Efficient Generation of Jacobian Matrices in OpenModelica

Using Jacobians for Simulation

Willi Braun, Bernhard Bachmann and Lennart Ochel

Department of Applied Mathematics
University of Applied Sciences Bielefeld
33609 Bielefeld, Germany

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Motivation

What are Jacobians useful for?

Motivation

What are Jacobians useful for?

For example

- Simulation
- Linear models
- Optimization
- Model analysis

Outline

Introduction: Jacobian

Which matrix is meant by the term Jacobian?

State-Space Equations

$$\begin{pmatrix} \underline{\dot{x}}(t) \\ \underline{y}(t) \end{pmatrix} = \begin{pmatrix} h(\underline{x}(t), \underline{u}(t), \underline{p}, t) \\ k(\underline{x}(t), \underline{u}(t), \underline{p}, t) \end{pmatrix}$$

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Linearization

$$\dot{\underline{x}}(t) = A(t) * \underline{x}(t) + B(t) * \underline{u}(t)$$
$$\underline{y}(t) = C(t) * \underline{x}(t) + D(t) * \underline{u}(t)$$

Linearization is done by Taylor series approximation and cancelling quadratic and higher order terms.

Jacobian matrices

- $A(t) = \frac{\partial h}{\partial \underline{x}}$
- $B(t) = \frac{\partial h}{\partial \underline{u}}$
- $C(t) = \frac{\partial k}{\partial \underline{x}}$
- $D(t) = \frac{\partial k}{\partial \underline{u}}$

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Simulation

- Many integration algorithms need "the Jacobian" : $\frac{\partial h}{\partial \underline{x}}$

Jacobian matrices

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Introduction: Differentiation

Numeric method

Differentiation methods

- Numeric
- Automatic
- Symbolic

Forward difference:

$$\dot{f}(x) = \lim_{\delta \to 0} \frac{(f(x+\delta) - f(x))}{\delta}$$

Drawback

Even if δ is selected optimal:

$$|\frac{\partial f(x)}{\partial x} - \frac{(f(x+\delta_{opt}) - f(x))}{\delta_{opt}}| \approx \sqrt{\epsilon_{RND}}$$

Some significant digits get lost by truncation.

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Forward difference:

$$\dot{f}(x) = \lim_{\delta \to 0} \frac{(f(x+\delta) - f(x))}{\delta}$$

Numerical Jacobian

Calculate the Jacobian numerical for a Modelica model needs $n+1$ call of the ODE-Block.

Introduction: Differentiation

automatic vs. symbolic differentiation

Differentiation methods

- Numeric
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Introduction: Differentiation

automatic vs. symbolic differentiation

Differentiation methods

- Numeric
- Automatic
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Basic differentiation rules

Chain rule:

$$\nabla \phi(u) = \dot{\phi}(u) \nabla u$$

Arithmetic operations:

$$\begin{aligned} \nabla(u \pm v) &= \nabla u \pm \nabla v \\ \nabla(uv) &= u \nabla v + v \nabla u \\ \nabla\left(\frac{u}{v}\right) &= \frac{(\nabla u - \frac{u}{v} \nabla v)}{v} \end{aligned}$$

Introduction: Differentiation

automatic vs. symbolic differentiation

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Example

$$y = f(x_1, x_2) = (x_1 x_2 + \sin(x_1))(x_2 + \cos(x_2))$$

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automatic vs. symbolic differentiation

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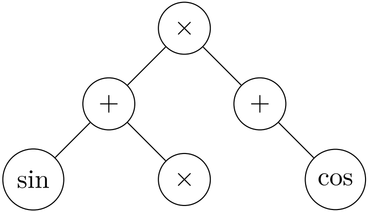
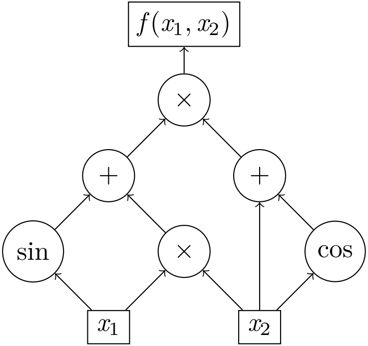


