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Certification Report on "Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations"

University of California

LOS ALAMOS SCIENTIFIC LABORATORY
Post Office Box 1663 Los Alamos, New Mexico 87545

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Certification Report on "Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations"

by Paul Swarztrauber and Roland Sweet

National Center For Atmospheric Research

Boulder, Colorado

Michael Steuerwalt

CERTIFICATION REPORT ON "EFFICIENT FORTRAN SUBPROGRAMS FOR THE SOLUTION OF ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS" BY PAUL SWARZTRAUBER AND ROLAND SWEET NATIONAL CENTER FOR ATMOSPHERIC RESEARCH BOULDER, COLORADO

by

Michael Steuerwalt

ABSTRACT

Paul Swarztrauber and Roland Sweet, National Center for Atmospheric Research, have developed a package of subroutines for solving a modified Helmholtz equation with simple boundary conditions on a rectangle in any of five coordinate frames. Because problems of this type arise frequently and because the testing of such a package is not trivial, five federal laboratories collaborated in certifying this package. This report documents the results of the certification effort. Although some difficulties were encountered during testing, the certification team judged the package to be good mathematical software. The team particularly commends its design, which permits users to communicate with it in familiar terms without having to grasp the mechanics of the discretization procedure.

INTRODUCTION

The problem of computing solutions to modified Helmholtz equations (or, more generally, separable linear elliptic equations) with simple boundary conditions on a rectangle in any of several coordinate frames arises frequently in applications and as an intermediate step in the solution of nonlinear and evolution problems. The importance of such problems, together with the recent development of fast direct methods for their solution, moved Paul Swarztrauber and Roland Sweet to develop a package of subroutines for solving them. The package was developed with the support of the National Center for Atmospheric Research (NCAR) between 1973 and 1975.[1]

The cost of developing, documenting, and testing such a package is not negligible. Therefore several federal laboratories that can profitably use the NCAR package chose to collaborate in its certification.

THE PACKAGE

Physically the NCAR package consists of about 4 700 lines of FORTRAN code (almost 40% are comments), 800 lines of example drivers, and 140 pages of documentation. The package cost about $300 000 to develop. In comparison, EISPACK has 11 500 lines of code (49% are comments), 10 000 lines of example drivers, 551 pages of documentation,[2] and cost about $900 000.

The heart of the NCAR package is the two routines POIS and BLKTRI, which solve the linear systems arising from standard second order finite difference approximations of separable elliptic boundary value problems on rectangles. These core routines embody variants of the Buneman direct algorithm, and on a mesh of MxN points do work proportional to $MN \log_2 N$. POIS is a faster but less general version of BLKTRI.

It is a straightforward but tedious, expensive, and error-prone process to develop the discrete system of difference equations from the given boundary value problem. The NCAR package, therefore, includes five drivers that build the discrete system from the least possible information: the differential equation and boundary conditions, the geometric region, and the number of (evenly spaced) mesh points in each direction. Most users will communicate with the core routines only through these drivers. The drivers with their associated equations are:

PWSCRT - Cartesian coordinates

$$u_{xx} + u_{yy} + \lambda u = f \tag{1}$$

PWSPLR - polar coordinates

$$(ru_r)_r/r + u_{\theta\theta}/r^2 + \lambda u = f \tag{2}$$

PWSCYL - cylindrical coordinates

$$(ru_r)_r/r + u_{zz} + \lambda u/r^2 = f \tag{3}$$

PWSCSP - spherical axisymmetric coordinates

$$(r^2 u_r)_r/r^2 + (u_\theta \sin\theta)_\theta/(r^2 \sin\theta) + \lambda u/(r^2 \sin^2\theta) = f \tag{4}$$

PWSSSP - spherical surface coordinates

$$(u_\theta \sin\theta)_\theta/\sin\theta + u_{\phi\phi}/\sin^2\theta + \lambda u = f \tag{5}$$

Note the nonstandard Helmholtz terms in (3) and (4). These terms arise naturally in treating a three-dimensional problem by a Fourier transform in the third variable.

Only PWSCSP calls on BLKTRI; the other drivers used POIS.

