Transformation of Differential Algebraic Array Equations to Index One Form

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Goal: Model and Simulate Large Systems (upto $10^4..10^6$ differential equations)

- Large multi-body systems with elastic bodies and contacts
- Large electrical circuits and power electronics
- Large thermo-fluid systems

Available algorithms for Modelica tools reaching their limits

↓

New algorithms are needed that move the limits!

How to reach the Goal?

- **No scalarization of array equations**
  $\rightarrow$ more efficient code generation + simulation.

- **No transformation to ODE form**
  Today: Transform ODAE (Overdetermined Differential Algebraic Equation System) from Pantelides algorithm to ODE form: $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$.
  Drawbacks:
  - Every evaluation of $\mathbf{f}(..)$ may require solution of algebraic equations
    $\rightarrow$ bad for implicit integrators (which solve algebraic equations in $\mathbf{f}(..)$).
  - Sparsity of original equations might get lost
    $\rightarrow$ bad for large systems.

- **How to solve ODAE, without transformation to ODE form?**
  $\rightarrow$ see next slides

- Start with solving the base problems above, afterwards more need to be done.

Differential Algebraic Array Equations

e.g. $\mathbf{r}_2 = \mathbf{r}_1 + \mathbf{n}s$

↓

new — **Removal of non-structural singularities**

↓

new — **Transformation algorithms on array equations (Pantelides, BLT)**

$$\text{e.g.}\quad \begin{aligned} \mathbf{r}_2 &= \mathbf{r}_1 + \mathbf{n}s \\ \dot{\mathbf{r}}_2 &= \dot{\mathbf{r}}_1 + \mathbf{n}\dot{s} \\ \ddot{\mathbf{r}}_2 &= \ddot{\mathbf{r}}_1 + \mathbf{n}\ddot{s} \end{aligned}$$

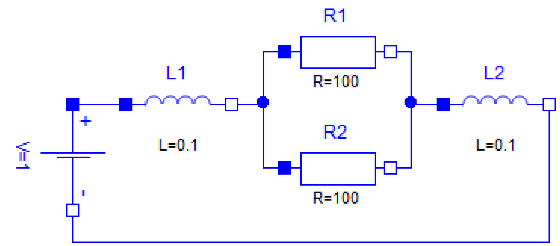
↓

new — **Transformation to special index 1 form**

$$\begin{bmatrix} \mathbf{f}_d(\dot{\mathbf{x}}, \mathbf{x}, t) \\ \mathbf{f}_c(\mathbf{x}, t) \end{bmatrix} = \mathbf{0} \qquad \begin{bmatrix} \dfrac{\partial \mathbf{f}_d}{\partial \dot{\mathbf{x}}} \\ \dfrac{\partial \mathbf{f}_c}{\partial \mathbf{x}} \end{bmatrix} \text{ is regular}$$

↓

DAE integrator with sparse matrix support



- remove equation: -L2.n.i - V.n.i = 0 (redundant)
- add equation : L2.n.v = 0 (arbitrary value)
- replace equation: -R1.p.i - R2.p.i - L1.n.i = 0
  with: -L1.p.i + L2.p.i = 0
  to make constraint structural
- details: see paper

- no scalarization of equations

- no algebraic equations solved
- no dynamic state selection (partial static state selection)
- sparseness is kept
- BDF iteration matrix can be scaled, so that it is regular for $h \to 0$

- algebraic equations only solved by DAE integrator (not in model, as of today)
- array equations intact (no scalarization)
- sparse matrix handling

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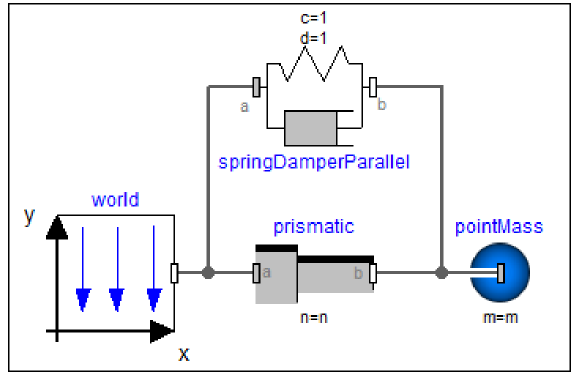
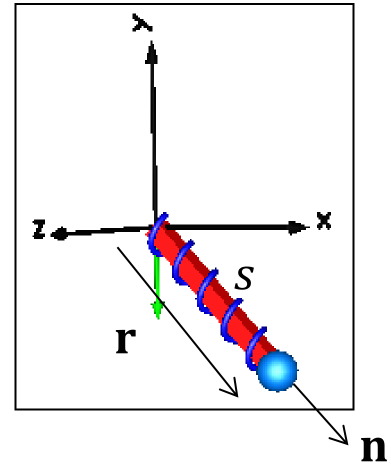
new algorithm