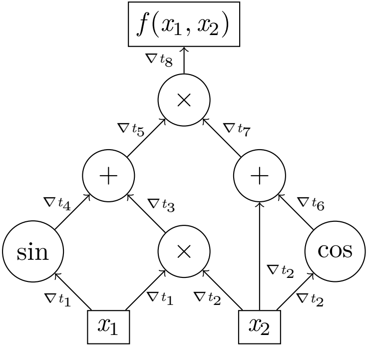
Introduction: Differentiation

automatic vs. symbolic differentiation



Introduction: Differentiation

automatic vs. symbolic differentiation



Operations	Differentiate(t_i, $\{x_1, x_2\}$)
$t_1 = x_1$	$\nabla t_1 = [1, 0]$
$t_2 = x_2$	$\nabla t_2 = [0, 1]$
$t_3 = t_1 t_2$	$\nabla t_3 = t_1 \nabla t_2 + \nabla t_1 t_2$
$t_4 = \sin(t_1)$	$\nabla t_4 = \cos(t_1) \nabla t_1$
$t_5 = t_3 + t_4$	$\nabla t_5 = \nabla t_3 + \nabla t_4$
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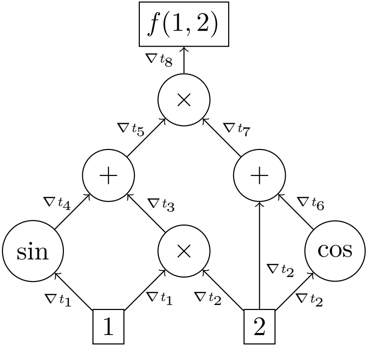
$t_8 = t_5 t_7$	$\nabla t_8 = \nabla t_5 t_7 + t_5 \nabla t_7$

Introduction: Differentiation

automatic vs. symbolic differentiation



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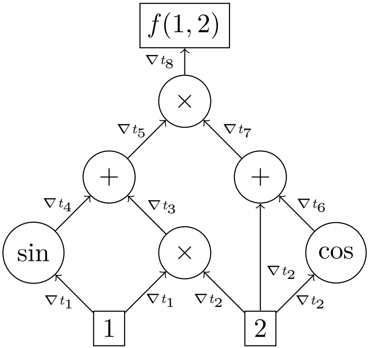
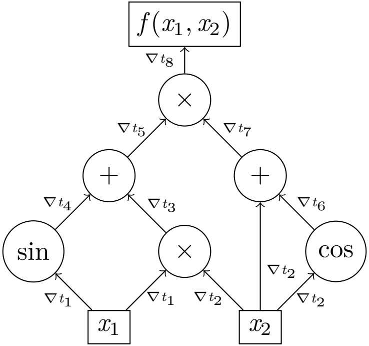


Operations	eval	Differentiate(t_i, $\{x_1, x_2\}$)	∇f
$t_1 = x_1$	1	$\nabla t_1 = [1, 0]$	$[1, 0]$
$t_2 = x_2$	2	$\nabla t_2 = [0, 1]$	$[0, 1]$
$t_3 = t_1 t_2$	2	$\nabla t_3 = t_1 \nabla t_2 + \nabla t_1 t_2$	$[2, 1]$
$t_4 = \sin(t_1)$	0.84	$\nabla t_4 = \cos(t_1) \nabla t_1$	$[0.54, 0]$
$t_5 = t_3 + t_4$	2.84	$\nabla t_5 = \nabla t_3 + \nabla t_4$	$[2.54, 1]$
$t_6 = \cos(t_2)$	-0.42	$\nabla t_6 = -\sin(t_2) \nabla t_2$	$[0, -0.91]$
$t_7 = t_6 + t_2$	1.58	$\nabla t_7 = \nabla t_6 + \nabla t_2$	$[0, 0.09]$
$t_8 = t_5 t_7$	4.50	$\nabla t_8 = \nabla t_5 t_7 + t_5 \nabla t_7$	$[4.02, 1.84]$

Introduction: Differentiation

automatic vs. symbolic differentiation



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$$\frac{\partial f(x1, x2)}{x_1} = \nabla t_8[1]$$

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$$
\begin{aligned}
\frac{\partial f(x1, x2)}{x_1} &= \nabla t_8[1] \\
\nabla t_8[1] &= (\nabla t_5[1] t_7 + t_5 \nabla t_7[1]) \\
\nabla t_8[1] &= (\nabla t_3[1] + \nabla t_4[1])(t_6 + t_2) + t_5(\nabla t_6[1] + \nabla t_2[1]) \\
\nabla t_8[1] &= (t_1 \nabla t_2[1] + \nabla t_1[1] t_2 + \cos(t_1) \nabla t_1[1])(\cos(t_2) + t_2) + t_5(-\sin(t_2) \nabla t_2[1]) \\
\nabla t_8[1] &= (t_2 + \cos(t_1))(\cos(t_2) + t_2) \\
\frac{\partial f(x1, x2)}{x_1} &= (x_2 + \cos(x_1))(\cos(x_2) + x_2)
\end{aligned}
$$

