SENSITIVITY ANALYSIS AND MODEL REDUCTION OF
NONLINEAR DIFFERENTIAL-ALGEBRAIC SYSTEMS

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FINAL PROGRESS REPORT

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1 Statement of the problem studied

Differential-algebraic equations arise in a wide variety of engineering and scientific problems. These types of systems occur frequently as initial value problems in the computer aided design and modeling of mechanical systems subject to constraints, electrical networks, chemical process simulation, flow of incompressible fluids and in many other applications. Much recent work has been devoted to understanding these systems and developing numerical methods and software for the simulation problem. Relatively little work has been done regarding sensitivity analysis and model reduction for this class of problems. Efficient methods for sensitivity analysis are required in model development and as an intermediate step in design optimization of engineering processes. Reduced order models are needed for modelling complex physical phenomena like turbulent reacting flows, where it is not feasible to use a fully-detailed model. The objective of this work has been to develop numerical methods and software for sensitivity analysis and model reduction of nonlinear differential-algebraic systems, including large-scale systems. The focus is on applications from chemical process modelling.

2 Summary of results

We have developed new algorithms and software for sensitivity analysis of DAE systems. The algorithms have several novel features which are particularly advantageous for the solution and sensitivity analysis of very large-scale DAE problems. The new algorithms have been analyzed and shown to achieve rapid convergence. A DAE solver DASPK3.0 incorporating the algorithms for sensitivity analysis and substantial improvements in other algorithms, for determining consistent initial conditions and dealing with higher index systems, is now available via our web site. The new solver is very efficient and easy to use. DASPK3.0 is also an important part of our optimization software described below. Generation of the sensitivity equations via automatic differentiation (ADIFOR) is included in the software, and has been extremely useful in generating the sensitivities for chemical kinetics problems in the mechanism reduction results described below. Due

to the wide range of scales and severe nonlinearities in these problems, it is sometimes difficult to select a finite-difference increment which would lead to acceptable errors.

To accomplish the nonlinear model reduction via the plan outlined in the proposal, a substantial capability for parameter estimation and optimal control of DAE systems is required. To this end, we have developed the COOPT algorithms and software for optimization of nonlinear DAE systems. The optimization is accomplished via an SQP method in a version of the software SNOPT by Gill, Murray and Saunders which has been modified for this purpose. The problem is discretized via a multiple-shooting type method which divides the original time interval into subintervals. The DAEs on each interval are solved by our DASPK3.0 algorithms and software including sensitivity analysis (needed for approximating the partial derivative matrices required by the SQP method). A fundamental problem with the multiple-shooting approach is its computational complexity for large-scale DAE systems. We have developed a modification of this method which maintains the robustness and stability of the original method but at a greatly reduced computational cost.

We have completed an implementation of the ideas outlined in the proposal for model reduction of chemically reacting mechanisms via an optimization approach. Several refinements have been made. The optimization problem generated by this approach is a nonlinear integer programming problem without convex or polynomial properties, for which there is a scarcity of available methods. Solutions to the continuous optimization problem are often not a good approximation to the discrete solutions. We found that adding nonlinear inequality constraints which force the solutions to be near to zero or one improves the performance. The GRI (Gas Research Institute) mechanism from GRI's Website, a well-known mechanism in the chemical engineering literature with 32 species and 177 reversible reactions, was reduced automatically to 17 species and 38 reactions with near perfect agreement. We have obtained similarly excellent results on an even larger mechanism obtained from Exxon. We have been investigating better measures for measuring the goodness of a reduced mechanism, attempting to reduce much larger mechanisms, improving the numerical methods and software, and investigating the effects of uncertainty due to using a reduced mechanism in more complicated

calculations.

3 List of Papers and Presentations

3.1 Papers

1. L. Petzold and W. Zhu, Model Reduction for Chemical Kinetics: An Optimization Approach, AIChE Journal, April 1999, pp. 869-886.
2. S. Li and L. Petzold, Software and Algorithms for Sensitivity Analysis of Large-Scale Differential Algebraic Systems, submitted, J. Comp. Appl. Math., 1999.
3. L. Petzold, P. Gill, L. Jay, M. Leonard and V. Sharma, An SQP Method for the Optimal Control of Large-Scale Dynamical Systems, to appear, special issue of J. Comp. Appl. Math.
4. W. Zhu and L. Petzold, Parallel Sensitivity Analysis for DAEs with Many Parameters, Concurrency: Practice and Experience 11, 1999, pp. 571-585.
5. S. Li, L. Petzold and W. Zhu, Sensitivity Analysis of Differential-Algebraic Equations: A Comparison of Methods on a Special Problem, to appear, Applied Numerical Mathematics, 1999.

