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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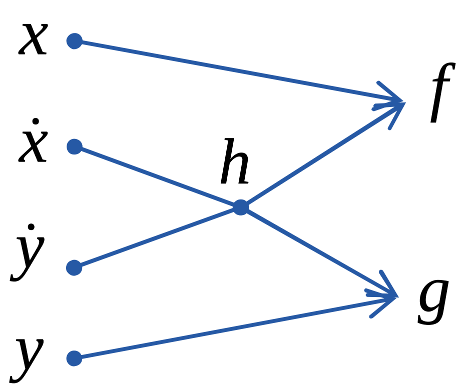
DAE Example

$$f\big(x, h(\dot{x}, \dot{y})\big) = 0$$
$$g\big(y, h(\dot{x}, \dot{y})\big) = 0$$
$$x, y, h, f, g \in \mathbb{R}$$

Corresponding computational graph



Jacobian

$$\frac{\partial(f, g)}{\partial(\dot{x}, \dot{y})} = \begin{pmatrix} \dfrac{\partial f}{\partial h} \\[2ex] \dfrac{\partial g}{\partial h} \end{pmatrix} \cdot \begin{pmatrix} \dfrac{\partial h}{\partial \dot{x}} & \dfrac{\partial h}{\partial \dot{y}} \end{pmatrix}$$

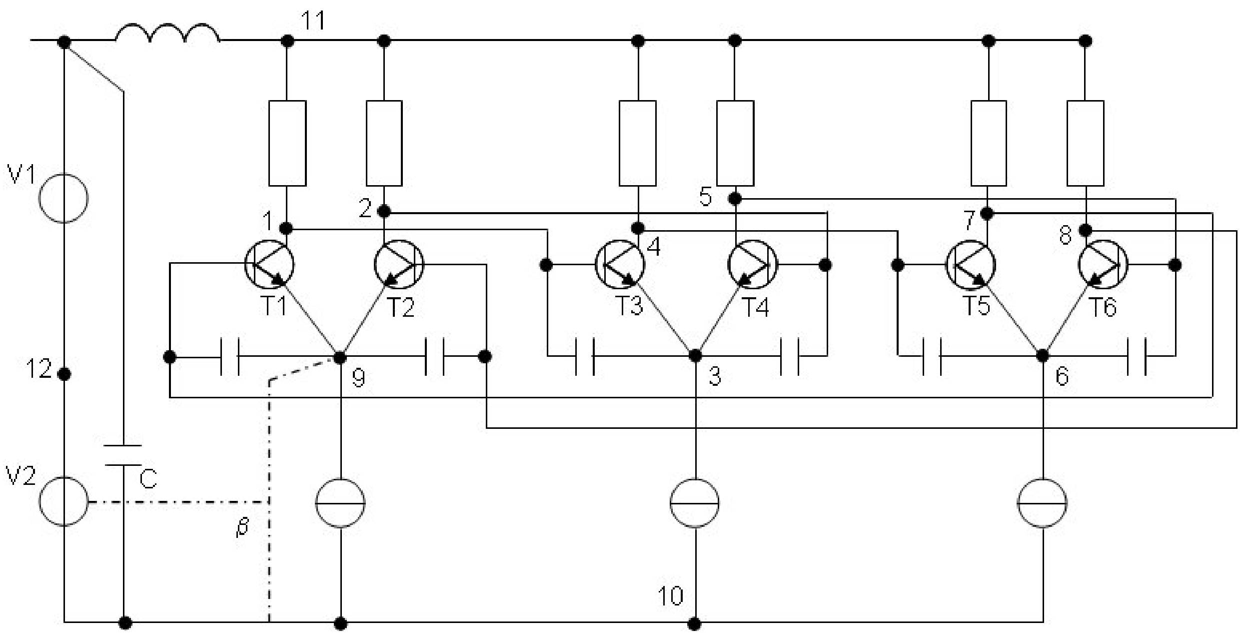
has rank ≤ 1

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

⇒ treated in second stage

DAEs given by the **general equation**:

$$f((d(x(t))', x(t)) = 0, \quad t \in I \qquad\qquad \bar{z}(t) = d(\bar{x}(t))'$$

