DAE Tools: An equation-oriented process modelling and optimization software

Introduction

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DAE Tools Project, http://www.daetools.com

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Outline

Outline

What is DAE Tools?

- Process modelling, simulation, optimization and parameter estimation software (www.daetools.com)
- Areas of application:
  - Initially: chemical process industry (mass, heat and momentum transfers, chemical reactions, separation processes, phase-equilibrium, thermodynamics)
  - Nowadays: multi-domain
- Hybrid approach between general-purpose programming languages (c++, Fortran, Java) and domain-specific modelling languages (Modelica, gPROMS...)

What can be done with DAE Tools?

- Simulation
  - Steady-State
  - Transient
- Optimization
  - NLP problems: IPOPT, NLOPT, OpenOpt, scipy.optimize
  - MINLP problems: BONMIN
- Parameter estimation: Levenberg–Marquardt algorithm (scipy.optimize)

Types of systems that can be modelled

- Initial value problems of implicit form: systems of linear, non-linear, and (partial-)differential algebraic equations
- Index-1 DAE systems
- With lumped or distributed parameters: Finite Difference or Finite Elements Methods
- Steady-state or dynamic
- Continuous with some elements of event-driven systems (discontinuous equations, state transition networks and discrete events)

Why yet another software?

Advantages:

1. Hybrid approach betwen DSL and GPPL
2. Programmatical generation of models
3. Runtime modification of objcts/models (operating procedures)
4. Introperability with 3rd party software packages/libraries
5. Code generation/Model exchange capabilities

Not a modelling language

- A set of software packages
- API for:
  - Model development
  - Results processing (plotting, various file formats)
  - Simulation, optimization and parameter estimation
  - Code generation for other DSLs and programming languages
  - Report generation (XML+MathML) and model exchange
- Large set of supported solvers (DAE, LA, NLP, MINLP)

Not a modelling language (cont'd)

- Allows easy interaction with other software libraries (two-way interoperability with other software, embedding in other software etc.)
- Free/Open source software (GNU GPL)
- Cross-platform (GNU/Linux, MacOS, Windows)
- Supports multiple architectures (32/64 bit x86, arm, any other with the GNU toolchain)
- Developed in c++ with Python bindings (Boost.Python)

Object-oriented modelling

- Everything is an object (models, parameters, variables, equations, state transition networks, simulations, solvers, ...)
- Models are classes derived from the base daeModel class (inheriting the common functionality)
- Hierarchical model decomposition allows creation of complex, re-usable model definitions
- All Object Oriented concepts supported (such as multiple inheritance, templates, polymorphism, ...) that are supported by the target language (c++, Python), except:
  - Derived classes always inherit all declared objects (parameters, variables, equations, ...)
  - All parameters, variables, equations etc. remain public

Equation-oriented (acausal) modelling

- Equations given in an implicit form (as a residual)

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

- Input-Output causality is not fixed:
  - Increased model re-use
  - Support for different simulation scenarios (based on a single model) by specifying different degrees of freedom
- For instance, equation given in the following form:

$$x_1 + x_2 + x_3 = 0$$

  can be used to determine either x_1, x_2 or x_3 depending on what combination of variables is known:

$$x_1 = -x_2 - x_3 \; or \; x_2 = -x_1 - x_3 \; or \; x_3 = -x_1 - x_2$$

Separation of models definition from operations on them

- The structure of the model (parameters, variables, equations etc.) given in the model classes ($daeModel$, $daeFiniteElementModel$)
- The runtime information in the simulation class ($daeSimulation$)
- Single model definition, but:
  - One or more different simulation scenarios
  - One or more optimization scenarios

Hybrid continuous/discrete systems

- Modelling of continuous systems with some elements of event-driven systems
    - Discontinuous equations
    - State transition networks
    - Discrete events

Code generation

- Model export from DAE Tools to other DSL/modelling/programming languages
    - Modelica
    - c99

Model Exchange

- Support for Functional Mock-up Interface for Model Exchange and Co-Simulation (FMI): https://www.fmi-standard.org
- FMI – a tool independent standard to support both model exchange and co-simulation of dynamic models using a combination of xml-files and compiled C-code
- Still in experimental phase

Model reports

- Automatic model documentation
- XML + MathML format
- XSL transformation used to to generate HTML code and visualize reports
- Two types:
  - Model description report (contains model definition)
  - Runtime report with all values and equations expanded (contains definition of the simulation)

Model reports (cont'd)

Parameters

Name	Units	Domains	Description
Q_b	Wm^{-2}		Heat flux at the bottom edge of the plate
Q_t	Wm^{-2}		Heat flux at the top edge of the plate
ρ	kgm^{-3}		Density of the plate
c_p	$JK^{-1}kg^{-1}$		Specific heat capacity of the plate
λ_p	$WK^{-1}m^{-1}$		Thermal conductivity of the plate