Problem restrictions, common to all the drivers, are mild:

- The geometric region must be a logical rectangle.
- On any edge of the region, the boundary condition must be simple: Dirichlet, Neumann, or periodic conditions are acceptable, but not mixed conditions such as $u + \beta u_x = g \quad (\beta \neq 0)$.
- The boundary conditions may be of different type on different edges.

In addition, the algorithms of the package require that the finite difference mesh of MxN panels must be evenly spaced in each direction, and at present that N have the factorization $N = 2^p 3^q 5^r$. Each driver has code to detect improper values of N, as well as certain other possible errors in the input parameters.

THE CERTIFICATION REPORT

Each of the five laboratories that had agreed to collaborate in the certification effort assumed responsibility for a particular driver:

PWSCRT - Air Force Weapons Laboratory, Kirtland Air Force Base, Albuquerque, New Mexico,
PWSPLR - Lawrence Livermore Laboratory, Livermore, California,
PWSCYL - Sandia Laboratories, Livermore, California,
PWSCSP - Sandia Laboratories, Albuquerque, New Mexico,
PWSSSP - Los Alamos Scientific Laboratory, Los Alamos, New Mexico.

Each laboratory agreed to:

(a) Compile the entire package.
(b) Verify the results of the seven NCAR example programs.
(c) Verify the correct working of the input error detection code.
(d) For its particular driver, run a test problem using
- several permissible regions,
- several mesh sizes in each direction,
- all possible boundary conditions,
- zero and nonzero values of λ.

(e) Evaluate the documentation.

It is important to note what we did not try to do:

(a) Explicitly test the core routines POIS and BLKTRI. Access to these routines was through the drivers alone.
(b) Make efficiency tests. The methods of the core routines are among the best direct methods available, but neither the authors nor the certifiers claim that there are no methods more efficient. In particular, we expect that higher order methods would be more efficient for a given (small enough) accuracy.
(c) Make severe tests of the package's robustness.

The schedule outlined above entails a considerable effort. Among the five laboratories there are perhaps 10 different FORTRAN compilers, so the simple compilation of the package is a good test of its portability. The testing implied by (d) is substantial. For example, the driver PWSSSP admits 9 different possible boundary conditions in the θ direction and 5 in the ϕ direction; not all combinations are compatible, and some are valid only for certain geometries. To complete part (d) for the PWSSSP routine, 8 different regions were used with all possible valid boundary conditions, and with 5 different mesh sizes in the θ direction and 4 in the ϕ direction, for a total of 2 360 runs per value of λ. Testing of the other drivers was similar. See Appendix A for details of the test problems.

RESULTS OF THE CERTIFICATION EFFORT

Some difficulties were encountered in the course of the testing effort.

Although the package had passed successfully through several compilers and FORTRAN verifiers before NCAR distributed it to us, it would not compile on some of our compilers. Most of the compilation errors were related to the order of declaration and dimension statements.

The laboratories had at least two different versions of what was purportedly the same package. It was difficult to decide which version was correct because none carried a date or sequence number.

Each of the core routines POIS and BLKTRI performs some preliminary computations that need not be repeated if certain problem parameters remain unchanged. Early versions of the package, therefore, included an initialization parameter INTL in the driver calling sequences to indicate whether these preliminary computations might be skipped. Our testing revealed program errors that could be avoided only by reinitializing every problem. Fortunately, initialization is expensive only for BLKTRI and PWSCSP (its cost is under 1% for the other routines).

In some places the documentation was misleading or incorrect

For instance, where Dirichlet and Neumann conditions are imposed on adjacent edges of the region, one must decide what to do at the mutual corner point. A scrupulous implementation of the decision table provided by the documentation almost invariably leads to wrong answers. The simple statement that Dirichlet conditions always have precedence would have clarified the documentation, which was obscure on this point. Most of the documentation errors, on the other hand, were minor and typographical.

