Solving large nonlinear generalized eigenvalue problems from Density Functional Theory calculations in parallel
The quantum mechanical ground state of electrons is described by Density Functional Theory, which leads to large minimization problems. An efficient minimization method uses a self-consistent field (SCF) solution of large eigenvalue problems. The iterative Davidson algorithm is often used, and we propose a new algorithm of this kind which is well suited for the SCF method, since the accuracy of the eigensolution is gradually improved along with the outer SCF-iterations. Best efficiency is obtained for small-block-size iterations, and the algorithm is highly memory efficient. The implementation works well on both serial and parallel computers, and good scalability of the algorithm is obtained. (C) 2001 IMACS. Published by Elsevier Science B.V. All rights reserved.
Numerical Solution of Differential Algebraic Equations

General information
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Authors: Thomsen, P. G. (Intern), Bendtsen, C. (Intern)
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Numerical Solution of Differential Algebraic Equations: A Ph.D. Course

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Authors: Wagner, F. J. (Intern), Hostrup, A. K. (Intern), Antonov, A. A. (Intern), Elmegaard, B. (Intern), Poulsen, M. Z. (Intern), Thomsen, P. G. (Intern), Bendtsen, C. (Intern)
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Tadiff, a flexible C++ package for automatic differentiation

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FADBAD, a flexible C++ package for automatic differentiation.

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Implementation of QR up- and downdating on a massively parallel computer
We describe an implementation of QR up- and downdating on a massively parallel computer (the Connection Machine CM-200) and show that the algorithm maps well onto the computer. In particular, we show how the use of corrected semi-normal equations for downdating can be efficiently implemented. We also illustrate the use of our algorithms in a new LP algorithm.
Storskala inversionsalgoritmer

Department of Informatics and Mathematical Modeling
Period: 01/12/1998 → 20/01/2003
Number of participants: 8
Phd Student:
Berglund, Eva Ann-Charlotte (Intern)
Supervisor:
Bendtsen, Claus (Intern)
Jacobsen, Bo Holm (Ekstern)
Madsen, Kaj (Intern)
Main Supervisor:
Hansen, Per Christian (Intern)
Examiner:
Nielsen, Hans Bruun (Intern)
Mosegaard, Klaus (Intern)
Rojas Larrazabal, Marielba de la Caridad (Intern)

Financing sources
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Name of research programme: Samarbejdsaftalefinans
Project: PhD

Parallele numeriske algoritmer til løsning af systemer af sædvanlige differentialligninger

Department of Informatics and Mathematical Modeling
Period: 01/07/1993 → 04/12/1996
Number of participants: 5
Phd Student:
Bendtsen, Claus (Intern)
Supervisor:
Skelboe, Stig (Ekstern)
Main Supervisor:
Thomsen, Per Grove (Intern)
Examiner:
Houbak, Niels (Intern)
Söderlind, Gustaf (Ekstern)

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Source: Internal funding (public)
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