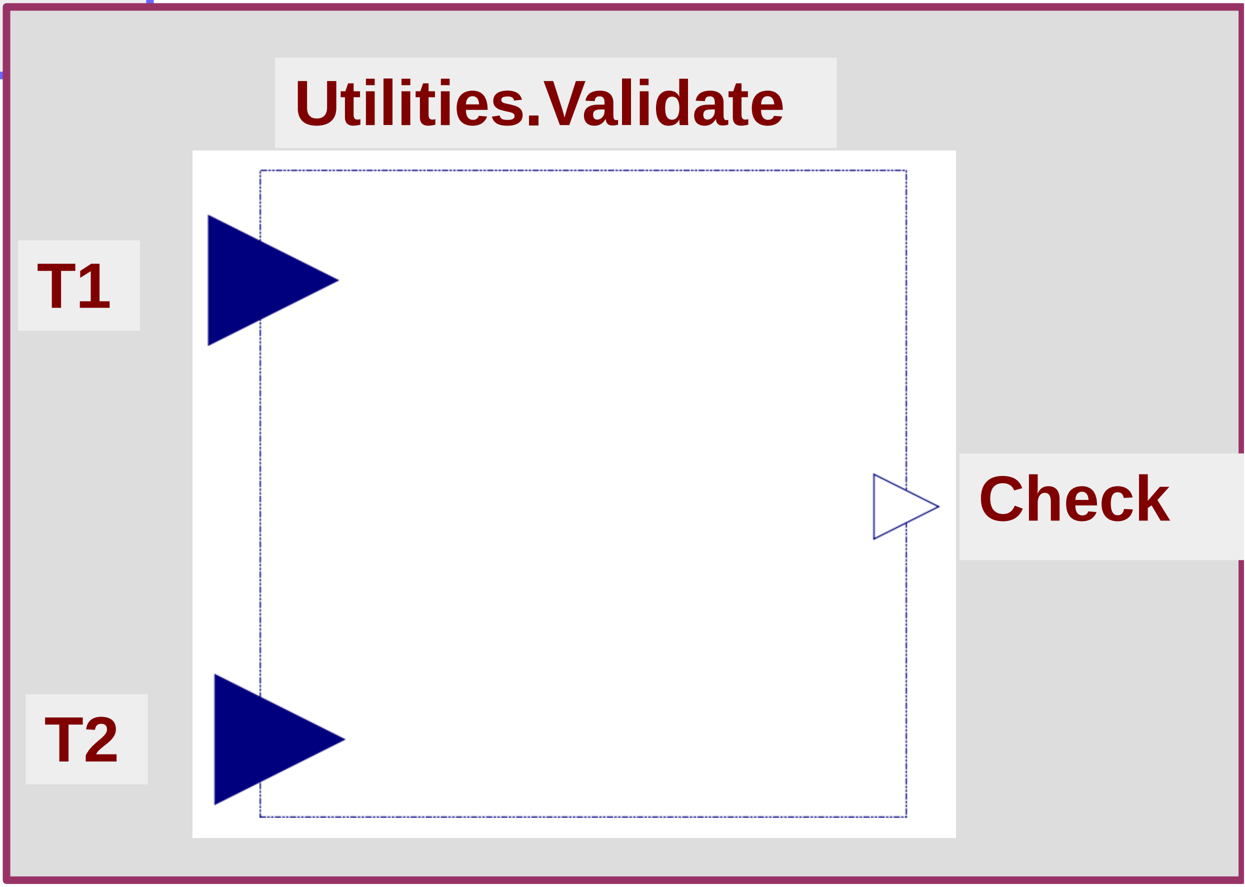
$$\int_{t0}^{t_f} |x_1(t) - x_2(t)|\,dt < A_{err}$$