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$$\frac{\partial f(x1, x2)}{x_1} = (x_2 + \cos(x_1))(x_2 + \cos(x_2))$$

$$\frac{\partial f(x1, x2)}{x_2} = (x_1(x_2 + \cos(x_2)) + (x_1 x_2 + \sin(x_1))(1 - \sin(x_2))$$

Efficent generation and evaluation of the Jacobian

Estimate complexity

Jacobian

$$J_A = \frac{\partial \underline{h}}{\partial \underline{x}} = \begin{pmatrix} \frac{\partial h_1}{\partial x_1} & \cdots & \frac{\partial h_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_n}{\partial x_1} & \cdots & \frac{\partial h_n}{\partial x_n} \end{pmatrix}$$

Determination of the full Jacobian depends at least on $O(n^2)$ using the presented method.

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Actually it is more than that!

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Determination of the full Jacobian depends at least on $O(n^2)$ using the presented method.

Actually it is more than that!

Determination of the full Jacobian depends at least on $O(n * m)$ where $m > n$ number of equation in the ODE-Block.

Efficent generation and evaluation of the Jacobian

A faster way

Operations	Differentiate(t_i, $\{x_1, x_2\}$)
$t_1 = x_1$	$\nabla t_1 = [1, 0]$
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Example

$$f(x_1, x_2) = (x_1 x_2 + \sin(x_1))(x_2 + \cos(x_2))$$

Efficent generation and evaluation of the Jacobian

A faster way

Operations	Differentiate(t_i, z)
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$t_2 = x_2$	$dt_2 = \frac{\partial x2}{\partial z}$
$t_3 = t_1 t_2$	$dt_3 = t_1 dt_2 + dt_1 t_2$
$t_4 = \sin(t_1)$	$dt_4 = \cos(t_1) dt_1$
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$$\frac{\partial f(x1, x2)}{\partial z}\left(\frac{\partial x1}{\partial z}, \frac{\partial x2}{\partial z}\right) = \quad ((x_1 \tfrac{\partial x2}{\partial z} + \tfrac{\partial x1}{\partial z} x_2) + (\cos(x_1) \tfrac{\partial x1}{\partial z}))(\cos(x_2) + x_2) +$$
$$((x_1 + x_2) + \sin(x_1))(\tfrac{\partial x2}{\partial z} - \sin(x_2) \tfrac{\partial x2}{\partial z})$$

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$$\frac{\partial f(x1, x2)}{\partial z}\left(\frac{\partial x1}{\partial z}, \frac{\partial x2}{\partial z}\right) = \quad ((x_1 \tfrac{\partial x2}{\partial z} + \tfrac{\partial x1}{\partial z} x_2) + (\cos(x_1) \tfrac{\partial x1}{\partial z}))(\cos(x_2) + x_2) +$$

$$((x_1 + x_2) + \sin(x_1))(\tfrac{\partial x2}{\partial z} - \sin(x_2) \tfrac{\partial x2}{\partial z})$$

$$\frac{\partial f(x1, x2)}{x_1}\left(\frac{\partial x1}{\partial z} = 1, \frac{\partial x2}{\partial z} = 0\right) = \quad (x_2 + \cos(x_1))(x_2 + \cos(x_2))$$

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$$f(x_1, x_2) = (x_1 x_2 + \sin(x_1))(x_2 + \cos(x_2))$$

$$\frac{\partial f(x1, x2)}{\partial z}(\frac{\partial x1}{\partial z}, \frac{\partial x2}{\partial z}) = ((x_1 \tfrac{\partial x2}{\partial z} + \tfrac{\partial x1}{\partial z} x_2) + (\cos(x_1) \tfrac{\partial x1}{\partial z}))(\cos(x_2) + x_2) +$$
$$((x_1 + x_2) + \sin(x_1))(\tfrac{\partial x2}{\partial z} - \sin(x_2) \tfrac{\partial x2}{\partial z})$$

$$\frac{\partial f(x1, x2)}{x_1}(\frac{\partial x1}{\partial z} = 1, \frac{\partial x2}{\partial z} = 0) = (x_2 + \cos(x_1))(x_2 + \cos(x_2))$$

$$\frac{\partial f(x1, x2)}{x_2}(\frac{\partial x1}{\partial x1} = 0, \frac{\partial x2}{\partial x2} = 1) = (x_1(x_2 + \cos(x_2)) +$$
$$(x_1 x_2 + \sin(x_1))(1 - \sin(x_2))$$

