LA-UR-76-2298

CONF-760740--1

TITLE: CERTIFICATION OF THE SWARZTRAUBER-SWEET ELLIPTIC PDE SOFTWARE PACKAGE

AUTHOR(S): B. L. BUZBEE

SUBMITTED TO: SPRINGER LECTURE SERIES,
Numerical Treatment of Differential Equations
Meeting, Freiburg, West Germany, July 6-8, 1976.

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

Form No. 836
St. No. 2629

UNITED STATES
ENERGY RESEARCH AND
DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

CERTIFICATION OF THE SWARZTRAUBER-SWEET ELLIPTIC PDE SOFTWARE PACKAGE

by

B. L. Buzbee*

University of California
Los Alamos Scientific Laboratory
Los Alamos, New Mexico, USA

The past ten years have seen the development of efficient direct methods for solving finite difference approximations to the Helmholtz equation on a rectangle with simple boundary conditions, i.e., strictly Dirichlet, Neumann, or periodic on any side. Because these techniques are direct and stable and because the associated class of problems is important, it is practical to incorporate these techniques into on-the-shelf software for general use. Many prospective users of such software are not familiar with the linear systems which result from finite difference approximations. Thus the software should be designed so that the user communicates with it in terms of familiar concepts such as the differential equation to be approximated, the region, mesh sizes, etc. Paul Swarztrauber and Roland Sweet of the National Center for Atmospheric Research in Boulder, Colorado, U.S.A., have developed such a package written in ANSI FORTRAN. The package consists of two nucleus routines and five drivers for various coordinate frames. Basically, the use of this package can be summarized as follows.

1. Choose the coordinate frame of interest and identify the associated driver.
2. Select a mesh and compute the right-hand side at the points of this mesh.
3. Input the discretized right-hand side to the associated driver, along with information describing the boundary conditions and region.

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*This work performed under the auspices of the U.S. Energy Research and Development Administration.

4. In turn, the driver generates the matrix equation corresponding to the finite difference equation that it embodies and proceeds to call the requisite nucleus routine.

5. The solution to the difference equation at all mesh points is returned to the user.

This package is documented in an NCAR report [1]. The report and the associated software are available from NCAR upon request. If you are interested in obtaining either, I will be happy to provide you with the appropriate address.

The report consists of seven chapters. The first five chapters discuss use of the drivers for various coordinate frames; chapters six and seven describe the nucleus routines. All chapters are self-contained in the sense that if one has a problem in Cartesian coordinates he will refer to that chapter only. In addition to describing the use of the driver, each chapter discusses the difference equations used, singular problems, and how to use these drivers in solving three-dimensional problems. Each chapter also contains a sample problem. Let's look now at each of the five drivers.

CHAPTER I — Cartesian Coordinates

The associated equation is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \lambda u = f(x,y) \quad .$$

Permissible boundary conditions are:

Dirichlet, Neumann, or periodic in either x or y.

CHAPTER II — Polar Coordinates

The associated equation is

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + \lambda u = f(r,\theta) \ .$$

Permissible boundary conditions are:

Dirichlet or Neumann in r (r=0 is acceptable and is treated as a special case);
Dirichlet, Neumann, or periodic in θ.

CHAPTER III — Cylindrical Coordinates

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{\partial^2 u}{\partial z^2} + \frac{\lambda}{r^2}u = f(r,z) .$$

Permissible boundary conditions are:

Dirichlet or Neumann in r (r=0 is acceptable and is treated as a special case);
Dirichlet, Neumann or periodic in z.

Note that this is not the standard Helmholtz equation

$$\nabla^2 u + \lambda u = f .$$

In three dimensions, Poisson's equation is:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2} = f(r,\theta,z) .$$

Thus to solve this problem, one does a discrete Fourier transform in the θ-direction, and solves the resulting family of two-dimensional problems with this driver. This explains the choice of the equation in both Chapters III and IV.

CHAPTER IV — Spherical (axisymmetric) Coordinates

The associated equation is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{\lambda}{r^2\sin^2\theta}u = f(\theta,r)$$

where θ is colatitude and r is the radial coordinate.

Permissible boundary conditions are:

Dirichlet or Neumann in r (r=0 is acceptable and is treated as a special case);
Dirichlet or Neumann in θ (θ=0 and θ=π are acceptable and are treated as special cases).

CHAPTER V — Spherical Surface Coordinates

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2} + \lambda u = f(\theta,\phi)$$

where θ is colatitude and ϕ is longitude.

Permissible boundary conditions are:

Dirichlet or Neumann in θ ($\theta=0$ and $\theta=\pi$ are acceptable and are treated as special cases); Dirichlet, Neumann, or periodic in ϕ.

At present, for the five coordinate frame drivers the number of mesh points in the y, θ, z, r, and ϕ directions, respectively, must have the form

$$N = 2^p 3^q 5^r \quad .$$

All other directions are unrestricted, and the above restriction will soon be removed.

This package required four to five man-years to develop and document. Thus, by today's standards, it cost approximately one quarter of a million dollars. Several ERDA laboratories need the capability of solving these types of problems. Adoption of this package by them is an obvious way to fulfill that need, especially in view of the developmental costs, as well as the special expertise required to develop such a package. Consequently, five laboratories are collaborating in testing and evaluating this package. They are:

Laboratory	Test Activity
Air Force Weapons Laboratory Albuquerque, New Mexico	Cartesian Driver
Lawrence Livermore Laboratory Livermore, California	R-θ Driver
Sandia Livermore Laboratory Livermore, California	R-Z Driver
Sandia Albuquerque Laboratory Albuquerque, New Mexico	Spherical Interior Driver
Los Alamos Scientific Laboratory Los Alamos, New Mexico	Spherical Surface Driver

Each laboratory will perform the following on its respective driver:

1. Test with two or three mesh sizes in each direction.
2. For each mesh, test all possible combinations of boundary conditions.

3. For each mesh and each boundary condition, test a zero and nonzero value of the Helmholtz constant.
4. Verify that all error flags work correctly.
5. Report implementation difficulties such as compilation failures.
6. Evaluate the documentation, e.g., sufficient, misleading, incorrect...
7. Run all of the NCAR tests and report the results.

This test list is modest compared to what can and has been done in software certification; for example, we are not investigating the package's robustness by deliberately introducing errors in its usage, nor are we examining its efficiency. Nevertheless, the program outlined above requires several hundred test cases per driver, and is sufficient for us to evaluate the reliability of the software and the adequacy of its documentation.

Our testing is about half complete and we expect to finish it by September of this year. Preliminary results suggest that the package is sound but the testing has pointed out several items that need improvement. Anyone who wishes a copy of the results may get them from me upon request.

REFERENCE

1. P. Swarztrauber and R. Sweet, "Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations," NCAR-TN/IA-109, National Center for Atmospheric Research, Boulder, CO, 1975.

Acknowledgement. This work is being done in collaboration with Marty Havens of the Air Force Weapons Laboratory, Niel Madsen of the Lawrence Livermore Laboratory, Melvin Scott of the Sandia Albuquerque Laboratory, Richard Basinger of the Sandia Livermore Laboratory, and Michael Steuerwalt of the Los Alamos Scientific Laboratory. Their cooperation and effort is essential and much appreciated.