Assimulo - a Python package for solving differential equations with interface to equation based languages

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Let's move the focus ...

Problem

Solver

User friendly description

$$\dot{x} = f(t, x)$$

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

$$x(0) = x_0$$
$$\dot{x}(0) = \dot{x}_0$$

$$t \in [t_0, t_\mathrm{e}]$$

$$\sum \alpha_i x_{n-1} - h \sum \beta_i \dot{x}_{n-1} = 0$$

Mathematical description

ODE and DAE solvers in two disjoint worlds

Industrial Simulation Tasks

- highly complex models
- high robustness standards
- high documentation standards
- long life cycle

$\longrightarrow$ *one or two ODE/DAE packages meet these requirements.*

Academic Simulation Tasks

- a few, low scale test models
- lab standard quality (validation of concept)
- good analyzed algorithms, poor code documentation
- short life cycle, often coupled on individual career steps.

$\longrightarrow$ *dozen of codes produced (and forgotten) this way.*

ODE and DAE solvers in two disjoint worlds

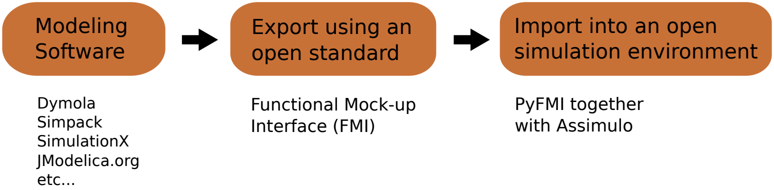
The harsh requirement that a useful numerical method must permit an efficient, robust, and reliable implementation has withered the beautiful flowers which bloomed on thousands of journal pages.

Hans Stetter in:
Mathematics of computation, 1943-1993: a half-century of computational mathematics : Mathematics of Computation 50th Anniversary Symposium, August 9-13, 1993, Vancouver, British Columbia

... highly valid still today.

Motivation

- Give the academic world access to complex models $\longrightarrow$ FMI
- Give the industrial world access to a variety of ODE/DAE codes (even experimental ones): $\longrightarrow$ ASSIMULO
- Give students in scientific computing an intuitive access to industrial standard solvers: $\longrightarrow$ ASSIMULO



Functional Mock-up Interface (FMI)

FMI is an open interface for model exchange with the idea that tools may generate and exchange dynamic system models.

The **FMI** supports model defined as discontinuous ordinary differential equations.

- **Model interface** The equations are evaluated and the model interaction is performed by standardized *C* functions.
- **Model description** The variable information of the model is contained in an XML-file.
- **Additional data** Model data, such as tables and maps may also exists.

$\Rightarrow$ Talk by Torsten Blochwitz on Wednesday.

Assimulo is written in Python, why?

Benefits of using Python:

- Open-source language
- Interpreted
- Object-oriented
- Many freely available packages
  - NumPy
  - SciPy
  - Matplotlib
  - Cython
- Highly flexible for interfacing to *C*, FORTRAN ...
- Ideal in teaching.

Assimulo

Python workbench for simulation of ordinary differential equations.

The intention is to provide a common high-level interface for a variety of different solvers.

Supports

- problems formulated as first or second order ordinary differential equations
- problems formulated as implicit ordinary differential equations including overdetermined problems.

ASSIMULO, problem formulations

- Explicit hybrid ODEs

$$\dot{y} = f(t, y, sw), \quad y(t_0) = y_0, \quad sw(t_0) = sw_0$$

- Implicit hybrid ODEs (also called DAEs)

$$F(t, y, \dot{y}, sw) = 0, \quad y(t_0) = y_0, \quad \dot{y}(t_0) = \dot{y}_0, \quad sw(t_0) = sw_0$$

- Mechanical systems in second order explicit ODE form

$$\ddot{p} = M(p)^{-1} f(t, p, \dot{p})$$

- Mechanical systems in (overdetermined) implicit ODE form

$$\begin{aligned} \dot{p} &= v \\ M(p)\dot{v} &= f(t, p, v) - G^T(p)\lambda \\ 0 &= g_{\mathrm{constr}}(p) \\ 0 &= G(p)v \end{aligned}$$

- Delay (retarded) differential equations.

ASSIMULO, solvers

Currently, solvers written in Python, FORTRAN and *C* are available.

- **IDA** - Multistep method for DAEs
- **CVode** - Multistep methods for ODEs
- **ODASSL** - Multistep methods for overdetermined DAEs
- **RADAU5** - Runge–Kutta method for DAEs
- **GLIMDA** - General linear methods methods for DAEs
- and we are working on a **"solver museum"** (oldest code in restoration 1983).