Testing AD vs. FD

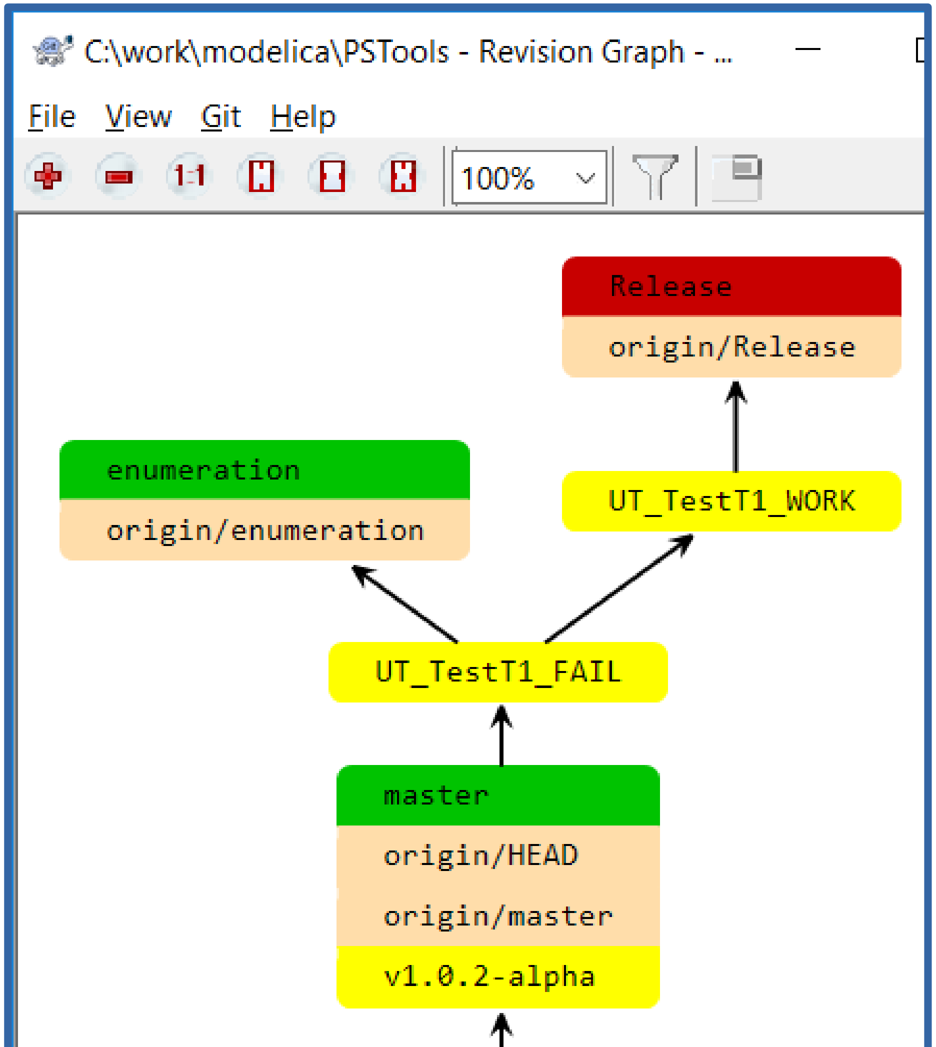
```
model TestT1BioProcess
  import PSTools.Utilities.unitVector;

  Utilities.Validate dmu_dKs(
        AccErr=1E-1,
        name="test T1.Processions dmu / dKs");

  PSTools.PS.T1.BioProcess.Bioprocess PSAD(
    NG=1,
    g_Ks=unitVector(1, NG));

  PSTools.PS.FD.BioProcess.BioProcess PSFD;
  ...
```

Visual unit testing

```
equation

  dmu_dKs.T1 = PSAD.g_mu[1];
  dmu_dKs.T2 = PSFD.g_mu[1];

end  TestT1BioProcess;
```