We did perform some testing of the package's robustness. The documentation clearly indicates that certain choices of boundary conditions are incompatible with particular geometries. For instance, in PWSSSP, three possible choices of the boundary condition at the final value of TF of θ require that TF = π. A sample problem was run with these choices of boundary condition but with TF < π. The package did not check for such illegal combinations, but simply computed--occasionally attempting to divide by zero, and always producing wrong answers.

All the difficulties we encountered were reported to Swarztrauber and Sweet (see Appendixes B-E), along with suggested corrections and changes. We think it is rather remarkable that <u>all</u> the changes we recommended have been incorporated into the new version of the package--which is prominently labeled version 2. We suspect that this is attributable more to the authors' good natures than to any collective wisdom on the part of the certification group.

Two changes in particular require comment. First, Swarztrauber and Sweet have chosen to handle the initialization problem by <u>always</u> doing the preliminary computations in POIS and the four drivers that call on it (PWSCRT, PWSPLR, PWSCYL, PWSSSP); INTL has been retained as a dummy parameter in the calling sequences of these routines to avoid disturbing an already large group of users. The option to skip the preliminary computations has been kept in BLKTRI and PWSCSP, where initialization is expensive; here INTL is not a dummy parameter.

Second, code has been added to the drivers to check illegal combinations of regions and boundary conditions. The drivers will compute, but will set an error flag if, say, $|TF-\pi|$ is "too large." We feel that the package's robustness is well enhanced by including this check, which has been done in a portable way and at little computing expense. On the other hand, we should remark that Swarztrauber and Sweet have indicated to us some uneasiness regarding the introduction of the imprecise and machine-dependent notion of "too large," and that no package, whatever its robustness or quality of documentation may be, can protect a user bent on self-immolation.

The documentation is neither so exhaustive as the EISPACK guide nor so rich in examples of the routines' uses. This is no handicap: use of the NCAR routines is straightforward, whereas EISPACK provides several options for doing many computations.

Version 2 of the package has been checked by the five laboratories to verify that all our suggestions have not improved it out of working order. We deem the package to be valuable software of good quality. We especially commend its design, which permits users to communicate with it in familiar terms so that they do not have to grasp the mechanics of the discretization procedure. We believe the documentation will help that user who only wants answers to his problems to get those answers while remaining in blissful ignorance of details peripheral to his interests.

ACKNOWLEDGMENTS

This work was done in collaboration with Martin Havens, Air Force Weapons Laboratory, Kirtland Air Force Base, Albuquerque, New Mexico; Niel Madsen, Lawrence Livermore Laboratory, Livermore, California; Melvin Scott and Alex Treadway, Sandia Laboratories, Albuquerque, New Mexico; Richard Basinger, Sandia Laboratories, Livermore, California; and Bill Buzbee, Los Alamos Scientific Laboratory, Los Alamos, New Mexico.

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1. P. Swarztrauber and R. Sweet, "Efficient FORTRAN Subprograms

for the Solution of Elliptic Partial Differential Equations," National Center for Atmospheric Research report NCAR-TN/1A-109, (1975).

2. B. T. Smith, J. M. Boyle, J. J. Dongarra, B. S. Garbow, Y. Ikebe, V. C. Klema, and C. B. Moler, Matrix Eigensystem Routines - EISPACK GUIDE, 2nd ed., Lecture Notes in Computer Science 6 (Springer-Verlag, New York, 1976).

APPENDIX A

DETAILS OF THE TEST PROBLEMS

Each driver may distinguish types of regions according to the geometry of the problem. Some combinations of boundary conditions and regions are not admissible. In this appendix we tabulate the valid combinations for each driver; in these tables the entry - indicates no legal combination. We also list the intervals whose Cartesian products form the regions used in the certification tests, and give the true solution u of the various boundary value problems. The appropriate boundary values and the function f can be determined for a given problem from u, λ, and the region. For all problems the values of λ, M, and N used were:

λ :	0.0	-1.0			
M :	9	18	36	72	144
N :	15	30	45	60	

PWSCRT

All 25 possible combinations of MBDCND and NBDCND are valid. The two regions used were

$$[A,B] = [-\frac{1}{2},\frac{1}{2}]$$

$$[C,D] = [-\frac{1}{2},\frac{1}{2}] \qquad [0,2] \quad .$$

The true solution was

$$u = \sin 2\pi(x + \frac{1}{8}) \cos 2\pi(y + \frac{1}{8}).$$

PWSPLR

This driver distinguishes two types of regions:

$0 < A$	P
$0 = A$	Z

The compatibility table has 34 entries:

MBDCND	NBDCND 0	1	2	3	4
1	PZ	PZ	PZ	PZ	PZ
2	PZ	PZ	PZ	PZ	PZ
3	P	P	P	P	P
4	P	P	P	P	P
5	Z	-	-	Z	-
6	Z	-	-	Z	-

The four regions used were

$$[A,B] = \quad [-\frac{1}{4},1] \qquad [0,1]$$

$$[C,D] = \quad [0,2\pi/3] \qquad [2\pi,8\pi/3] \quad .$$

The true solution was

$$u = r^3 \cos(\frac{4\pi}{D-C}\theta + \frac{\pi}{4}).$$

PWSCYL

This driver distinguishes two types of regions:

$0 < A$	P
$0 = A$	Z

The compatibility table has 40 entries:

MBDCND	NBDCND 0	1	2	3	4
1	PZ	PZ	PZ	PZ	PZ
2	PZ	PZ	PZ	PZ	PZ
3	P	P	P	P	P
4	P	P	P	P	P
5	Z	Z	Z	Z	Z
6	Z	Z	Z	Z	Z

Two regions were used:

$[A,B] = \quad [1,2] \qquad [0,1]$

$[C,D] = \quad [0,2\pi]$

The true solution was

$$u = r^2 \cos(z + \frac{\pi}{4}).$$

<u>PWSCSP</u>

This driver recognizes eight types of regions:

	$0 < RS$	$0 = RS$
$0 < TS,\ TF < \pi$	A	E
$0 = TS,\ TF < \pi$	B	F
$0 < TS,\ TF = \pi$	C	G
$0 = TS,\ TF = \pi$	D	H

The compatibility table has 72 entries:

MBDCND \ NBDCND	1	2	3	4	5	6
1	ABCD	ABCD	ABCD	ABCD	-	-
2	AB	AB	AB	AB	-	-
3	A	A	A	A	E	E
4	AC	AC	AC	AC	-	-
5	BD	BD	BD	BD	-	-
6	B	B	B	B	F	F
7	CD	CD	CD	CD	-	-
8	C	C	C	C	G	G
9	D	D	D	D	H	H

Eight regions were used:

[TS,TF] = $[-\frac{\pi}{4},\frac{\pi}{2}]$ $[0,\frac{\pi}{2}]$ $[\frac{\pi}{2},\pi]$ $[0,\pi]$

[RS,RF] = [1,2] [0,1]

The true solution was

$$u = r^4 \cos^4 \theta .$$

PWSSSP

This driver distinguishes four types of regions:

$0 < TS, TF < \pi$	A
$0 = TS, TF < \pi$	B
$0 < TS, TF = \pi$	C
$0 = TS, TF = \pi$	D

There are 59 entries in the compatibility table:

MBDCND	NBDCND 0	1	2	3	4
1	ABCD	ABCD	ABCD	ABCD	ABCD
2	AB	AB	AB	AB	AB
3	A	A	A	A	A
4	AC	AC	AC	AC	AC
5	BD	-	-	BD	-
6	B	-	-	B	-
7	CD	-	-	CD	-
8	C	-	-	C	-
9	D	-	-	D	-

The tests used eight regions:

$[TS,TF] = [\frac{\pi}{4},\frac{\pi}{2}] \quad [0,\frac{\pi}{2}] \quad [\frac{\pi}{2},\pi] \quad [0,\pi]$

$[PS,PF] = [\frac{\pi}{2},\frac{3\pi}{2}] \quad [0,2\pi]$

The true solution was

$u = \sin^2 \theta \cos 2\phi.$

APPENDIX B

LETTER TO P. SWARZTRAUBER FROM B. BUZBEE, SEPTEMBER 8, 1976

The certification of your Poisson package is nearing completion and our preliminary results show that some corrections need to be made to the package. The required corrections are enumerated below.