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

$$A(t) = \frac{\partial f}{\partial z}(\bar{z}(t), \bar{x}(t)), \qquad B(t) = \frac{\partial f}{\partial z}(\bar{z}(t), \bar{x}(t)), \qquad D(t) = \frac{\partial d}{\partial x}(\bar{x}(t))$$

Continuous matrix function sequence:

$$\begin{aligned} G_0 &:= AD, \qquad B_0 := B, \\ G_{i+1} &:= G_i + B_i Q_i \\ &= (G_i + W_i B_i Q_i)(I + G_i^- B_i Q_i), \\ B_{i+1} &:= (B_i - G_{i+1} D^- \underline{(D P_0 \dots P_{i+1} D^-)'} D P_0 \dots P_{i-1}) P_i \end{aligned}$$

(if det(G_{i+1}) <> 0
return index = i + 1)

Originally: differentiation approximated by finite differences!!!

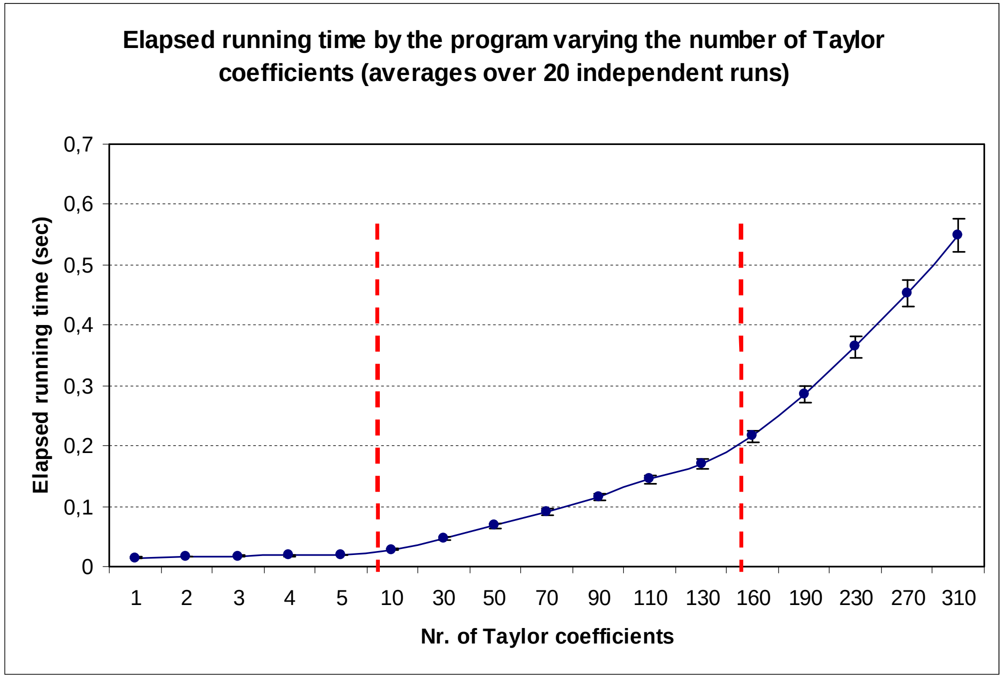
Repeated Differentiations $\cong$ **Taylor series arithmetic + Shift op.** on original specification!!

"Algorithmic Differentiation" yields the matrices of polynomials $A(t), B(t), D(t)$

