SENSITIVITY ANALYSIS AND MODEL REDUCTION OF NONLINEAR DIFFERENTIAL-ALGEBRAIC SYSTEMS

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

In collaboration with Peter Brown and Alan Hindmarsh of LLNL, we developed an algorithm for finding consistent initial conditions for several widely occuring classes of differential-algebraic equations(DAEs). The new algorithm is much more robust than the previous algorithm. It is also very easy to use, having been designed to require almost no information about the differential equation, Jacobian matrix, etc. in addition to what is already needed to take the subsequent time steps. The new algorithm has been implemented in a version of our software for solution of large-scale DAEs, DASPK, which has been made available on the internet. The new methods and software have been used to solve a Tokamak edge plasma problem at LLNL which could not be solved with the previous methods and software because of difficulties in finding consistent initial conditions. The capability of finding consistent initial values is also needed for the sensitivity and

optimization efforts described below.

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 in DASPK. The new algorithms have been analyzed and shown to achieve rapid convergence. Versions of the DAE solvers DASSL and DASPK have been implemented incorporating the new algorithms for sensitivity analysis. The new solvers are very efficient and easy to use. Experimental versions are available via anonymous ftp; the sensitivity solver based on DASPK is an important part of our optimization software described below. Generation of the sensitivity equations via automatic differentiation (ADIFOR) has recently been added to 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 a preliminary version of the DASOPT algorithms and software for optimization of nonlinear DAE systems in collaboration with P. Gill and J. B. Rosen. 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 DASPK algorithms and software which have been modified to include 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. The new method has been implemented and performed excellently in preliminary testing.

We have completed a preliminary 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. With the follow-on grant, we are 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 a fluid flow calculation.

3 List of Papers and Presentations

3.1 Papers

1. L. Petzold, J. B. Rosen, P. E. Gill, L. O. Jay and K. Park, *Numerical Optimal Control of Parabolic PDEs using DASOPT*, Large Scale Optimization with Applications, Part II: Optimal Design and Control, Eds. L. Biegler, T. Coleman, A. Conn and F. Santosa, IMA Volumes in Mathematics and its Applications, Vol. 93, (1997), 271-300.

2. P. N. Brown, A. C. Hindmarsh and L. R. Petzold, *Consistent Initial Condition Calculation for Differential- Algebraic Systems*, to appear, SIAM J. Sci. Comput.

3. S. F. Ashby, S. L. Lee, L. R. Petzold, P. E. Saylor and E. Seidel, *Computing Spacetime Curvature via Differential-Algebraic Equations*, to appear, Applied Numerical Mathematics.

4. T. Maly and L. R. Petzold, *Numerical Methods and Software for Sensitivity Analysis of Differential-Algebraic Systems*, Applied Numerical Mathematics 20 (1996), 57-79.

5. A. C. Hindmarsh and L. R. Petzold, *Algorithms and Software for Ordinary Differential Equations and Differential-Algebraic Equations*, Part I and Part II, Computers in Physics, 1995.

6. P. E. van Keken, L. R. Petzold and D. A. Yuen, *A New High Order and Adaptive Time-Integration Technique with Applications to Mantle Convection with Strongly Temperature- and Pressure-Dependent Rheology*, Geophys. Astrophys. Fluid Dyn. 80 (1995), 57-74.

7. L. R. Petzold, Y. Ren and T. Maly, *Regularization of higher-index differential-algebraic equations with rank-deficient constraints*, to appear, SIAM J. Sci. Comput.

8. P. N. Brown, A. C. Hindmarsh and L. R. Petzold, *Using Krylov Methods in the Solution of Large-Scale Differential-Algebraic Systems*, SIAM J. Sci. Comput. (1994), 1467-1488.

9. W. Zhu and L. R. Petzold, *Asymptotic Stability of Linear Delay Differential Algebraic Equations and Numerical Methods*, to appear, Applied Numerical Mathematics.

10. W. Zhu and L. R. Petzold, *Asymptotic Stability of Hessenberg Delay Differential-Algebraic Equations of Retarded or Neutral Type*, to appear, Applied Numerical Mathematics.