Symbolic Transformation of Array Equations

Example: Array equations of a sliding mass

parameters: $c, d, m, \mathbf{n}, \mathbf{g}$
unknowns: $s, \mathbf{r}, \mathbf{v}, \mathbf{f}, \mathbf{u}$





$$\mathbf{r} = \mathbf{n}s$$
$$\mathbf{v} = \dot{\mathbf{r}}$$
$$m\dot{\mathbf{v}} = \mathbf{f} + m\mathbf{g} + \mathbf{u}$$
$$0 = \mathbf{n} \cdot \mathbf{f}$$
$$\mathbf{u} = -(cs + d\dot{s})\mathbf{n}$$

Pantelides algorithm:
Determine, how often every equation must be differentiated until the highest derivative variables can be uniquely assigned to the highest derivative equations

Idea: Assign array variables to array equations

No scalar equation contains **scalar** s → array equation must be scalarized

Scalar equation has **no scalar** unknown → array unknown $\mathbf{f}$ must be scalarized

→ **Idea does not work**

1. (Conceptually) scalarize using **incidence of original array equations**
2. Apply **Pantelides**

scalarized, highest derivative equations	*unknowns (incidence)*	*assigned variables*
...	...	...
$u_1 = -(cs + d\dot{s})\, n_1$	u_1, u_2, u_3	u_1
$u_2 = -(cs + d\dot{s})\, n_2$	u_1, u_2, u_3	u_2
$u_3 = -(cs + d\dot{s})\, n_3$	u_1, u_2, u_3	u_3

3. **Sort** highest derivative equations (**BLT**)
   → **array elements** are in the same algebraic loop (= **BLT block**)

BLT block	*unknowns*
$u_1 = -(cs + d\dot{s})\, n_1$ $u_2 = -(cs + d\dot{s})\, n_2$ $u_3 = -(cs + d\dot{s})\, n_3$	u_1, u_2, u_3
...	...

4. (Conceptually) transform **back to arrays**

BLT block	*solve for*
$\mathbf{u} = -(cs + d\dot{s})\mathbf{n}$	$\mathbf{u}$
$\ddot{\mathbf{r}} = \mathbf{n}\ddot{s}$ $\dot{\mathbf{v}} = \ddot{\mathbf{r}}$ $m\dot{\mathbf{v}} = \mathbf{f} + m\mathbf{g} + \mathbf{u}$ $0 = \mathbf{n} \cdot \mathbf{f}$	$\ddot{s}, \ddot{\mathbf{r}}, \dot{\mathbf{v}}, \mathbf{f}$

5. Analytically differentiate array equations

new algorithm

Transformation to Special Index 1 DAE Form

Example: Multi-Body Systems

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{v} \\ \mathbf{M}(\mathbf{q},t)\dot{\mathbf{v}} + \mathbf{G}^T(\boldsymbol{q},t)\boldsymbol{\lambda} &= \mathbf{h}(\boldsymbol{q},\boldsymbol{v},t) \\ \mathbf{0} &= \mathbf{g}(\boldsymbol{q},t) \end{aligned}$$

$\mathbf{G} = \frac{\partial \mathbf{g}}{\partial \mathbf{q}}, \mathbf{M} = \mathbf{M}^T > \mathbf{0}$

Pantelides algorithm

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{v} \\ \mathbf{M}\dot{\mathbf{v}} + \mathbf{G}^T\boldsymbol{\lambda} &= \mathbf{h}(\mathbf{q},\mathbf{v},t) \\ \mathbf{0} &= \mathbf{g}(\mathbf{q},t) \\ \mathbf{0} &= \dot{\mathbf{g}} = \mathbf{G}\,\dot{\mathbf{q}} + \mathbf{g}^{(1)}(\mathbf{q},t) \\ \mathbf{0} &= \ddot{\mathbf{g}} = \mathbf{G}\,\ddot{\mathbf{q}} + \mathbf{g}^{(2)}(\mathbf{q},\dot{\mathbf{q}},t) \\ \ddot{\mathbf{q}} &= \dot{\mathbf{v}} \end{aligned}$$