Case Study 1 PSTools Library



UT_TestT1_FAIL

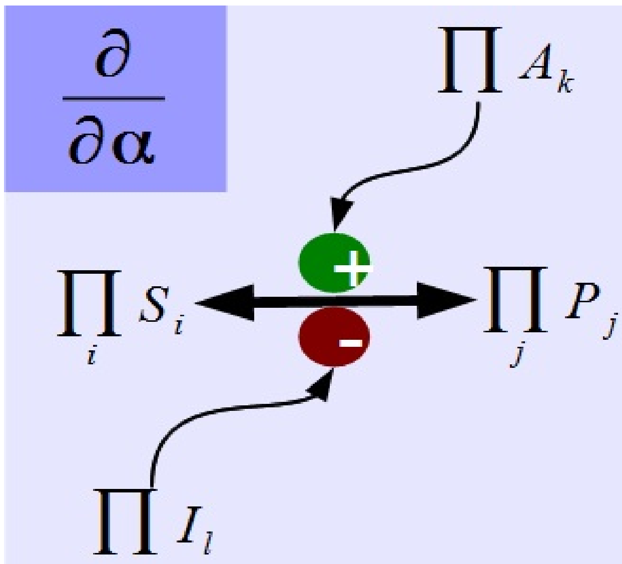
```
// der(VS) = -qS * VX;
 g_VS[i] =  -g_qS[i] * VX
                    - qS * g_VX[i];
```

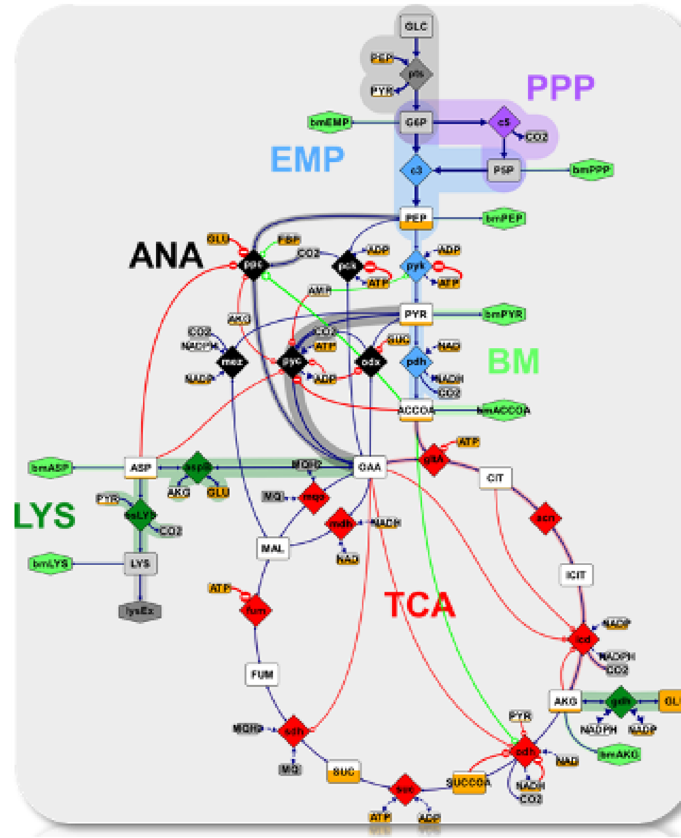
UT_TestT1_WORK

```
// der(VS) = -qS * VX;
 der(g_VS[i]) =  -g_qS[i] * VX
                    - qS * g_VX[i];
```

GenKinetics

2018 R 1.0-alpha





$$v = \prod_a \frac{K_{A_a}+[A_a]}{K_{A_a}} \cdot \prod_b \frac{K_{I_b}}{K_{I_b}+[I_b]} \cdot \frac{V^{fwd}_{max}\prod_i \frac{[S_i]}{K_{mS_i}} - V^{bwd}_{max}\prod_j \frac{[P_j]}{K_{mP_j}}}{V^{fwd}_{max}\prod_i 1+\frac{[S_i]}{K_{mS_i}} + V^{bwd}_{max}\prod_j 1+\frac{[P_j]}{K_{mP_j}} - 1}$$

