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The NASTI User's Manual

P. W. Gaffney

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THE NASTI USER'S MANUAL

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TABLE OF CONTENTS

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The NASTI User's Manual

P. W. Gaffney

ABSTRACT

The purpose of this report is to explain how to use the NASTI data base. Specifically, NASTI is a Numerical Analysis Software Tutorial Inquirer. It is an interactive program which is designed to inform computer users of some of the state-of-the-art mathematical routines that exist at Oak Ridge. The information that is provided by NASTI is intended to help users, with mathematical problems, to make the correct choice of a numerical routine. Moreover, in addition to providing help to these users, NASTI is designed to reduce the possibility of acquiring software that already exists at Oak Ridge. This is an important feature of NASTI and members of all divisions at Oak Ridge are urged to consult NASTI before acquiring mathematical subroutines.

1. INTRODUCTION

The purpose of this report is to explain how to use the NASTI data base. Specifically, NASTI is a Numerical Analysis Software Tutorial Inquirer. It is an interactive program which is designed to inform computer users of some of the state-of-the-art mathematical routines that exist at Oak Ridge. Moreover, for each problem area, NASTI presents the author's ranking of the three subroutine libraries HARWELL, IMSL and NAG.

At present NASTI contains information on approximately eighty routines. Consequently, a number of quality routines are not described in NASTI. However, since NASTI is continually being updated, it is intended that the number of such omissions will be minimized.

The information that is provided by NASTI is a shorter version of that contained in the report, "Information and Advice on the Numerical Software Available for the Fusion Energy Program at Oak Ridge," by P. W. Gaffney, ORNL/CSD/TM-93. Consequently, users are encouraged to consult this report and/or to contact the author for a detailed description of the software and advice on its use. In addition to providing help to users, NASTI is designed to reduce the possibility of acquiring software that already exists at Oak Ridge. Therefore, members of all divisions at Oak Ridge are urged to consult NASTI before acquiring mathematical routines. However, if a particular routine is not listed in NASTI, then it is advisable to search alternative sources (for example, the Key Word Index of Numerical Software by M. T. Heath) before acquiring any routines.

The heart of NASTI is a data base which is managed by the System 1022 Data Base Management System.[1] Therefore, it is advisable, though not necessary, to have some knowledge of the 1022 system before using NASTI. In Section 2, we describe how to use NASTI. In Section 3, we explain how the information on the mathematical routines is organized within NASTI. In Appendix A, we list the reports that can be used with NASTI. Finally, in Appendix B we list the abbreviations that are used in NASTI.

2. HOW TO USE NASTI

Introduction

In this section we describe how to use NASTI. To do this we have used some examples of situations where NASTI may be applied. However, in order to realize the full potential of the System 1022 Data Base Management System, users are urged to consult the 1022 manual.

To Begin a Session with NASTI

NASTI is available through the PDP-10 computers at X-10 and Y-12. On the FED PDP-10, NASTI is available on DSKB while on the X-10 PDP-10, it is available on DSKD. Therefore, in order to commence a NASTI session, a user must log on to at least one of these machines. When this is accomplished, the commands

```
R 1022
OPEN NASTI[200,23000]          On FED PDP-10
     or
OPEN NASTI[6137,463]           On X-10 PDP-10
```

will open the data base in preparation for examination.

Examining NASTI

When the data base has been opened, a user has a number of ways of obtaining information from NASTI. The most common and recommended way is to search for the routines in a particular problem area. A list of the problem areas allowed by NASTI may be obtained, at the user's terminal, by typing the command:

USE NASTI.PRB[200,23000] On FED PDP-10

USE NASTI.PRB[6137,463] On X-10 PDP-10

An example of the output generated by this command is shown in Figure 1. In addition to the problem areas the figure also shows the number of routines that are listed under each problem area. Thus, it can be seen that there are still many areas which lack quality numerical routines. NASTI will be updated when appropriate routines are available for these areas.