$\mathbf{g}^{(1)} = \frac{\partial \mathbf{g}}{\partial \mathrm{t}}, \mathbf{g}^{(2)} = \dot{\mathbf{G}}\,\dot{\mathbf{q}} + \dot{\mathbf{g}}^{(1)}$

Target equations

$$\begin{bmatrix} \mathbf{f}_d(\dot{\mathbf{x}},\mathbf{x},t) \\ \mathbf{f}_c(\mathbf{x},t) \end{bmatrix} = \mathbf{0} \qquad \begin{bmatrix} \frac{\partial \mathbf{f}_d}{\partial \dot{\mathbf{x}}} \\ \frac{\partial \mathbf{f}_c}{\partial \mathbf{x}} \end{bmatrix} \text{ is regular}$$

$$\mathbf{0} = \begin{bmatrix} \mathbf{f}_d(\dot{\mathbf{x}},\mathbf{x},t) \\ \mathbf{f}_c(\mathbf{x},t) \end{bmatrix} = \begin{bmatrix} \dot{\mathbf{q}} - \mathbf{v} + \mathbf{G}^{\mathrm{T}}\dot{\boldsymbol{\mu}}_{int} \\ \mathbf{M}\,\dot{\mathbf{v}} + \mathbf{G}^{\mathrm{T}}\,\dot{\boldsymbol{\lambda}}_{int} - \mathbf{h}(\mathbf{q},\mathbf{v},t) \\ \hline \mathbf{g}(\mathbf{q},t) \\ \dot{\mathbf{g}} = \mathbf{G}\,\mathbf{v} + \mathbf{g}^{(1)}(\mathbf{q},t) \end{bmatrix}$$

$\mathbf{x} = [\mathbf{q};\mathbf{v};\boldsymbol{\lambda}_{int};\boldsymbol{\mu}_{int}],\ \boldsymbol{\lambda} := \dot{\boldsymbol{\lambda}}_{int}$

(Gear/Gupta/Leimkuhler 1985; Gear 1988)

Can be generalized to any DAE (where Pantelides algorithm can be applied, details see paper)

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Variant of dummy derivative method → Index 1 DAE
(Mattsson/Söderlind 1993)

Example:

Result of Pantelides algorithm:

BLT blocks	*solve for*
$\mathbf{u} = -(cs + d\dot{s})\mathbf{n}$	$\mathbf{u}$
$\ddot{\mathbf{r}} = \mathbf{n}\ddot{s}$ $\dot{\mathbf{v}} = \ddot{\mathbf{r}}$ $m\dot{\mathbf{v}} = \mathbf{f} + m\mathbf{g} + \mathbf{u}$ $\mathbf{0} = \mathbf{n} \cdot \mathbf{f}$	$\ddot{s}, \ddot{\mathbf{r}}, \dot{\mathbf{v}}, \mathbf{f}$

BLT Block 1		*solve for*
	$\mathbf{u} = -(cs + d\dot{s})\mathbf{n}$	$\mathbf{u}$
BLT Block 2		
	BLT Block 2.1	
	$\mathbf{r} = \mathbf{n}s$	$s, \mathbf{r}$
	BLT Block 2.2	
	$\dot{\mathbf{r}} = \mathbf{n}\dot{s}$ $\mathbf{v} = \dot{\mathbf{r}}$	$\dot{s}, \dot{\mathbf{r}}, \mathbf{v}$
	BLT Block 2.3	
	$\ddot{\mathbf{r}} = \mathbf{n}\ddot{s}$ $\dot{\mathbf{v}} = \ddot{\mathbf{r}}$ $m\dot{\mathbf{v}} = \mathbf{f} + m\mathbf{g} + \mathbf{u}$ $\mathbf{0} = \mathbf{n} \cdot \mathbf{f}$	$\ddot{s}, \ddot{\mathbf{r}}, \dot{\mathbf{v}}, \mathbf{f}$