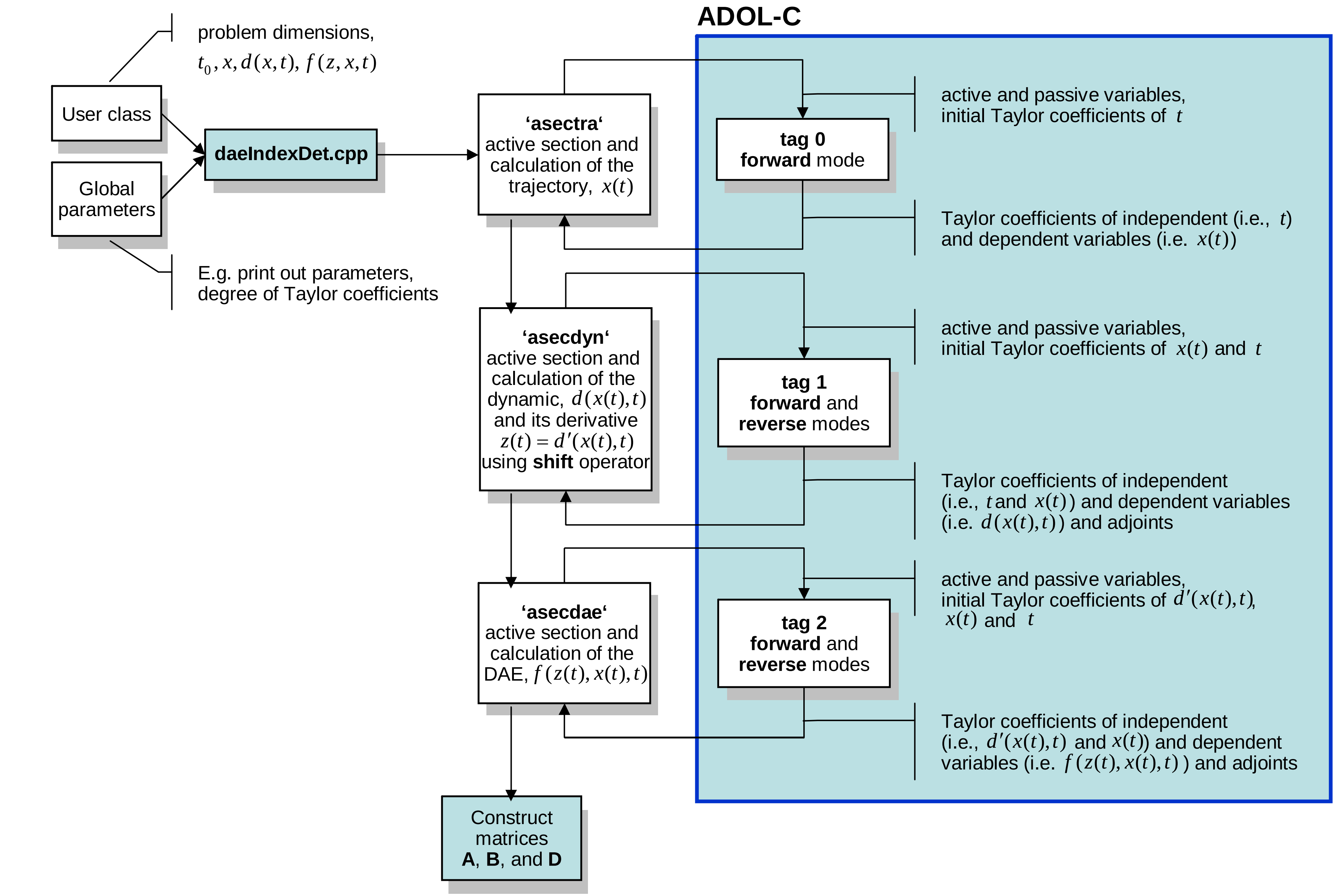
No truncation errors

Term	$Q_{1,13}$ *rel.err.*
$(t - 1)^0$	0.0
$(t - 1)^1$	5.000e-16
$(t - 1)^2$	2.000e-16
$(t - 1)^3$	1.478e-15
$(t - 1)^4$	6.153e-15
Term	$Q_{2,13}$ *rel.err.*
$(t - 1)^0$	6.790e-14
$(t - 1)^1$	1.404e-13
$(t - 1)^2$	2.094e-13
$(t - 1)^3$	2.785e-13
$(t - 1)^4$	–

Quadratic complexity in degree



Use of Algorithmic Differentiation techniques



Example: Bike Dynamo

(In cooperation with project D13) **(Index 4)**

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

p : position of the mass point

v : velocity

e : voltage

ϕ : magnetic flow

j_L : conductance

m, k, k_0, C, G are known

with

$$\tilde{f}(v, j_L, t) = \frac{f_{mech}}{m} + \frac{2\pi}{mk} k_0 j_L \sin(2\pi kvt)$$
$$\phi_L(v, t) = k_0 r \cos(2\pi kvt)$$