NASTI PROBLEM AREAS DATE = MAY 31, 1979

83 RECS FOUND.

APPROXIMATION OF SPECIAL FUNCTIONS	(1)
COMPLEX ARITHMETIC	(3)
CURVE AND SURFACE FITTING	(3)
DETERMINANTS	(1)
EIGENVALUES AND EIGENVECTORS	(4)
INTEGRAL EQUATIONS	(2)
INTERPOLATION	(5)
MATRIX OPERATIONS	(1)
MESH GENERATORS	(1)
MINIMIZING OR MAXIMIZING A FUNCTION	(5)
MULTIPLE PRECISION ROUTINES	(1)
NUMERICAL DIFFERENTIATION	(1)
ORDINARY DIFFERENTIAL EQUATIONS	(18)
PARTIAL DIFFERENTIAL EQUATIONS	(11)
QUADRATURE	(3)
ROOTS OF ONE OR MORE TRANSCENDENTAL EQUATIONS	(3)
SIMULTANEOUS LINEAR EQUATIONS	(13)
SOFTWARE TOOLS	(4)
STATISTICS	(1)
SUMMATION OF SERIES	(1)
ZEROS OF POLYNOMIALS	(1)

Figure 1. Output from NASTI.PRB

When the following command

FIND PROBLEM "PROBLEM AREA"

is issued, all of the routines that are listed under the problem area "PROBLEM AREA" are selected in preparation for (i) output and/or (ii) further searching.

(i) OUTPUT

If at this stage the user wishes to see the names of the selected routines, then the command:

TYPE NAME

may be used to produce, at the user's terminal, a list of the names of all of the routines in "PROBLEM AREA". Alternatively, either of the commands

USE NASTI.TYP[200,23000]	On FED PDP-10
USE NASTI.TYP[6137,463]	*On X-10 PDP-10*

or

USE NASTI.FIL[200,23000]	On FED PDP-10
USE NASTI.FIL[6137,463]	*On X-10 PDP-10*

will produce a report which contains all of the information about all of the routines in the currently selected "PROBLEM AREA". The difference between the above two commands is that NASTI.TYP types this information at the user's terminal and NASTI.FIL generates a file, called NASTI.OUT, which contains the information. In order to see the result of one of these commands, say NASTI.FIL, we consider a simple example.

EXAMPLE 1

Suppose that a user wishes to inquire about the routines in the problem area QUADRATURE. Then, the following commands:

```
R 1022
OPEN NASTI[200,23000]
FIND PROBLEM "QUADRATURE"
USE NASTI.FIL[200,23000]
```

will produce the file NASTI.OUT in the user's area on the PDP-10 at Y-12. This file is shown in Figure 2.

```
      THE NUMERICAL ANALYSIS SOFTWARE TUTORIAL INQUIRER...NASTI

   *** THE LAST UPDATE OF NASTI OCCURRED ON THE 29TH. MAY 1979 ***

 FOR FURTHER INFORMATION PLEASE CONTACT P.W.GAFFNEY, TELEPHONE: 4-0630


       THE FOLLOWING SUBROUTINE LIBRARIES HAVE BEEN RANKED,
       BY THE AUTHOR, FOR THE PROBLEM AREA:

       QUADRATURE

                          1.  NAG
                          2.  HARWELL
                          3.  IMSL

SOME ADDITIONAL SOFTWARE AVAILABLE AT OAK RIDGE:


NAME    = QAGS
PURPOSE = COMPUTES THE INTEGRAL FROM A TO B OF F(X) WHERE A AND B ARE
          FINITE NUMBERS.
PROBLEM = QUADRATURE
METHOD  = NON-LINEAR EXTRAPOLATION TECHNIQUE BASED ON THE EPSILON
          ALGORITHM
ORIGIN  = QUADPACK
VERSION = JANUARY  1, 1979


NAME    = QAINF
PURPOSE = COMPUTES THE INTEGRAL FROM A TO B OF F(X) WHERE A AND/OR B
          MAY BE INFINITE.
PROBLEM = QUADRATURE
METHOD  = NON-LINEAR EXTRAPOLATION TECHNIQUE BASED ON THE EPSILON
          ALGORITHM
ORIGIN  = QUADPACK
VERSION = JANUARY  1, 1979


NAME    = QUANC8
PURPOSE = ADAPTIVE QUADRATURE ROUTINE FOR APPROXIMATING THE INTEGRAL
          FROM A TO B OF F(X).DEPENDING ON THE ACCURACY REQUIRED A
          LARGE NUMBER OF FUNCTION EVALUATIONS MAY BE USED TO COMPUTE
          THE INTEGRAL, SO BEWARE
PROBLEM = QUADRATURE
METHOD  = NEWTON COTES 8-PANEL RULE
ORIGIN  = FMM(J.LYNESS)
VERSION = JANUARY  1, 1978


FURTHER SOURCES:

1.   THE REPORT ORNL/CSD/TM-93 ENTITLED
     "INFORMATION AND ADVICE ON THE NUMERICAL SOFTWARE AVAILABLE
      FOR THE FUSION ENERGY PROGRAM AT OAK RIDGE" BY P.W.GAFFNEY

2.   "THE KEY WORD INDEX OF NUMERICAL SOFTWARE" BY M.T.HEATH

   *** END OF NASTI REPORT ***
```

