Sujet TP1 : SUNDIALS & the Test Set for Initial Value Problems of CWI

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Abstract

The Test Set for Initial Value Problems of CWI represents a source of problems that SUNDIALS, a suite of non linear differential/algebraic equation solvers, can solve. The purpose of this TP is first to explore the capabilities of CVODE and to solve some of the test cases of CWI thanks to the FORTRAN interface to the CVODE solver from SUNDIALS (called FCVODE).

1 Information concerning the reports to write for the session

For the TPs, a report (written in english !!!) answering the questions in pdf format have to be provided. The FORTRAN source codes associated to the different exercises have also to be provided. These must be COMMENTED, DOCUMENTED AND A MAKEFILE FOR THE COMPILATION AND THE LINKING HAVE TO BE WRITTEN. The different outputs of the codes must be clear and self-explaining. Finally, the solution curves must be plotted with GNUPLOT.

2 SUNDIALS and CVODE

2.1 CVODE

SUNDIALS is a solver for non linear differential/algebraic equations written in C. In this work we will focus on CVODE, a solver for stiff and nonstiff ordinary differential equation (ODE) systems (initial value problem) given in explicit form $\frac{\partial y}{\partial t} = f(t, y)$.

To obtain the source code of SUNDIALS, you must go to its home page `http://www.llnl.gov/CASC/sundials/main.html` and download the source code from the whole distribution after having registered.

Describe how you realize the compilation of the distribution with the C and the FORTRAN compilers (icc, and ifort) from intel. The examples and the shared libraries must be compiled.

FCVODE (the FORTRAN interface to the C routines of CVODE) is composed of different kinds of solvers (direct and iterative) for serial and parallel use. Please describe the main process for the resolution of a Initial Value problem, and the different choices you have to solve a dense non linear system (direct/iterative solver) and their different options (methods/preconditionning).

2.2 FCVODE example : fcvdenx.f

In the SUNDIALS distribution some examples written in FORTRAN 77 are given. One of these is the fcvdenx.f. Convert this source code to FORTRAN 90 and remove the statements concerning the root finding.

Change the solver for the GMRES Krylov without preconditionning and compare the solutions found by both solvers.

3 CWI Test Set

At the URL : `http://pitagora.dm.uniba.it/~testset//` you can find the Test Set of Initial Value Problems. Some ODE problems are given under the following form:

- The description of the problem in pdf format.
- The FORTRAN routine containing some subroutines for the evaluation of the right-hand side and the Jacobian. The final solution is also provide to compare the solution found to the real one.

Choose one of them, and give a short description.

The goal is to solve the problem choosen with the FCVODE subroutines with either the direct of the iterative solver of your choice. The produced source code must be written in FORTRAN 90.

Compare your final solution and the real one given in the problem.

Plot the obtained components of the solution corresponding to the ones given on the page of your problem.