Efficent generation and evaluation of the Jacobian

A faster way

Jacobian

$$J_A = \frac{\partial \underline{h}}{\partial \underline{x}} = \begin{pmatrix} \frac{\partial h_1}{\partial x_1} & \cdots & \frac{\partial h_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_n}{\partial x_1} & \cdots & \frac{\partial h_n}{\partial x_n} \end{pmatrix}$$

Evaluate the Jacobian

$$J_A = \frac{\partial \underline{h}}{\partial z}(\underline{e}_k)$$

$\underline{e}_k \in R^n := k -$ th coordinate vector

Efficent generation and evaluation of the Jacobian

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Evaluate the Jacobian

$$J_A = \frac{\partial \underline{h}}{\partial z}(\underline{e}_k)$$

$\underline{e}_k \in R^n := k -$ th coordinate vector

Evaluation while the simulation still takes n call.

Efficent generation and evaluation of the Jacobian

Which color has the Jacobian?

Jacobian

$$J = \begin{pmatrix} j_{11} & j_{12} & 0 & 0 & j_{15} \\ 0 & 0 & j_{23} & 0 & 0 \\ 0 & j_{32} & j_{33} & j_{34} & 0 \\ j_{41} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & j_{54} & j_{55} \end{pmatrix}$$

Efficent generation and evaluation of the Jacobian

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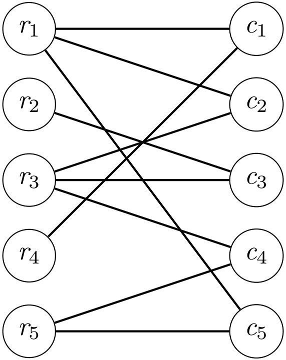

Efficent generation and evaluation of the Jacobian

Which color has the Jacobian?

Jacobian

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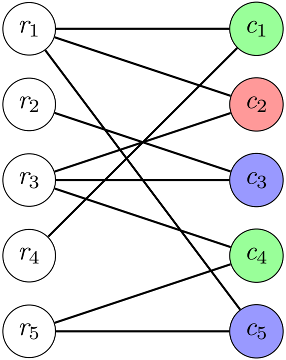


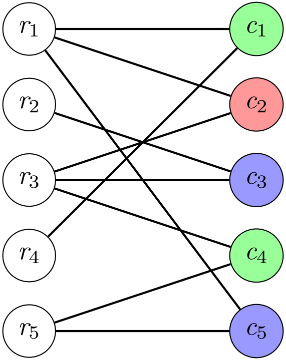
Efficent generation and evaluation of the Jacobian

Which color has the Jacobian?

Jacobian

$$J = \begin{pmatrix} j_{11} & j_{12} & 0 & 0 & j_{15} \\ 0 & 0 & j_{23} & 0 & 0 \\ 0 & j_{32} & j_{33} & j_{34} & 0 \\ j_{41} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & j_{54} & j_{55} \end{pmatrix}$$

$$J_R = \begin{pmatrix} j_{11} & j_{12} & j_{15} \\ 0 & 0 & j_{23} \\ j_{34} & j_{32} & j_{33} \\ j_{41} & 0 & 0 \\ j_{54} & 0 & j_{55} \end{pmatrix}$$

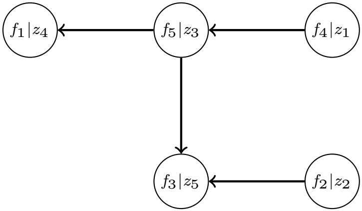


Efficent generation and evaluation of the Jacobian

Explore the sparse pattern

Example system

$$\underline{z}(t) = \underline{f}(\underline{x}(t), t)$$

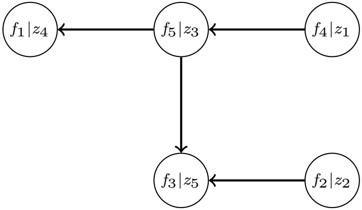


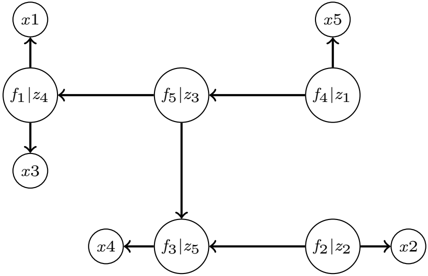
Efficent generation and evaluation of the Jacobian