Figure 2. NASTI.OUT for Example 1

Figure 2 shows that the file NASTI.OUT also contains information about the subroutine libraries that are suitable for the problem area. These are ranked according to the author's recommendations. Figure 2 also provides an example of one of the abbreviations, namely FMM, which is employed in NASTI. A complete list of these abbreviations together with their meanings is given in Appendix A.

(ii) FURTHER SEARCHING

After a FIND command, a user may wish to continue to search the selected records. In this case the SEARCH command in combination with the operator CONTAINS, which may be abbreviated to CT, is very useful. To see this, consider the following example.

EXAMPLE 2

Suppose that a user wishes to know the available routines for ordinary differential equations. Then, the following commands

```
R 1022
OPEN NASTI[200,23000]
FIND PROBLEM "ORDINARY DIFFERENTIAL EQUATIONS"
```

will produce the message that there are 18 routines in this problem area. Now suppose that the user wishes to know the names of those routines which use a Runge-Kutta method. In this case the user can type the command:

```
SEARCH METHOD CT "RUNGE"
```

to select those records which contain the word RUNGE in the description of METHOD, and then

```
TYPE NAME
```

to obtain the names:

```
RKF45
GERK .
```

As before, the command,

```
USE NASTI.FIL[200,23000]
```

will generate a file called NASTI.OUT for the currently selected records. Thus, in this case it contains information about the subroutine libraries for the problem area ORDINARY DIFFERENTIAL EQUATIONS and the additional software RKF45 and GERK (see Figure 3).

TERMINATING A NASTI SESSION

To terminate a NASTI session, type the command:

```
QUIT .
```

```
      THE NUMERICAL ANALYSIS SOFTWARE TUTORIAL INQUIRER...NASTI

   *** THE LAST UPDATE OF NASTI OCCURRED ON THE 29TH. MAY 1979 ***

 FOR FURTHER INFORMATION PLEASE CONTACT P.W.GAFFNEY, TELEPHONE: 4-0630


       THE FOLLOWING SUBROUTINE LIBRARIES HAVE BEEN RANKED,
       BY THE AUTHOR, FOR THE PROBLEM AREA:

       ORDINARY DIFFERENTIAL EQUATIONS

                              1.  NAG
                              2.  IMSL

SOME ADDITIONAL SOFTWARE AVAILABLE AT OAK RIDGE:


NAME    = GERK
PURPOSE = INTEGRATES A SYSTEM OF N FIRST ORDER ORDINARY DIFFERENTIAL
          EQUATIONS GIVEN INITIAL CONDITIONS. PROVIDES A RELIABLE AND
          EFFICIENT ESTIMATE OF THE GLOBAL ERROR IN THE SOLUTION
          RETURNED.
PROBLEM = ORDINARY DIFFERENTIAL EQUATIONS
METHOD  = RUNGE-KUTTA-FEHLBERG(4-5) WITH STEPSIZE CONTROL AND GLOBAL
          ERROR
ORIGIN  = SHAMPINE,WATTS
VERSION = JULY  1, 1978


NAME    = RKF45
PURPOSE = INTEGRATES A SYSTEM OF N FIRST ORDER ODES GIVEN INITIAL
          CONDITIONS. SHOULD NOT BE USED IF THE RIGHT HAND SIDE OF THE
          ODES IS EXPENSIVE TO EVALUATE AND/OR HIGH ACCURACY IS
          REQUESTED.
PROBLEM = ORDINARY DIFFERENTIAL EQUATIONS
METHOD  = RUNGE-KUTTA-FEHLBERG(4-5) WITH STEPSIZE CONTROL
ORIGIN  = FMM
VERSION = JANUARY  1, 1978


FURTHER SOURCES:

1.   THE REPORT ORNL/CSD/TM-93 ENTITLED
     "INFORMATION AND ADVICE ON THE NUMERICAL SOFTWARE AVAILABLE
      FOR THE FUSION ENERGY PROGRAM AT OAK RIDGE" BY P.W.GAFFNEY


2.   "THE KEY WORD INDEX OF NUMERICAL SOFTWARE" BY M.T.HEATH

   *** END OF NASTI REPORT ***
```