MAJOR CONCERNS

1. In the process of testing the package we discovered that at least two laboratories had different versions of it. We strongly

urge you to incorporate version numbers into the package so that users can determine which one they have.

2. Specification of the input content of array F(I,J) is ambiguous at the corners and must be clarified. Careful implementation of the documentation as written on this matter will usually yield incorrect results.

3. A list of untested internal error flags is attached.

4. The input parameter INTL does not work as advertised and its merit is questionable in some cases.

5. A nonzero value in the output parameter PERTRB is the only indication of a singular problem. Some remark about normalization of the computed solution would be useful. Also, no guidance is given as to when the user should become concerned about the magnitude of this parameter.

6. The routines do not check for illegal boundary conditions with respect to some geometric regions (e.g., for PWSSSP, MBDCND in {7,8,9} is illegal if $TF \neq \pi$), but simply go ahead and compute--sometimes producing a zero divisor in TRID, and always producing wrong answers.

SECONDARY CONSIDERATIONS

1. The equations of Chapters 3 and 4 are not Helmholtz, i.e., Helmholtz means

$$\Delta^2 u + \lambda u = f$$

We suggest the term "modified Helmholtz" as well as some discussion at the beginning of each chapter indicating why this particular form was chosen.

2. Most chapters include a list of entry points, some of which are unknown to the user. We suggest that you replace this list by a list of subroutines required from the package by the driver.

3. A list of unreferenced variables is attached.

4. Type statements should appear before DIMENSION statements; at least one version of the package would not compile until this ordering was accomplished.

5. One version did not include IERROR=11. See attached note from Scott.

In general, we find that your package is a good piece of mathematical software. The above corrections should increase its value to most prospective users.

APPENDIX C

LETTER TO B. BUZBEE FROM P. SWARZTRAUBER, OCTOBER 15, 1976

In responding to your report we are repeating your concerns and following each with our response.

1. In the process of testing the package we discovered that at least two laboratories had different versions of it. We strongly urge you to incorporate version numbers into the package so that users can determine which one they have.

Each major program now contains a header which includes the version number (2), date, date of errata, cross reference to the documentation, and the origin of the package.

2. Specification of the input content of array F(I,J) is ambiguous at the corners and must be clarified. Careful implementation of the documentation as written on this matter will usually yield incorrect results.

The errata will contain an underlined note which removes the ambiguity at the corner; see errata number 5.

3. A list of untested internal error flags is attached.

It is unnecessary to test the internal error flags since the errors reported by these flags would have been detected earlier. For example, in SUBROUTINE PWSCS1, following statement number 375, the parameter, IERROR, is not tested. The reason is that either the appropriate error tests have been made earlier in SUBROUTINE PWSCSP or it is known that for the particular problem of solving the Poisson equation on the interior of the sphere that a particular error (in this case IERROR=4 in BLKTRI) will not occur.

4. The input parameter INTL does not work as advertised and its merit is questionable in some cases.

The use of INTL has been essentially eliminated from the drivers with the exception of PWSCSP and BLKTRI where initialization takes a significant portion of the computing time. In addition these programs have been corrected so that they function as described in the documentation. Also, in one case, the documentation has been corrected; see errata number 20.

5. A nonzero value in the output parameter, PERTRB, is the only indication of a singular problem. Some remark about normalization of the computed solution would be useful. Also, no guidance is given as to when the user should become concerned about the magnitude of this parameter.

Errata number 7 indicates that PERTRB should be small with respect to the right side F and stresses the importance of making this comparison. It also indicates that the solution is not normalized. The reason is that it would require an increase in computing with no apparent value to geophysical scientists.

6. The routines do not check for illegal boundary conditions with respect to some geometric regions (e.g., for PWSSSP, MBDCND in [7,8,9] is illegal if TF $\neq \pi$), but simply go ahead and compute--sometimes producing a zero divisor in TRID and always producing wrong answers.

