D7 : (old title) Numerical simulation of integrated circuits for future chip generations

(new title) Index determination and structural analysis using Algorithmic Differentiation

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Dagmar Monett* (M. Selva until 09/2006)
René Lamour, Lutz Lehmann (since 09/2007)

**DAE Example**

\[
\begin{align*}
 f(x, h(x, y)) &= 0 \\
 g(y, h(x, y)) &= 0 \\
 x, y, h, f, g &\in \mathbb{R}
\end{align*}
\]

Jacobian

\[
\frac{\partial (f, g)}{\partial (\dot{x}, \dot{y})} = \begin{pmatrix}
 \frac{\partial f}{\partial h} \\
 \frac{\partial g}{\partial h}
\end{pmatrix} \cdot \begin{pmatrix}
 \frac{\partial h}{\partial \dot{x}} & \frac{\partial h}{\partial \dot{y}}
\end{pmatrix}
\]

has rank \( \leq 1 \)

**Transformation to ODE for** \((\dot{x}, \dot{y})\) **impossible!**

**Structural Analysis à la Pantelides fails!!!**
Some applications

- Circuit simulation (focus of original project)
- Electromechanical problems (dynamo, plate condenser)
- Multiple pendulum
- Robotic arm

Criteria for index 3 or higher:

CV-loops & LI-cutsets
D7 history

- First funding period
  - Circuit-device coupled simulations
  - Determination of suitable discretizations
- Second funding period, first stage (Tischendorf)
  - Incorporation of a system integrator
  - Discretization of new semiconductor device models
  - Inclusion of 2D models by applying the Scharfetter-Gummel approach

Occurring challenges

- Determination of the tractability index
- Computation of consistent initial values

D7: Numerical simulation of integrated circuits for future chip generations
DAEs given by the general equation:

\[ f \left( (d(x(t)))', x(t) \right) = 0, \quad t \in I \quad \bar{z}(t) = d(\bar{x}(t))' \]

“Random” path \( \bar{x}(t) \) yields linearized system with coefficients:

\[
A(t) = \frac{\partial f}{\partial \bar{z}} (\bar{z}(t), \bar{x}(t)), \quad B(t) = \frac{\partial f}{\partial \bar{z}} (\bar{z}(t), \bar{x}(t)), \quad D(t) = \frac{\partial d}{\partial x} (\bar{x}(t))
\]

Continuous matrix function sequence:

\[
G_0 := AD, \quad B_0 := B,
\]

\[
G_{i+1} := G_i + B_i Q_i \quad \text{(if det} (G_{i+1}) \not\equiv 0 \text{ return index } i + 1)
\]

\[
= (G_i + W_i B_i Q_i)(I + G_i^{-1} B_i Q_i),
\]

\[
B_{i+1} := (B_i - G_{i+1} D^{-1}(DP_0 \ldots P_{i+1} D^{-1})'DP_0 \ldots P_{i-1})P_i
\]

Originally: differentiation approximated by finite differences!!!
Repeated Differentiations $\cong$ **Taylor series arithmetic + Shift op. on original specification!!**

**“Algorithmic Differentiation”** yields the matrices of polynomials $A(t), B(t), D(t)$

No truncation errors

<table>
<thead>
<tr>
<th>Term</th>
<th>$Q_{1,13}$ rel.err.</th>
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<td>$(t - 1)^4$</td>
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<table>
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<td>2.785e-13</td>
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<tr>
<td>$(t - 1)^4$</td>
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**Quadratic complexity in degree**

Elapsed running time by the program varying the number of Taylor coefficients (averages over 20 independent runs)
Use of Algorithmic Differentiation techniques

- User class
- daeIndexDet.cpp
- Global parameters

- ‘asectra’ active section and calculation of the trajectory, $x(t)$
- ‘asecdyn’ active section and calculation of the dynamic, $d(x(t), t)$ and its derivative $z(t) = d'(x(t), t)$ using shift operator
- ‘asecdae’ active section and calculation of the DAE, $f(z(t), x(t), t)$

- Construct matrices $A$, $B$, and $D$

ADOL-C

- tag 0 forward mode
  - active and passive variables, initial Taylor coefficients of $t$
  - Taylor coefficients of independent (i.e., $t$) and dependent variables (i.e., $x(t)$)

- tag 1 forward and reverse modes
  - active and passive variables, initial Taylor coefficients of $x(t)$ and $t$
  - Taylor coefficients of independent (i.e., $t$ and $x(t)$) and dependent variables (i.e., $d(x(t), t)$) and adjoints

- tag 2 forward and reverse modes
  - active and passive variables, initial Taylor coefficients of $d'(x(t), t)$, $x(t)$ and $t$
  - Taylor coefficients of independent (i.e., $d'(x(t), t)$ and $x(t)$) and dependent variables (i.e., $f(z(t), x(t), t)$) and adjoints
Example: Bike Dynamo

\begin{align*}
\dot{p} &= v \\
\dot{v} &= \tilde{f}(v, j_L, t) - \lambda \\
0 &= p - z(t) \\
C\dot{e} + Ge - j_L &= 0 \\
\dot{\phi} - e &= 0 \\
\phi &= \phi_L(v, t).
\end{align*}

with
\begin{align*}
\tilde{f}(v, j_L, t) &= \frac{f_{\text{mech}}}{m} + \frac{2\pi}{mk} k_0 j_L \sin(2\pi kt) \\
\phi_L(v, t) &= k_0 r \cos(2\pi vt)
\end{align*}