Figure 3. NASTI.OUT for Example 2

3. NASTI DESIGN

The Organization of Information Within NASTI

In this section we describe how the information on numerical software is organized within NASTI. To do this, we recall that NASTI is managed by the System 1022 data base management system. Therefore, there are 'attributes' associated with each piece of information that is stored in NASTI. We have defined six attributes for each item of software. These attributes are described in the following table.

Table 1. NASTI Attributes

ATTRIBUTE	DESCRIPTION
NAME	The name that is commonly associated with the software.
PURPOSE	A short description of the software and some brief advice on its use.
PROBLEM*	The problem area under which the software is listed.
METHOD	The numerical method that is used by the software.
ORIGIN	The origin of the software.
VERSION	The approximate date that the software was received in Oak Ridge.

The table shows that PROBLEM is a keyed attribute. This means that the data base can be scanned rapidly by the command

FIND PROBLEM "PROBLEM NAME" .

---

*Keyed Attribute.

Alternatively, it may be examined by using the command:

SEARCH ATTRIBUTE "ATTRIBUTE NAME".

However, in this case the SEARCH command must be preceded by a FIND command, for example:

FIND ALL

SEARCH NAME "RKF45" .

In most cases the attribute PURPOSE contains some brief advice on the correct use of the routine. For further information and advice, users should consult the report by Gaffney.[2]

REFERENCES

1. "System 1022 Data Base Management System," Software House, Cambridge, Massachusetts 02138

2. "Information and Advice on the Numerical Software Available for the Fusion Energy Program at Oak Ridge," P. W. Gaffney, ORNL/CSD/TM-93, June 1979.

APPENDIX A. NASTI Reports

In this appendix, we provide the data programming language listings of the reports that we have written for NASTI. We believe that these listings may be useful to users creating data bases with the 1022 system. Consequently, in general, NASTI users may skip this section.

NASTI.PRB

NASTI.PRB can be used to obtain the problem areas that are allowed by NASTI. A listing of NASTI.PRB is shown in Figure 4.

```
 TYPE SYSDATE FMT // 5T  ' NASTI PROBLEM AREAS     DATE = ' D1 / END.
FIND ALL.
VALUES PROBLEM.
```