3.2 Technical Reports

1. S. Li and L. Petzold, Design of New DASPK for Sensitivity Analysis, UCSB Dept. of CS Tech. Report 1999.

3.3 Presentations

1. L. Petzold, MIT Department of Chemical Engineering Seminar, "Model Reduction for Chemical Kinetics: An Optimization Approach", Octo-

ber, 1999.

2. L. Petzold, MIT Department of Chemical Engineering Colloquium, "Algorithms and Software for Dynamic Optimization with Application to Chemically Reacting Stagnation Flows", October, 1999.
3. L. Petzold, IMA Workshop on Mathematical and Computational Strategies for Simplifying Complex Kinetics, "Model Reduction for Chemical Kinetics: An Optimization Approach", October, 1999.
4. L. Petzold, UCSB Nonequilibrium Physics seminar, "Algorithms and Software for Sensitivity Analysis and Optimal Control of Large-Scale Differential-Algebraic Systems, with Applications to Chemical Vapor Deposition Processes", October, 1999.
5. L. Petzold, IMA Workshop on Decision Making under Uncertainty, Minneapolis, MN "Model Reduction and Assessment for Nonlinear Networked Systems", September, 1999.
6. L. Petzold, Lawrence Livermore National Laboratory CASC, Livermore, CA, "Algorithms and Software for Sensitivity Analysis and Optimal Control of Large-Scale Differential-Algebraic Systems", September, 1999.
7. L. Petzold, ANODE99, Auckland Numerical Ordinary Differential Equations workshop, Auckland, New Zealand (2 hours plenary lecture), "Algorithms and Software for Sensitivity Analysis and Optimal Control of Large-Scale Differential-Algebraic Systems, with Applications", August, 1999.
8. L. Petzold, SciCADE99, International Conference on Scientific Computing and Differential Equations, Queensland, Australia (plenary lecture), "Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics", August, 1999.
9. L. Petzold, ICIAM International Meeting, Edinburgh, Scotland, "Algorithms and Software for Sensitivity Analysis and Optimal Control of Large-Scale Differential-Algebraic Systems", July 1999.

10. L. Petzold, Argonne National Laboratory, Reduced Mechanisms in Turbulent Combustion Workshop, "Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics", June 1999.
11. L. Petzold, Workshop on Computational Sciences and Engineering, Ascona, Switzerland, "Algorithms and Software for Sensitivity Analysis and Optimal Control of Large-Scale Differential-Algebraic Systems, with Application to Chemical Vapor Deposition", May 1999.
12. L. Petzold, UC Davis, Institute of Theoretical Dynamics, "Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics", April 1999.
13. L. Petzold, Conference on Nonlinear Dynamics and Scientific Computing, UCSB, "Algorithms and Software for Sensitivity Analysis and Optimal Control of Large-Scale Differential Algebraic Systems, with Application to Chemical Vapor Deposition", April 1999.
14. L. Petzold, University of Colorado Boulder, Dept. of Chemical Engineering and Dept. of Applied Mathematics joint seminar, "Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics", February 1999.
15. L. Petzold, RPI SCOREC Seminar, New York, "Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics", February 1999.
16. L. Petzold, IGPP/NPACI Workshop on Accurate Simulation and Modeling of Physical Systems, San Diego, "Modeling and Sensitivity Analysis for Physical Systems", November 1998.
17. L. Petzold, DOE Predictability Workshop, Albuquerque, "Sensitivity Analysis for Large-Scale Differential-Algebraic Systems", October 1998.
18. L. Petzold, SIAM Annual Meeting minisymposium, "Model Reduction and Uncertainty", July 1998.
19. L. Petzold, Argonne Automatic Differentiation Workshop, "Automatic Differentiation in Sensitivity Analysis and Optimal Control of Differential-Algebraic Systems", May 1998.

20. L. Petzold, Workshop on Control and Computation, UCSB, "Model Reduction for Chemical Kinetics", April 1998.

4 Awards

L. Petzold received the Dahlquist Prize for numerical solution of differential equations in 1999.

5 List of all participating scientific personnel

The personnel participating in this project were: PI: Linda Petzold, Graduate Research Assistants: Wenjie Zhu, Postdoctoral Research Associates: Sheng-tai Li. Wenjie Zhu completed his Ph.D. in Computer Science at University of Minnesota on this topic in 1999.

6 Report of inventions

None.