E.g. $t = 0$  \rightarrow  Singular point

The new method correctly computes the index even at problem singularities!!!
Example: Bipolar ring oscillator with inductor

\[ G(e_1 - e_{11}) + j_{C1} + j_{B_3} + j_{1,3} = 0 \]
\[ G(e_2 - e_{11}) + j_{C2} + j_{B_4} + j_{2,3} = 0 \]
\[ j_{E_3} + j_{E_4} + i - j_{1,3} - j_{2,3} = 0 \]
\[ G(e_4 - e_{11}) + j_{C3} + j_{B_5} + j_{4,6} = 0 \]
\[ G(e_5 - e_{11}) + j_{C4} + j_{B_6} + j_{5,6} = 0 \]
\[ j_{E_5} + j_{E_6} + i - j_{4,6} - j_{5,6} = 0 \]
\[ G(e_7 - e_{11}) + j_{C5} + j_{B_1} + j_{7,9} = 0 \]
\[ G(e_8 - e_{11}) + j_{C6} + j_{B_2} + j_{8,9} = 0 \]
\[ j_{E_1} + j_{E_2} + i - j_{7,9} - j_{8,9} = 0 \]
\[ j_y - 3i = 0 \]
\[ u_{10} + v = 0 \]
\[ L j_L' + e_{11} = 0 \]
\[ G(6e_{11} - e_1 - e_2 - e_4 - e_5 - e_7 - e_8) - j_L = 0 \]
Main achievements

▷ Exact differentiations without explicit specification of derivatives expressions

▷ High accurate results (e.g. checking eps-conditions: equal to 0 up to machine precision). Accurate calculation of the index / consistent initial values (for the linear case)

▷ New matrix-algebra operations to deal with AD (e.g. implementation of special matrix-matrix multiplications, QR decomposition of matrices of Taylor polynomials, etc.) with operator overloading in C++

▷ New program and library for the index determination and the consistent initialization
Cooperations within application area

D13 (higher index problems, device models for electrical circuits)

Cooperations with other application areas

C12 (software development, AD issues, algebraic equations solving)

External Cooperations

1st half (until 09/2006):
- A. Jüngel (Univ. Mainz)
- M. Günther (Univ. Wuppertal)
- R. Riaza (Univ. Madrid, Spain)
- C. Führer (Univ. Lund, Sweden)

2nd half:
- C. Tischendorf, M. Selva (Univ. Cologne)
- F. Mazzia (Università di Bari, Italy)
- J. D. Pryce (Cranfield Univ., UK)
- N. S. Nedialkov (McMaster Univ., Canada)
- S. Campbell (North Carolina State Univ., USA)
- P. Barton (MIT, USA)
- H. G. Bock (Univ. Heidelberg)
- A. Walther (Univ. Dresden)
1. Computation of consistent initial values
   ▶ Nonlinear case, via [März/Lamour] (3 months)

2. Sparse implementation
   ▶ Sparse LU-based implementation of [März/Lamour]
     using Taylor arithmetic (6 months)
   ▶ Investigate connections to approaches of [Campbell] & [Kunkel/Mehrmann]

3. Structural analysis
   ▶ Exploration of extension of [Pantelides/Pryce]
     to computational graphs (3 months)

4. If 3. promising
   Development and implementation of method (in additional year)
Plans for 2008/2009 and beyond

Solution of introductory example based on graph

Expanded system

\[
\begin{align*}
z - h(x, y) &= 0 \\
f(x, z) &= 0 \\
g(y, z) &= 0
\end{align*}
\]

Maximal Degree of Variables

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
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Solution of introductory example based on graph

Expanded system

\[ z - h(x, \dot{y}) = 0 \]
\[ f(x, z) = 0 \]
\[ g(y, z) = 0 \]

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Occurrence of derivatives determines structural index via maximal transversal

Combinatorial subtasks:
- Identification of replicated subgraphs
- Maximal Weighted Matching on DAG
- Linear Assignment Problem on Matrix
Refereed Publications 2006-2008: 1
Submitted Preprints: 1
Books: 1
Conference Proceedings: 4
Further publications: 4

PhD Thesis (completed): 1 (first stage)
Habilitations: –

Plenary Lectures: –
Invited talks: 2

Offers (Prof. and similar): –
Public funding

BMBF project
Multiskalensysteme in Mikro- und Optoelektronik: Numerische Simulation von Hochfrequenzschaltungen der Kommunikationstechnik (until 09/2006, C. Tischendorf and M. Selva continued the cooperation)

BMBF project
NOVOEXP (Numerische Optimierung ... für optimale Versuchsplanung ...) im Förderschwerpunkt: Mathematik für Innovationen in Industrie und Dienstleistungen together with Univ. Heidelberg, TU Berlin, Univ. Marburg, BASF, Knauer
Cooperation topic: AD for DAEs
External Industrial Cooperations

Infineon Technologies, Quimonda

(mainly accomplished until 09/2006, first stage)
Software

**MECS**: Multiphysical Electric Circuit Simulator
A Matlab-program for the simulation of electrical circuits
http://www.mi.uni-koeln.de/~mselva/software.html
(Initiated inside D7 and further developed at the University of Cologne)

daeIndexDet: Program for the index determination in DAEs
indexdet: Corresponding library
Using Algorithmic Differentiation techniques (ADOL-C package for AD)
http://www.mathematik.hu-berlin.de/~monett/indexdet/indexdet.html

Internal Workshop

**Index computations and structural analysis of DAEs** (18/02/2008)
Invited guests:
- R. März (Humboldt-Univ. zu Berlin)
- C. Tischendorf (Univ. zu Köln)
- J. Pryce (Cranfield University, UK)