Variables

Name	Type	Domains	Description
T	temperature_t	x, y	Temperature of the plate, K
$test$	temperature_t		

Equations

$HeatBalance:$

$$\rho \cdot c_p \cdot \frac{dT(x,y)}{dt} - \lambda_p \cdot \left(\frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2} \right) = 0 ; \forall x \in (x_0, x_n), \forall y \in (y_0, y_n)$$

Heat balance equation. Valid on the open x and y domains

$BC_{bottom}:$

$$((-\lambda_p)) \cdot \frac{\partial T(x,y)}{\partial y} - Q_b = 0 ; \forall x \in [x_0, x_n], y = y_0$$

Boundary conditions for the bottom edge

$BC_{top}:$

$$((-\lambda_p)) \cdot \frac{\partial T(x,y)}{\partial y} - Q_t = 0 ; \forall x \in [x_0, x_n], y = y_n$$

Boundary conditions for the top edge

Model reports (cont'd)

BC_{right} **:**

$$\frac{\partial T(x,y)}{\partial x} = 0 ; x = x_n, \forall y \in (y_0, y_n)$$

Boundary conditions for the right edge

Expanded into:

$$\frac{3 \cdot tutorial1.T(25,1) - 4 \cdot tutorial1.T(24,1) + tutorial1.T(23,1)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,2) - 4 \cdot tutorial1.T(24,2) + tutorial1.T(23,2)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,3) - 4 \cdot tutorial1.T(24,3) + tutorial1.T(23,3)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,4) - 4 \cdot tutorial1.T(24,4) + tutorial1.T(23,4)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,5) - 4 \cdot tutorial1.T(24,5) + tutorial1.T(23,5)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,6) - 4 \cdot tutorial1.T(24,6) + tutorial1.T(23,6)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,7) - 4 \cdot tutorial1.T(24,7) + tutorial1.T(23,7)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,8) - 4 \cdot tutorial1.T(24,8) + tutorial1.T(23,8)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,9) - 4 \cdot tutorial1.T(24,9) + tutorial1.T(23,9)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,10) - 4 \cdot tutorial1.T(24,10) + tutorial1.T(23,10)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

$$\frac{3 \cdot tutorial1.T(25,11) - 4 \cdot tutorial1.T(24,11) + tutorial1.T(23,11)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

Equation is: Linear

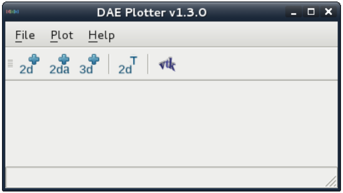
$$\frac{3 \cdot tutorial1.T(25,12) - 4 \cdot tutorial1.T(24,12) + tutorial1.T(23,12)}{tutorial1.x[25] - tutorial1.x[23]} = 0$$

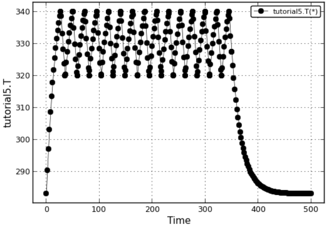
Multi-domain

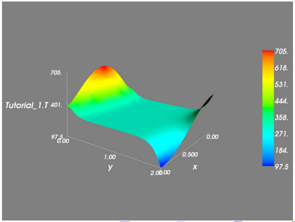
- From chemical processing industry to biological neural networks
- DAE Tools is not a DSL but defines the basic modelling concepts such as models, parameters, variables, various types of equations (ordinary, differential, partial differential, discontinuous), state transition networks etc. that can be used as building blocks for a specific domain
- Example: a reference implementation simulator for NineML (xml-based modelling language for describing networks of spiking neurons)
- The key concepts from NineML are based on DAE Tools concepts: Neurone, Synapse, Population of neurones, Layers, Projections etc

DAE Plotter

- 2D plots (Matplotlib)
- Animated 2D plots
- 3D plots (Mayavi)







Solvers

Supported DAE solvers@

- Sundials IDAS (https://computation.llnl.gov/casc/sundials/main.html)

Supported FE libraries:

- deal.II (http://dealii.org)

Supported optimization solvers:

- IPOPT (https://projects.coin-or.org/Ipopt)
- Bonmin (https://projects.coin-or.org/Bonmin)
- NLOPT (http://ab-initio.mit.edu/wiki/index.php/NLopt)

Solvers

Supported LA solvers:

- Sundials dense LU, Lapack
- Trilinos Amesos (http://trilinos.sandia.gov/packages/amesos)
- Trilinos AztecOO (http://trilinos.sandia.gov/packages/aztecoo)
- SuperLU SuperLU-MT (http://crd.lbl.gov/ xiaoye/SuperLU/index.html)
- Umfpack (http://www.cise.ufl.edu/research/sparse/umfpack)
- MUMPS (http://graal.ens-lyon.fr/MUMPS)
- CUSP (http://code.google.com/p/cusp-library)
- Intel Pardiso (http://software.intel.com/en-us/articles/intel-mkl)

Outline

Approaches to process modelling

- Two approaches to process modelling:
  - Domain Specific Language (DSL)
  - General-purpose programming language (such as c, c++, Java or Python)

Domain Specific Languages

- Special-purpose programming or specification languages dedicated to a particular problem domain
- Designed to directly support the key concepts from that domain
- Specifically created to solve problems in a particular domain
- (Usually) not intended to solve problems outside that domain (although that may be technically possible in some cases)
- Commonly lack low-level functions for filesystem access, interprocess control, and other functions that characterize full-featured programming languages, scripting or otherwise
- Examples: Modelica, gPROMS, SpeedUp, Ascend, GAMS ...

General-purpose programming languages

- Created to solve problems in a wide variety of application domains
- Do not support key concepts from any domain
- Have low-level functions for filesystem access, interprocess control etc.
- Examples: c, c++, Fortran, Python, Java etc.
- Typical scenario: solving a DAE system
    - Choose a solver (Sundials IDA, DASSL, RADAU5, DAEPACK etc)
    - Implement user functions to manually calculate residuals and derivatives for a Jacobian matrix, apply boundary conditions etc
    - Create an executable program

DAE Tools approach

A sort of the hybrid approach:

- Applies general-purpose programming languages such as c++ and Python
- Offers a class-hierarchy/API that resembles a syntax of a DSL as much as possible.
- Provides low-level concepts such as parameters, variables, equations, ports, models, state transition networks, discrete events etc.
- Concepts from new application domains can be added on top of its low level concepts (for instance the simulator for biological neural networks - NineML, as it will be shown later in Use Case section)
- Enables an access to the low-level functions and a large

gPROMS vs. Modelica

```
PARAMETER
  Density as Real
  CrossSectionalArea as Real
  Alpha as Real

VARIABLE
  HoldUp as Mass
  FlowIn as Flowrate
  FlowOut as Flowrate
  Height as Length

EQUATION
  # Mass balance
  $HoldUp = FlowIn - FlowOut;

  # Relation betwee liquid level and holdup
  HoldUp = CrossSectionalArea * Height * Density;

  # Relation between pressure drop and flow
  FlowOut = Alpha * sqrt(Height);
```

Model developed in gPROMS
http://www.psenterprise.com

```
model BufferTank
  /* Import libs */
  import Modelica.Math.*;

  parameter Real Density;
  parameter Real CrossSectionalArea;
  parameter Real Alpha;

  Real HoldUp(start = 0.0);
  Real FlowIn;
  Real FlowOut;
  Real Height;

equation
// Mass balance
  der(HoldUp) = FlowIn - FlowOut;

// Relation betwee liquid level and holdup
  HoldUp = CrossSectionalArea * Height * Density;

// Relation between pressure drop and flow
  FlowOut = Alpha * sqrt(Height);

end BufferTank;
```

The same model in OpenModelica
https://www.openmodelica.org

DAE Tools

```python
class BufferTank(daeModel):
    def __init__(self, Name, Parent = None, Description = ""):
        daeModel.__init__(self, Name, Parent, Description)

        self.Density = daeParameter("Density", unit(), self)
        self.Area    = daeParameter("Area",    unit(), self)
        self.Alpha   = daeParameter("Alpha",   unit(), self)

        self.HoldUp  = daeVariable("HoldUp",  no_t, self)
        self.FlowIn  = daeVariable("FlowIn",  no_t, self)
        self.FlowOut = daeVariable("FlowOut", no_t, self)
        self.Height  = daeVariable("Height",  no_t, self)

    def DeclareEquations(self):
        # Mass balance
        eq = self.CreateEquation("MassBalance")
        eq.Residual = self.HoldUp.dt() - self.FlowIn() + self.FlowOut()

        # Relation between liquid level and holdup
        eq = self.CreateEquation("LiquidLevelHoldup")
        eq.Residual = self.HoldUp() - self.Area() * self.Height() * self.Density()

        # Relation between pressure drop and flow
        eq = self.CreateEquation("PressureDropFlow")
        eq.Residual = self.FlowOut() - self.Alpha() * Sqrt(self.Height())
```

Key modelling concepts & grammar

DSL/Modelling languages

- Domain-specific languages allow solutions to be expressed in the idiom and at the level of abstraction of the problem domain (direct support for all modelling concepts by the language syntax)

