SENSITIVITY ANALYSIS AND MODEL REDUCTION OF NONLINEAR DIFFERENTIAL-ALGEBRAIC SYSTEMS

FINAL PROGRESS REPORT

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December 30, 1997

U.S. DEPARTMENT OF ENERGY

CONTRACT/GRANT NUMBER DE-FG02-92ER25130

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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 occurring 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


### 3.2 Presentations


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.