Explore the sparse pattern

Example system

$$\underline{z}(t) = \underline{f}(\underline{x}(t), t)$$



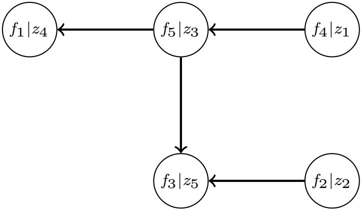


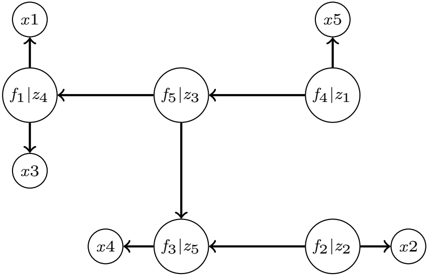
Efficent generation and evaluation of the Jacobian

Explore the sparse pattern

Example system

$$\underline{z}(t) = \underline{f}(\underline{x}(t), t)$$

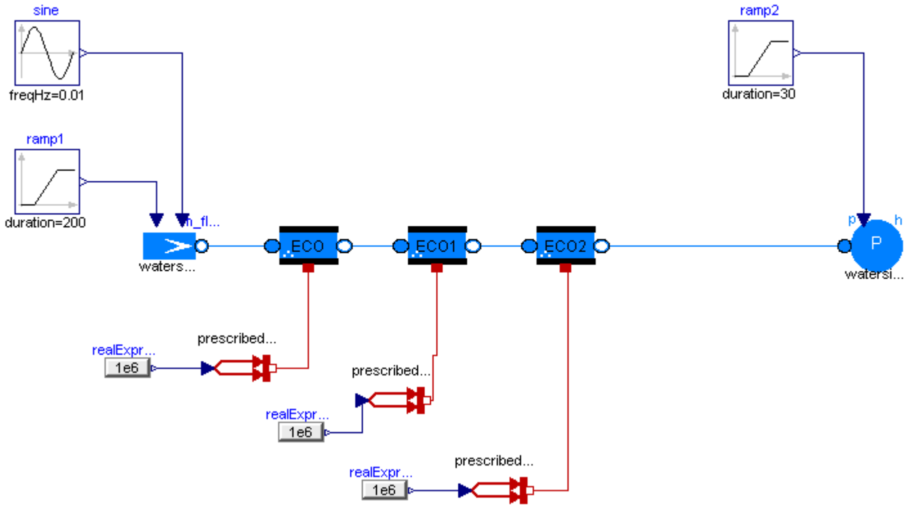




$$J = \begin{pmatrix} * & 0 & * & 0 & 0 \\ 0 & * & 0 & * & 0 \\ 0 & 0 & 0 & * & 0 \\ * & 0 & * & * & * \\ * & 0 & * & * & 0 \end{pmatrix}$$

Results

Model for Testing



Results

Model for Testing

sparse pattern

$$
\begin{pmatrix}
* & * & * & * & * & * & * & & & & & & & & \\
* & * & * & & & * & * & * & * & * & * & & & & \\
* & * & * & & & * & * & & & * & * & * & * & * & * \\
* & & & * & & * & & & & & & & & & \\
* & & & & * & & * & & & & & & & & \\
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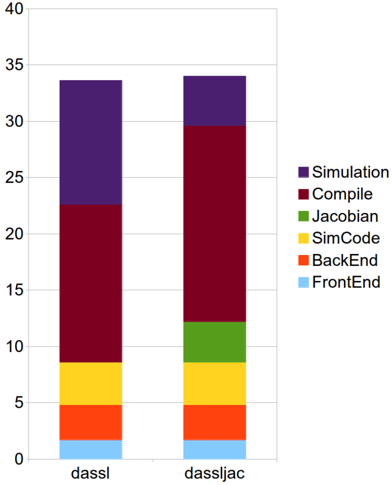
& & * & & & & & & & & * & * & & * & * \\
& & * & & & & & & & & & & * & * & *
\end{pmatrix}
$$

