NUMERICAL OPTIMAL CONTROL OF PARABOLIC PDES USING DASOPT*

LINDA PETZOLD[†], J. BEN ROSEN[‡], PHILIP E. GILL[§], LAURENT O. JAY[¶], AND KIHONG PARK^{||}

Abstract. This paper gives a preliminary description of DASOPT, a software system for the optimal control of processes described by time-dependent partial differential equations (PDEs). DASOPT combines the use of efficient numerical methods for solving differential-algebraic equations (DAEs) with a package for large-scale optimization based on sequential quadratic programming (SQP). DASOPT is intended for the computation of the optimal control of time-dependent nonlinear systems of PDEs in two (and eventually three) spatial dimensions, including possible inequality constraints on the state variables. By the use of either finite-difference or finite-element approximations to the spatial derivatives, the PDEs are converted into a large system of ODEs or DAEs. Special techniques are needed in order to solve this very large optimal control problem. The use of DASOPT is illustrated by its application to a nonlinear parabolic PDE boundary control problem in two spatial dimensions. Computational results with and without bounds on the state variables are presented.

Key words. differential-algebraic equations, optimal control, nonlinear programming, sequential quadratic programming, partial differential equations.

AMS(MOS) subject classifications. 34A09, 34H05, 49J20, 49J15, 49M37, 49D37, 65F05, 65K05, 90C, 90C30, 90C06, 90C90

1. Introduction. We describe a numerical method (DASOPT) for finding the solution of a general optimal control problem. We assume that the problem is described with an objective function that must be minimized subject to constraints involving a system of DAEs and (possibly) inequality constraints. The numerical method uses the general-purpose packages DASPKSO (§4) and SNOPT (§3) in an essential way, and takes full advantage of their capabilities.

In the method proposed, large-scale nonlinear programming is used to

^{*} This research was partially supported by National Science Foundation grants CCR-95-27151 and DMI-9424639, National Institute of Standards and Technology contract 60 NANB2D 1272, Department of Energy grant FG02-92ER25130, Office of Naval Research grants N00014-90-J-1242 and N00014-96-1-0274, the Army High Performance Computing Research Center ARL Cooperative agreement DAAH04-95-2-0003 and contract DAAH04-95-C-0008, and the Minnesota Supercomputing Institute.

[†] Department of Computer Science, University of Minnesota, Minneapolis, Minnesota 55455.

[‡] Department of Computer Science, University of Minnesota, Minneapolis, Minnesota 55455, and Department of Computer Science and Engineering, University of California, San Diego, La Jolla, California 92093-0114.

[§] Department of Mathematics, University of California, San Diego, La Jolla, California 92093-0112.

 $[\]P$ Department of Computer Science, University of Minnesota, Minneapolis, Minnesota 55455.

^{||} School of Mechanical Engineering, Kookmin University, Seoul, Korea.

L. T. Biegler et al. (eds.), Large-Scale Optimization with Applications

[©] Springer-Verlag New York, Inc. 1997

solve the optimization/optimal control problem. The original time interval is divided into subintervals in a multiple-shooting type approach that provides a source of parallelism. (For other approaches, see, e.g., Dickmanns and Well [11], Kraft [20], Hargraves and Paris [19], Pesch [28], Lamour [21], Betts and Huffman [3], von Stryk and Bulirsch [35], Bulirsch *et al.* [9], von Stryk [34], Betts [2], Brenan [6], Schulz, Bock and Steinbach [30], Tanartkit and Biegler [32], Pantelides, Sargent and Vassiliadis [27], and Gritsis, Pantelides and Sargent [18].)

The associated finite-dimensional optimization problem is characterized by: (a) many variables and constraints; (b) sparse constraint and objective derivatives; and (c) many constraints active at the solution. The optimization problem is solved using the package SNOPT (§3), which is specifically designed for this type of problem. SNOPT uses a sequential quadratic programming (SQP) method in conjunction with a limitedmemory quasi-Newton approximation of the Lagrangian Hessian. There has been considerable interest elsewhere in extending SQP methods to the large structured problems. Much of this work has focused on reduced-Hessian methods, which maintain a dense quasi-Newton approximation to a smaller dimensional *reduced* Hessian (see, e.g., Biegler, Nocedal and Schmidt [4], Eldersveld [12], Tjoa and Biegler [33], and Schultz [29]). Our preference for approximating the full Hessian is motivated by substantial improvements in reliability and efficiency compared to earlier versions of SNOPT based on the reduced-Hessian approach.

The function and derivative computations for the optimization involve computing the solution of a large-scale DAE system, and solution sensitivities with respect to the initial conditions and the control parameters. The general-purpose package DASPKSO (§4) is used to compute the DAE solution and sensitivities. The sensitivity equations can be solved very efficiently, and in parallel with the original DAE.

In §5, a typical application is described, consisting of a nonlinear parabolic PDE in two spatial dimensions, with boundary control of the interior temperature distribution. This application serves as an initial test problem for DASOPT, and has the important feature that the size of the problem is readily increased by simply using a finer spatial grid size. It is shown in §5 how the PDE is reduced to a suitable finite-dimensional optimization problem. The numerical results, obtained by DASOPT for ten related cases, are summarized in §6. These results are displayed in ten figures that show, as a function of time, the optimal control and the temperatures at interior points obtained with different constraints and degrees of nonlinearity.

We assume that the continuous problem is given in the form

 $\begin{array}{lll} \underset{u,v}{\text{minimize}} & \phi(u) & = & \int_{0}^{t_{\max}} \psi(v,u,t) \, dt \\ \text{subject to} & v(0) & = & v_{0}, \end{array}$