PACKAGE ID - 000848MLTPL00 DDASAC

KWIC TITLE - Double Precision Differential/Algebraic Sensitivity Analysis Code

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LIMITATION CODE -UNL **AUDIENCE CODE -** UNL

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DESCRIPTION - DDASAC solves nonlinear initial-value problems involving stiff implicit systems of ordinary differential and algebraic equations. Purely algebraic nonlinear systems can also be solved, given an initial guess within the region of attraction of a solution. Options include automatic reconciliation of inconsistent initial states and derivatives, automatic initial step selection, direct concurrent parametric sensitivity analysis, and stopping at a prescribed value of any user-defined functional of the current solution vector. Local error control (in the max-norm or the 2-norm) is provided for the state vector and can include the sensitivities on request.

PACKAGE CONTENTS - Media Directory; Software Abstract; DDASAC Readme File; Appendix A, DDASAC Software Package Documentation; Compiling and Linking Instructions; Media Includes Source Code, Readme File, Sample Problem Input and Output Data;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - Reconciliation of initial conditions is done with a damped Newton algorithm adapted from Bain and Stewart (1991). Initial step selection is done by the first-order algorithm of Shampine (1987), extended here to differential-algebraic equation systems. The solution is continued with the DASSL predictor-corrector algorithm (Petzold 1983, Brenan et al. 1989) with the initial accleration phase deleted and with row scaling of the Jacobian added. The backward-difference formulas for the predictor and corrector are expressed in divide-difference form, and the fixed-leading-coefficient form of the corrector (Jackson and Sacks-Davis 1980, Brenan et al. 1989) is used. Weights for error tests are updated in each step with the user's tolerances at the predicited state. Sensitivity analysis is performed directly on

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METHOD OF SOLUTION -(CONT) the corrector equationsar in Catacotsios and Stewart (1985) and is extended here to the initialization when needed.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - DDASAC is in use on a wide variety of machines and operating systems.

PROGRAMMING LANGUAGES - Written in Fortran and conforms largely to the Fortran 77 standard.

SOFTWARE LIMITATIONS - This algorithm, like DASSL, performs well on differential-algebraic systems of index 0 and 1 but not on higher-index systems; see Brenan et al. (1989). The user assigns the work array lengths and the output unit. The machine number range and precision are determined at run time by a call to the LAPACK subroutine DLAMCH.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Parametric sensitivity analysis; automatic reconciliation of initial states and derivatives; row scaling of the Jacobian to improve numerical stability; flexible error control (see Method of Solution), and accurate stopping a designated value of a functional of the state vector. The latter feature allows repeated stopping on a value of a solution component or derivative, to obtain a Poincare' map of the solution.

RELATED SOFTWARE - This code is an extension and revision of DASSL (Petzold 1983). An earlier version of DDASAC has been distributed by Sandia Livermore Laboratories for use in their package SENKIN. The new DDASAC is different in many respects, including the error controls, the initialization options, the calling sequence for DDASAC, the tasks of the user's subroutines, and the adoption of LAPACK in place of LINPACK for the linear algebra computations. The LAPACK and BLAS codes used by DDASAC are collected in a seperate file LAPACK.FOR on the same diskette.

OTHER PROG/OPER SYS INFO - The notation Filename.FOR on the diskette denotes a Fortran source file, and Filename.DTA denotes the output data file. The .FOR files, when compiled and linked, suffice for execution of the four test problems given in the users' manual, Appendix A. The .DTA files correspond to the printed outputs of the four examples, given in Appendix A. These results were computed on a VAXstation 3200.

HARDWARE REQS - No special hardware requirements.

TIME REQUIREMENTS - Each of the examples has been run in less than 1 minute on a 486/33 personal computer.

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REFERENCES - User's guide on media

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SPONSOR - DOE/ER

PACKAGE TYPE - AS - IS