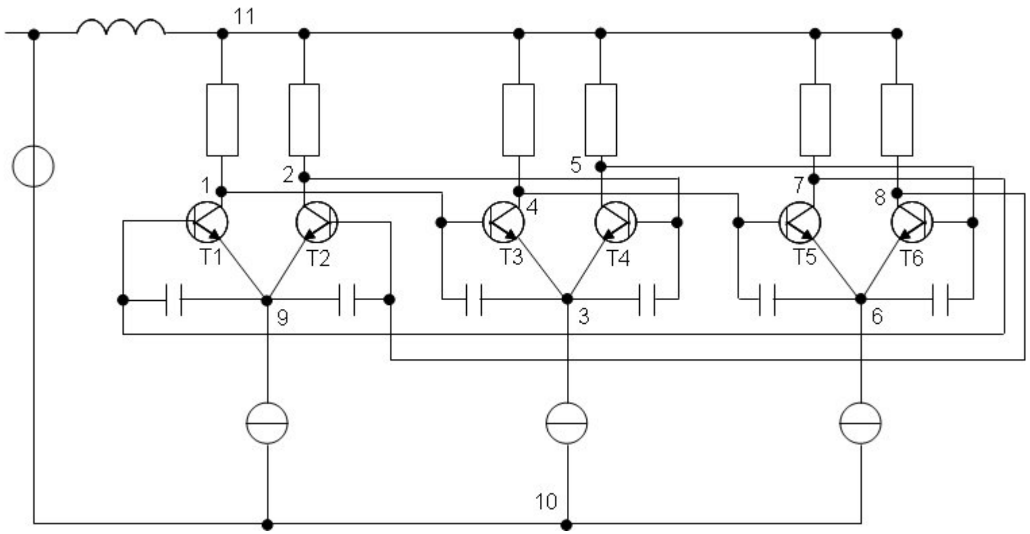
$$f_{mech} = gm\tan(\alpha)$$

E.g. $t = 0$ ⇨ Singular point

The new method correctly computes the index even at problem singularities!!!

Example: Bipolar ring oscillator with inductor

(**Index 2**)



$$j_{a,b} = \dot{q}(e_a - e_b) \qquad q(v) = -4\cdot 10^{-11} v_B \sqrt{1 - \frac{v}{v_B}}$$

$$j_B = j_{BE} + j_{BC}$$

$$= \frac{I_S}{\alpha}\left(e^{\frac{v_{BE}}{v_T}} - 1\right) + \frac{I_S}{\alpha_r}\left(e^{\frac{v_{BC}}{v_T}} - 1\right)$$

$$j_C = \alpha j_{BE} - (1 + \alpha_r) j_{BC}$$

$L, \alpha, \alpha_r, v, v_T, v_B, G, I_S, i$ are known

$$G(e_1 - e_{11}) + j_{C1} + j_{B3} + j_{1,3} = 0$$
$$G(e_2 - e_{11}) + j_{C2} + j_{B4} + j_{2,3} = 0$$
$$j_{E3} + j_{E4} + i - j_{1,3} - j_{2,3} = 0$$
$$G(e_4 - e_{11}) + j_{C3} + j_{B5} + j_{4,6} = 0$$
$$G(e_5 - e_{11}) + j_{C4} + j_{B6} + j_{5,6} = 0$$
$$j_{E5} + j_{E6} + i - j_{4,6} - j_{5,6} = 0$$
$$G(e_7 - e_{11}) + j_{C5} + j_{B1} + j_{7,9} = 0$$
$$G(e_8 - e_{11}) + j_{C6} + j_{B2} + j_{8,9} = 0$$
$$j_{E1} + j_{E2} + i - j_{7,9} - j_{8,9} = 0$$
$$j_v - 3i = 0$$
$$u_{10} + v = 0$$
$$Lj'_L + e_{11} = 0$$
$$G(6e_{11} - e_1 - e_2 - e_4 - e_5 - e_7 - e_8) - j_L = 0$$

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 MATHEON and externally

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)

Plans for 2008/2009 and beyond

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**)

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4. If 3. promising

   ⇨ Development and implementation of method (**in additional year**)

Solution of introductory example based on graph

Expanded system

$$z - h(\dot{x}, \dot{y}) = 0$$

$$f(x, z) = 0$$

$$g(y, z) = 0$$

Maximal Degree of Variables

x	y	z
1	1	0
0	–	0
–	0	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

Statistics I: Publications, Talks, etc

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 ... in der Chemie ...) 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)