$$\begin{bmatrix} \mathbf{f}_d(\dot{\mathbf{x}}, \mathbf{x}, t) \\ \mathbf{f}_c(\mathbf{x}, t) \end{bmatrix}$$

$$\mathbf{x} = [s; \dot{s}]$$

$$\begin{aligned}
\mathbf{r} &:= \mathbf{n}s \\
\dot{\mathbf{r}} &:= \mathbf{n}\dot{s} \\
\mathbf{v} &:= \dot{\mathbf{r}} \\
\ddot{\mathbf{r}} &:= \mathbf{n}\ddot{s} \\
\dot{\mathbf{v}} &:= \ddot{\mathbf{r}} \\
\mathbf{u} &:= -(cs + d\dot{s})\mathbf{n} \\
\mathbf{f} &:= m\dot{\mathbf{v}} - m\mathbf{g} - \mathbf{u}
\end{aligned}$$

With tearing on every BLT block, constraint equations are explicitly solved (here) and are local equations:

new algorithm

Tearing

Tearing with retained solution space

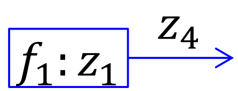
(Elmqvist/Otter 1999 (unpublished), Bender/Fineman/Gilbert/Tarjan 2016)

$$\mathbf{0} = \boldsymbol{g}(\boldsymbol{z}) \xrightarrow[\text{solve explicitly}]{} \begin{array}{l} \boldsymbol{z}_e := \boldsymbol{g}_e(\boldsymbol{z}_e, \boldsymbol{z}_t) \\ 0 = \boldsymbol{g}_r(\boldsymbol{z}_e, \boldsymbol{z}_t) \end{array}$$

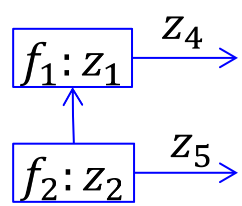
Observation:
$(z_{e,i}, g_{e,i})$ nodes of a Directed Acyclic Graph,
so **no cycles**

Example:

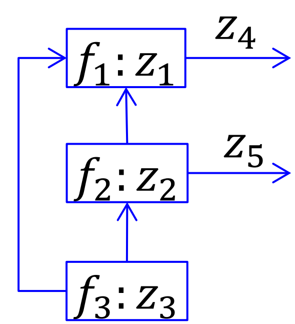
$$\begin{aligned} z_1 &= f_1(z_4) \\ z_2 &= f_2(z_1, z_5) \\ z_3 &= f_3(z_2, z_1) \\ z_4 &= f_4(z_3, z_2) \end{aligned}$$



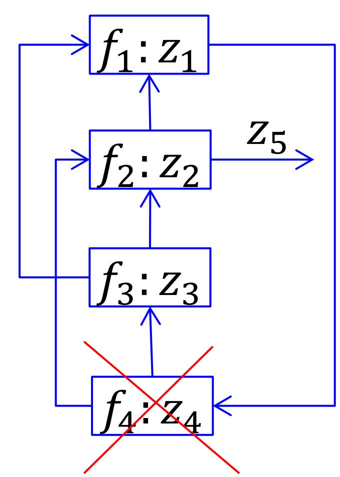
cycles?



cylces?



cycles?



cycles?

Try all combinations of variables
that can be explicitly solved for and check
whether a cycle is present (with Depth First Search).
Faster search with incremental cycle detection (Bender et al. 2016)

Conclusions and Future Work

- Several new algorithms developed to improve symbolic processing of Modelica tools (should allow to support larger Modelica models)
- Test implementation and evaluation of the algorithms in Modia (= domain specific extension of the Julia programming language; see companion paper „Innovations for future Modelica").
- Tests/evaluation with large, difficult models not yet done. Will be performed in the near future.
- Initialization of index 1 DAEs not discussed: Could be performed with all equations from Pantelides algorithm (as today). Evaluation of a new method to handle Dirac impulses in any DAE: $\mathbf{x}(t_0 - \epsilon) \rightarrow$ changes discontinuously to $\mathbf{x}(t_0 + \epsilon) \rightarrow$ Dirac impulses in $\dot{\mathbf{x}}(t_0)$
- Modia, including the implementations of the algorithms, to become available from https://github.com/modiasim under MIT license.