IDA and CVode are production quality solvers from the **SUNDIALS** suite.

ASSIMULO, overview

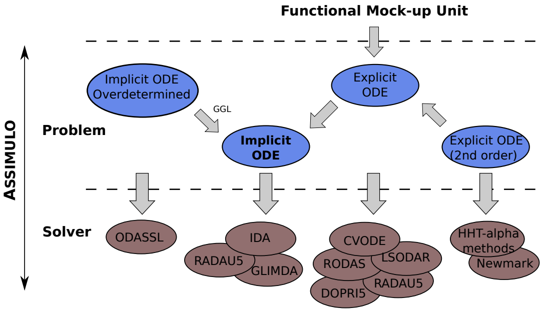


Figure : Connection between the different problem formulations and the different solvers available in ASSIMULO. The connection of the Functional Mock-up Interface to ASSIMULO is also shown.

Simple example workflow

Make a problem

```
def rhs(t,y):
  A = array([[0, 1], [-2, -1]])
  yd = N.dot(A, y)
  return yd

y0 = array([1.0, 1.0])
t0 = 0.0

linmodel = Explicit_Problem(rhs, y0, t0)
```

Create a solver instance

```
sim = CVode(linmodel)
```

... and simulate

```
t, y = sim.simulate(tfinal)
```

Assimulo can be quite verbose...

```
Final Run Statistics: Linear Test ODE

 Number of Error Test Failures              = 4
 Number of F-Eval During Jac-Eval           = 0
 Number of Function Evaluations             = 153
 Number of Jacobian Evaluations             = 0
 Number of Nonlinear Convergence Failures   = 0
 Number of Nonlinear Iterations             = 149
 Number of Root Evaluations                 = 0
 Number of Steps                            = 84

Solver options:

 Solver                    :  CVode
 Linear Multistep Method   :  Adams
 Nonlinear Solver          :  FixedPoint
 Maxord                    :  12
 Tolerances (absolute)     :  1e-06
```

Controlling the method

```
sim.atol=N.array([1.0,0.1])*1.e-5
sim.rtol=1.e-8
sim.maxord=3
sim.discr='BDF'
sim.iter='Newton'
```

Discontinuities – a Continuous Challenge

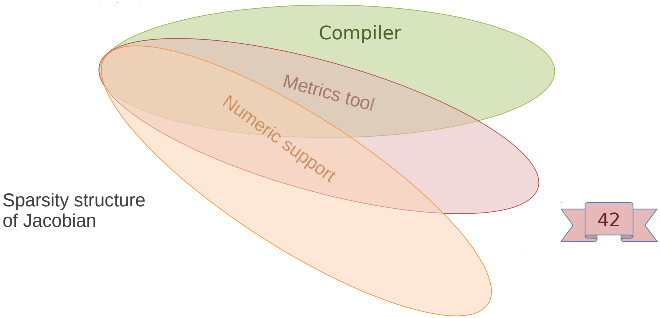
```
class Extended_Problem(Explicit_Problem):
  #Sets the initial conditions directly into the problem
  y0 = [0.0, -1.0, 0.0]
  sw0 = [False,True,True]

  #The right-hand-side function (rhs)
  def rhs(self, t, y, sw):
      ....

  #The event function
  def state_events(self, t, y, sw):
     event_0 = y[1] - 1.0
      ...
     return array([event_0,event_1,event_2])

  #Responsible for handling the events.
  def handle_event(self, solver, event_info):
    event_info = event_info[0]
    while True: #Event Iteration
      self.event_switch(solver, event_info) #Turns the swi
       ...
```

Languages have the potential to inform

- Are there discontinuities?
- State/Time events?
- Are there linear components?
- What are differential, what are algebraic variables? ("loop closure" conditions versus algebraic equations)
- Derivatives?

The compiler might know more

Why extensible compilers?



(Sorry Görel for changing your slide ...)

Plans/ideas/wishes for the future

- Would like to stimulate to open the **FMI** for a wider range of problem formulations - higher index DAES(?)
- Continue to expand the solvers available in ASSIMULO
  - Work on the museum.
  - Introduce problem formulation for delay differential equations
  - Generalize solvers for discontinuity handling
- Potentials of language/compiler aided numerics.
- Automatic differentiation: a separate tool or an integrated part of the language-solver chain?

Thank you!

... and feel free to try it out!

- **Assimulo** www.assimulo.org
- **PyFMI** www.pyfmi.org