

Code Abstract for IDAS v1.0.0

1. Identification

Software acronym: IDAS v1.0.0

Short title: Stiff DAE integrator with sensitivity analysis capabilities

2. Developer name(s) and affiliations

Radu Serban (CASC, LLNL)

3. Software Completion Date

November 26, 2007

4. Brief description

IDAS is a general purpose (serial and parallel) solver for differential algebraic equation (DAE) systems or implicit ordinary differential equation (ODE) systems with sensitivity analysis capabilities. It provides both forward and adjoint sensitivity analysis options.

5. Method of solution

Integration is by the BDF method. Corrector iteration is by Newton iteration. For the solution of linear systems within Newton iteration, users can select a dense solver, a band solver, or a preconditioned iterative solver (GMRES, BiCG-Stab, or TFQMR). The IDAS forward sensitivity module implements a simultaneous corrector method and a staggered corrector method. The adjoint sensitivity provides the infrastructure required for the backward integration in time of multiple systems of differential equations dependent on the solution of the original DAEs. It employs a checkpointing scheme for efficient reproduction of forward solutions during the backward integration and provides a choice of either a cubic Hermite or a variable-order polynomial interpolation scheme.

6. Computer(s) for which software is written

IDAS should run on any computer with an ANSI C compiler. The appropriate precision (single, double, or extended) is selected at the configuration phase.

7. Operating system

No system-dependency in the software itself. But installation is system-dependent. The package supplied consists of a single archived file. Installation from this file assumes a system with the tar utility. Configuration is done through a configure script. Compilation of libraries is done by way of makefiles.

8. Programming language(s) used

ANSI C (100%)

9. Software limitations

none

10. Unique features of the software

IDAS is organized in a highly modular manner. The basic integrator and sensitivity modules are separate from, and independent of, the linear system solvers, as well as the vector operation modules. Thus the set of linear solvers can be expanded and the internal vector representation can be replaced with no impact

on the main solver.

11. Related and auxiliary software

IDAS is part of SUNDIALS (Suite of Nonlinear and Differential/Algebraic equation Solvers).

12. Other Programming or Operating Information or Restrictions

none

13. Hardware Requirements

none

14. Time Requirements

Timing is highly dependent on machine and problem.

15. References

Document provided with the distribution

- R. Serban and C. Petra, "User Documentation for IDAS v1.0.0," LLNL technical report UCRL-SM-234051, August 2007.

Additional background references

- A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker, and C. S. Woodward, "SUNDIALS, Suite of Nonlinear and Differential/Algebraic Equation Solvers," ACM Trans. Math. Softw., 31, pp. 363–396, 2005.
- Y. Cao, S. Li, L.R. Petzold, and R. Serban, "Adjoint sensitivity analysis for differential-algebraic equations: the adjoint DAE and its numerical solution," SIAM J. Sci. Comp., 24(3), pp. 1076-1089, 2003.
- T. Maly and L.R. Petzold, "Numerical methods and software for sensitivity analysis of differential-algebraic systems," Appl. Numer. Math., 20, pp. 57-79, 1996
- W.F. Feehery, J.E. Tolsma, and P.I. Barton, "Efficient sensitivity analysis of large- scale differential-algebraic systems," Appl. Numer. Math., 25, pp. 41-54, 1997