Formal unit testing procedure

1) a unit test model for each component C using

    - Example of a small model employing C
    - Equivalent model implemented only by equations

2) Execute all unit tests by *.mos & OMShell

    - after each significant modification

3) Investigate errors , if any

Most useful when the component checks but the UT does not translate or simulate

A library is shipped with its unit tests

All unit tests are within a package called UnitTests

Currently about 40 unit tests distributed GenKinetics

Case Study 2 ADGenKinetics Library

OMC 1.12.0

A = product({KA[i] / (KA[i] + mc_A[i].c) for i in 1:NA});

2012

OMC 1.13.0

A = product({ **(KA .+ mc_A.c) ./ KA** for i in 1:NA});

2019

Case Study 3 GenKinetics / Biochem Libraries

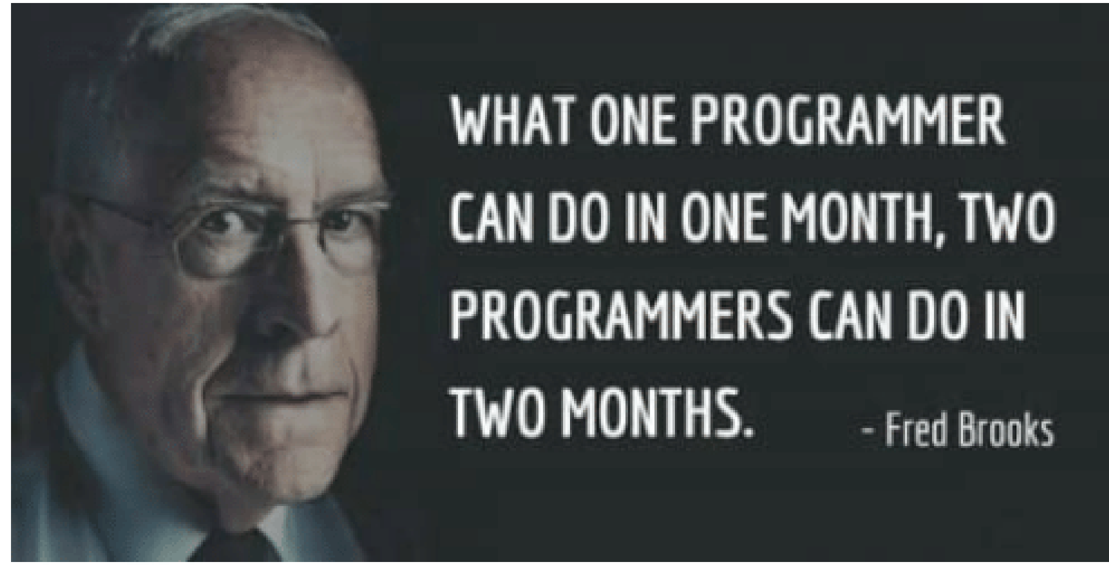
Numerical Problem

```
der(c) = if
        (c < tolerance) then 0 else r_net;
```

Solution

```
der(c) = if
        (c < tolerance and r_net < 0) then 0 else r_net;
```

Advantages



- Simplicity
- Purely Modelica
- Suitability
  - individual developers of Modelica libraries
    - GenKinetics https://github.com/AtiyahElsheikh/GenKinetics
    - PSTools
  - small-scale developments
  - Minimum constraints get done
  - Shipping Unit Tests with the product

Outlook

- a user experience report from GenKinetics
- Combine Relative Error w. Absolute Error

  Asghar, Adeel, Andreas Pfeiffer, Arunkumar Palanisamy, Alachew Mengist, Martin Sjölund, Adrian Pop, and Peter Fritzson.
  "Automatic Regression Testing of Simulation Models and Concept for Simulation of Connected FMUs in PySimulator."
  In*Proceedings of the 11th International Modelica Conference, Versailles.* 2015.

- Continuous Integration Solution