We discussed this concept at considerable length when the package was in its initial design phase. The question at that time was whether to test for the condition of TS=0, TS=π, or RS=0 or to have the user specify that those conditions existed by adding additional options to the boundary value parameters MBDCND,NBDCND. Due to the difficulty of testing whether TF=π or not, or for that matter when TS=0, it was decided to introduce these options at the expense of making the description of the parameters somewhat more complex. However, in recognition of the difficulty outlined in (6) above, the documentation included additional guidance in the use of these boundary options. For example, on page 61, if the user anticipates using a derivative boundary condition (such as MBDCND=3), he is directed to a note which, in turn, leads to an alternate boundary condition if TF=0.

Additional secondary considerations:

1. The equations of Chapters 3 and 4 are not Helmholtz; i.e., Helmholtz means

$$\Delta^2 u + \lambda u = f$$

We suggest the term "modified Helmholtz" as well as some discussion at the beginning of each chapter indicating why this particular form was chosen.

See errata numbers 1, 2, 11, 12.

2. Most chapters include a list of entry points, some of which are unknown to the user. We suggest that you replace this list by a list of subroutines required from the package by the driver.

See errata numbers 6, 17, 33. The entry points also advise the user of any conflict in program names.

3. A list of unreferenced variables is attached.

These variables have been deleted.

4. Type statements should appear before DIMENSION statements; at least one version of the package would not compile until this ordering was accomplished.

This reordering has been done.

5. One version did not include IERROR=11.

This has been corrected.

APPENDIX D

LETTER TO P. SWARZTRAUBER FROM M. STEUERWALT, DECEMBER 9, 1976

We have several remarks concerning your responses to our letter of September 8.

Response 4. Does this change the calling sequence in any of the drivers? Such a change might be expected, but the list of errata doesn't reflect this.

Response 5. We would like the documentation to include some further remark about the distinction between normalized and unnormalized solutions.

Response 6. This is a good example of the tension between a desideratum and its implementation. We agree with your remarks about the practical difficulties of implementing the boundary condition checks. On the other hand, the package's robustness may be well enhanced by the addition of another value to the error flag IERROR, indicating the untrustworthiness of the computer answer for certain combinations of geometry and boundary condition if, say, $|TF-\pi|$ is "too large." The addition of this test would not be a significant programming expense; counterbalancing the expense, however trivial, is the fact that no package, whatever its robustness or quality of documentation may be, can protect a user bent on self-immolation.

Secondary 2. The documentation uses the term "entry points" where the meaning intended is "package subroutines used." This is a confusing use of a well defined Fortran term. We suggest the alternate phrase "subroutines used" on pages 5, 23, 43, 66, 86, 98, 117.

Erratum 16. This change requires corresponding alterations on page 77, analogous to those of errata 29-30 and 37-38.

Implementation of our suggestion regarding boundary condition checks may require that you add to the package a routine that computes a particular machine-dependent number (usually called macheps). Portable routines of this kind exist. Simple, mildly nonportable alternatives are available.

Except for these points, the five laboratories involved in the testing agree that the questions we raised have all been well answered. Verification of the final changes in the package should go quite smoothly, once you send us the latest version.

APPENDIX E

LETTER TO M. STEUERWALT FROM P. SWARZTRAUBER, DECEMBER 22, 1976

This letter is in response to your letter dated December 9, 1976. The new errata list is attached.

Response 4. The vestigial parameter INTL remains in the list so that current users will not have to modify their programs. Any changes between version 1 and 2 were intended to require no modifications of the user program.

Response 5. If we had been able to determine a description of the "unnormalization" which was satisfactory to us, we would have included it. Instead, we merely state: "This solution plus any constant is also a solution; hence, the solution is not unique. See errata number 7.

Response 6. Although we are somewhat uneasy about the implementation of this recommendation, it now exists in version 2. See errata numbers 19 and 27. We also recognize the value of this error detection and we are optimistic that in at least 99.9% of the cases, the test will function correctly.

If an error is incorrectly sensed, a solution will still be obtained since the error is issued only as a warning. Nevertheless, in this unlikely event, the user will probably be somewhat confused.

Secondary 2. This suggestion has been implemented. See errata number 8.

Erratum 16. This has been corrected. See errata 24.