Results

Evaluation measurements

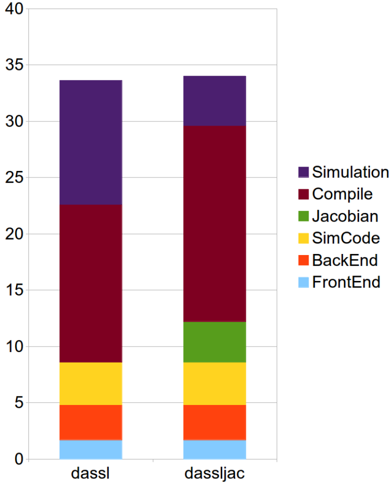


Details

N	19
states	231
equations	1006
JacElements	53361
NonZero	3032
Colors	79

Results

Evaluation measurements



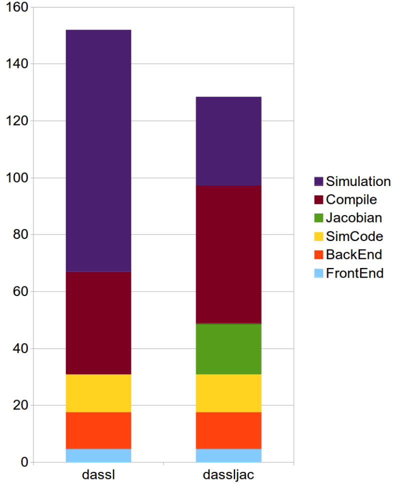
Details

N	19
states	231
equations	1006
JacElements	53361
NonZero	3032
Colors	79

Dymola $\approx 1 sec$

Results

Evaluation measurements

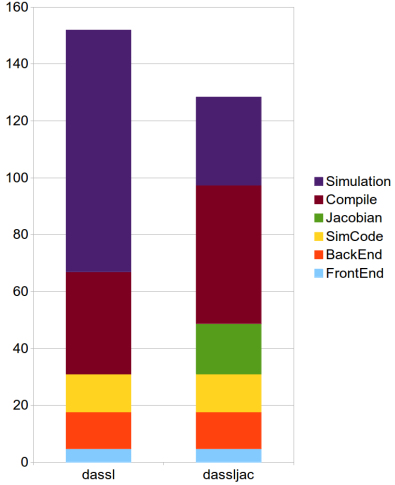


Details

N	50
states	603
equations	2587
JacElements	363609
NonZero	17261
Colors	203

Results

Evaluation measurements



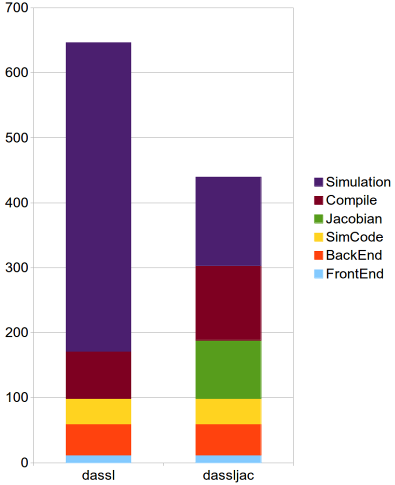
Details

N	50
states	603
equations	2587
JacElements	363609
NonZero	17261
Colors	203

Dymola $\approx 7sec$

Results

Evaluation measurements

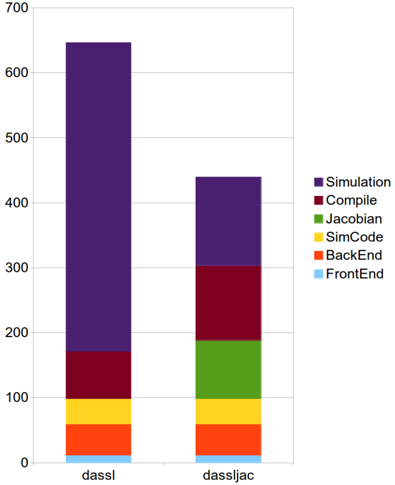


Details

N	100
states	1203
equations	5137
JacElements	1447209
NonZero	64511
Colors	403

Results

Evaluation measurements



Details

N	100
states	1203
equations	5137
JacElements	1447209
NonZero	64511
Colors	403

Dymola $\approx 35sec$

Summary

- OpenModelica generates Jacobians efficently.
- Simulation speed can be increased using Jacobians.

Summary

- OpenModelica generates Jacobians efficently.
- Simulation speed can be increased using Jacobians.

- Outlook
  - Utilize the Jacobian for FMI 2.0.
  - Improving the usability.
  - Improving the algorithms.