DAE Tools

- Modelling concepts cannot be expressed directly in the programming language and have to be emulated in the API or in some other way

Verbosity

DSL/Modelling languages

- Clean, concise, ellegant and natural way of building model descriptions: the code can be self documenting

DAE Tools

- The support for modelling concepts is much more verbose and less elegant; however, DAE Tools can generate XML+MathML based model reports that can be either rendered in XHTML format using XSLT transformations (representing the code documentation) or used as an XML-based model exchange language

Maintainability & portability

DSL/Modelling languages

- Domain-specific languages could enhance quality, productivity, reliability, maintainability and portability

DAE Tools

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Simulators & programming languages

DSL/Modelling languages

- DSLs could be and often are simulator independent making a model exchange easier

DAE Tools

- Programming language dependent; however, a large number of scientific software libraries exposes its functionality to Python via Python wrappers

Need for a compiler/parser/interpreter

DSL/Modelling languages

- Cost of designing, implementing, and maintaining a domain-specific language as well as the tools required to develop with it (IDE): a compiler/lexical parser/interpreter must be developed with all burden that comes with it (such as error handling, grammar ambiguities, hidden bugs etc)

DAE Tools

- A compiler/lexical parser/interpreter is an integral part of the programming language (c++, Python) with a robust error handling, universal grammar and massively tested

Need for a new language syntax

DSL/Modelling languages

- Cost of learning a new language vs. its limited applicability: users are required to master a new language (yet another language grammar)

DAE Tools

- No learning of a new language required (everything can get done in a favourite programming language)

Interoperability with the 3^{rd} party software

DSL/Modelling languages

- Increased difficulty of integrating the DSL with other components: calling external functions/libraries and interaction with other software is limited by the existence of wrappers around a simulator engine (for instance some scripting languages like Python or javascript)

DAE Tools

- Calling external functions/libraries is a natural and straightforward Interaction with other software is natural and straightforward

Runtime generation & modification

DSL/Modelling languages

- Models usually cannot be created in the runtime/on the fly (or at least not easily) and cannot be modified in the runtime

DAE Tools

- Models can be created in the runtime/on the fly and easily modified in the runtime

Simulation setup

DSL/Modelling languages

- Setting up a simulation (ie. the values of parameters values, initial conditions, initially active states) is embedded in the language and it is typically difficult to do it on the fly or to obtain the values from some other software (for example to chain several software calls where outputs of previous calls represent inputs to the subsequent ones)

DAE Tools

- Setting up a simulation is done programmaticaly and the initial values can be obtained from some other software in a natural way (chaining several software calls is easy since a large number of libraries make Python wrappers available)

Operating procedures

DSL/Modelling languages

- Simulation operating procedures are not flexible; manipulation of model parameters, variables, equations, simulation results etc is limited to only those operations provided by the language

DAE Tools

- Operating procedures are completely flexible (within the limits of a programming language itself) and a manipulation of model parameters, variables, equations, simulation results etc can be done in any way which a user cosiders suitable for his/her problem

Outputs

DSL/Modelling languages

- Only the type of results provided by the language/simulator is available; custom processing is usually not possible or if a simulator does provide a way to build extensions it is limited to the functionality made available to them

DAE Tools

- The results processing can be done in any way which a user considers suitable(again within the limits of a programming language itself)

Outline

Available modules

- pyDAE:
  - pyCore (key modelling concepts)
  - pyActivity (simulation, optimization)
  - pyDataReporting (results handling)
  - pyIDAS (DAE solver)
  - pyUnits ($unit$ and $quantity$ concepts)

- FE Solvers:
  - pyDealII

Available modules (cont'd)

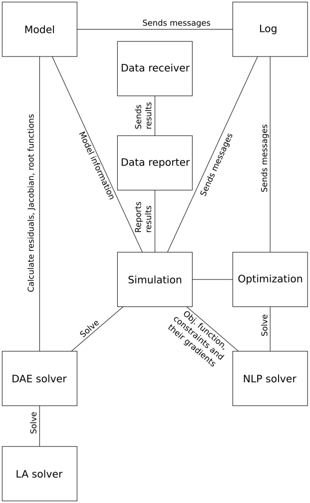
- LA Solvers:
  - pySuperLU
  - pySuperLU_MT
  - pyTrilinos (Amesos, AztecOO)
  - pyIntelPardiso

- NLP/MINLP Solvers:
  - pyIPOPT
  - pyBONMIN
  - pyNLOPT

Available components

- Model
- Simulation
- Optimization
- DAE solver
- LA solver
- NLP solver
- Log
- Data reporter
- Data receiver

Available components (cont'd)



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