3.2 Presentations

1. L. Petzold, Stanford University, Scientific Computing and Computational Math Colloquium, *Model Reduction for Chemical Kinetics: An Optimization Approach*, December, 1997.

2. L. Petzold, Caltech, Workshop on Theoretical Foundations of Virtual Engineering and Complex Systems, *DAEs in Simulation and Design of Complex Systems*, November, 1997.

3. L. Petzold, University of California, Santa Barbara, Mathematics Colloquium, *Model Reduction for Chemical Kinetics: An Optimization Approach*, November, 1997.

4. L. Petzold, University of Minnesota, IMA Workshop on Multiple Time-Scale Dynamical Systems, *Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics*, October, 1997.

5. L. Petzold, AIChE National Meeting, Los Angeles, California, *Model Reduction for Chemical Kinetics: An Optimization Approach*, November, 1997.

6. L. Petzold, University of Minnesota, IMA Workshop on Automatic Differentiation, *Automatic Differentiation in Sensitivity Analysis and Optimal Control of Large-Scale Dynamical Systems*, July, 1997.

7. L. Petzold, Canadian Applied Mathematics Society National Meeting, *Model Reduction for Nonlinear Dynamical Systems from Chemical Kinetics*, May, 1997.

8. L. Petzold, University of Arizona, Dept. of Mathematics, *Parallel Numerical Methods for Optimization and Control of Large-Scale Differential-Algebraic Systems*, February 15, 1996.

9. L. Petzold, SIAM Conf. on Optimization, Victoria, British Columbia, *Numerical Optimal Control of Parabolic PDEs using DASOPT*, May 20, 1996.

10. L. Petzold, Volterra Centennial Conference, Arizona State University, Tempe, Arizona, *Delay-differential-algebraic equations and their numerical solution*, May 27, 1996.

11. L. Petzold, C3AD Colloquia Em Computacao Cientifica De Alto Desempenho, Laboratorio Nacional de Computacao Cientifica, Rio de Janeiro, Brazil, *Numerical Methods and Software for Optimization and Control of Large-Scale Differential-Algebraic Systems*, July 10, 1996.

12. L. Petzold, Universidade Federal do Rio de Janeiro, *Numerical Methods and Software for Optimization and Control of Large-Scale Differential-Algebraic Systems*, July 12, 1996.

13. L. Petzold, University of Wisconsin LaCrosse, Department of Mathematics, *Numerical Optimal Control of Parabolic PDEs using DASOPT*, September 27, 1996.

14. L. Petzold, Parallel Numerical Methods for Optimization and Control of Large-Scale Differential-Algebraic Systems, Dept. of Mathematics, UC San Diego, December, 1995.

15. L. Petzold, Parallel Numerical Methods for Optimization and Control of Large-Scale Differential-Algebraic Systems, Dept. of Mathematics, Princeton University, December, 1995.

16. L. Petzold, Parallel Numerical Methods for Optimization and Control of Large-Scale Differential-Algebraic Systems, University of Heidelberg, November, 1995.

17. L. Petzold, Parallel Numerical Methods for Optimization and Control of Large-Scale Differential-Algebraic Systems, Air Products and Chemicals Corp., October 1995.

18. L. Petzold, Parallel Solution and Sensitivity Analysis for Large-Scale Differential-Algebraic Systems, Minisymposium lecture, ICIAM 95, Hamburg (1995).

19. L. Petzold, Parallel Numerical Methods for Optimization and Control of Large-Scale Differential-Algebraic Systems, IMA Workshop on Large-Scale Optimization, Minneapolis, July, 1995.

20. L. Petzold, Numerical Methods and Software for Sensitivity Analysis of Differential-Algebraic Systems, Method of Lines for Partial Differential Equations Workshop, University of Kentucky, (1995).

21. L. Petzold, Krylov Methods in the Solution of Large-Scale DAE Systems, North Carolina State University, Workshop on Krylov Methods (1995).

4 List of all participating scientific personnel

The personnel participating in this project were: PI: Linda R. Petzold, Graduate Research Assistants: Wenjie Zhu. Wenjie Zhu is expected to complete his Ph.D. on this topic in approximately one year.

5 Report of inventions

None.