Figure 4. NASTI.PRB

NASTI.FIL

NASTI.FIL is the main report that can be used to obtain information from NASTI. This information is given in the disk file NASTI.OUT. A listing of NASTI.FIL is shown in Figure 5.

```
REPORT START.
SECTION INITIAL.
LET FLAG EQ 0.
SORT BY NAME.
INIT 1 NASTI.OUT.
SECTION GETREC.
GETREC ENDS.
SECTION HEADING.
ON START PRINT FMT / 7T ' THE NUMERICAL ANALYSIS SOFTWARE TUTORIAL INQUIRER...NASTI ' //
 5T '*** THE LAST UPDATE OF NASTI OCCURRED ON THE 29TH. MAY 1979 ***' //
 2T ' FOR FURTHER INFORMATION PLEASE CONTACT P.W.GAFFNEY, TELEPHONE: 4-0630'// END.
IF FLAG EQ 1 THEN BEGIN.
IF PROBLEM EQ "MULTIPLE PRECISION ROUTINES" THEN NOSUB.
IF PROBLEM EQ "SOFTWARE TOOLS" THEN NOSUB.
IF PROBLEM EQ "MESH GENERATORS" THEN NOSUB.
PRINT PROBLEM FMT // 8T ' THE FOLLOWING SUBROUTINE LIBRARIES HAVE BEEN RANKED,'
/ 8T ' BY THE AUTHOR, FOR THE PROBLEM AREA:' // 9T A  / END.
IF PROBLEM EQ "COMPLEX ARITHMETIC" THEN S1.
IF PROBLEM EQ "ZEROS OF POLYNOMIALS" THEN S2.
IF PROBLEM EQ "ROOTS OF ONE OR MORE TRANSCENDENTAL EQUATIONS" THEN S3.
IF PROBLEM EQ "SUMMATION OF SERIES" THEN S3.
IF PROBLEM EQ "QUADRATURE" THEN S3.
IF PROBLEM EQ "ORDINARY DIFFERENTIAL EQUATIONS" THEN S4.
IF PROBLEM EQ "PARTIAL DIFFERENTIAL EQUATIONS" THEN S1.
IF PROBLEM EQ "NUMERICAL DIFFERENTIATION" THEN S1.
IF PROBLEM EQ "INTEGRAL EQUATIONS" THEN S1.
IF PROBLEM EQ "INTERPOLATION" THEN S3.
IF PROBLEM EQ "CURVE AND SURFACE FITTING" THEN S3.
IF PROBLEM EQ "MINIMIZING OR MAXIMIZING A FUNCTION" THEN S5.
IF PROBLEM EQ "MATRIX OPERATIONS" THEN S13.
IF PROBLEM EQ "EIGENVALUES AND EIGENVECTORS" THEN S6.
IF PROBLEM EQ "DETERMINANTS" THEN S15.
IF PROBLEM EQ "SIMULTANEOUS LINEAR EQUATIONS" THEN S3.
IF PROBLEM EQ "STATISTICS" THEN S17.
IF PROBLEM EQ "APPROXIMATION OF SPECIAL FUNCTIONS" THEN S6.
```

Figure 5. NASTI.FIL

```
GOTO ADD.
S1: PRINT FMT 30T '1.  NAG '  / END.
GOTO ADD.
S2: PRINT FMT 30T '1.  IMSL' / 30T '2.  HARWELL' / 30T '3.  NAG' / END.
GOTO NOADD.
S3: PRINT FMT 30T '1.  NAG' / 30T '2.  HARWELL' / 30T '3.  IMSL' / END.
GOTO ADD.
S4: PRINT FMT 30T '1.  NAG' / 30T '2.  IMSL' / END.
GOTO ADD.
S5: PRINT FMT 30T '1.  NAG' / 30T '2.  HARWELL' / END.
GOTO ADD.
S6: PRINT FMT 30T '1.  NAG' / 30T '2.  IMSL' / 30T '3.  HARWELL' / END.
GOTO ADD.
S13: PRINT FMT 30T '1.  NAG' / 30T '2.  HARWELL' / 30T '3.  IMSL' END.
GOTO NOADD.
S15: PRINT FMT 30T '1.  NAG' / 30T '2.  IMSL' / 30T '3.  HARWELL' END.
GOTO NOADD.
S17: PRINT FMT 30T '1.  IMSL' / 30T '2.  NAG' / END.
NOADD: PRINT FMT / 2T ' NO ADDITIONAL SOFTWARE AT PRESENT. ' / END.
GOTO ENDS.
ADD: PRINT FMT / 2T 'SOME ADDITIONAL SOFTWARE AVAILABLE AT OAK RIDGE:'
 // END.
NOSUB: LET FLAG EQ 1.
BEGIN: SECTION PRINT.
PRINT NAME PURPOSE PROBLEM METHOD ORIGIN VERSION FMT ' NAME    = ' A /
 ' PURPOSE = ' S60 / ' PROBLEM = ' S60 / ' METHOD  = ' S60 /
' ORIGIN  = ' A / ' VERSION = ' D1 // END.
ENDS: SECTION TOTALS.
ON END PRINT FMT / 2T 'FURTHER SOURCES:' // 2T '1.   THE REPORT ORNL/CSD/TM-93 ENTITLED ' /
7T '^"INFORMATION AND ADVICE ON THE NUMERICAL SOFTWARE AVAILABLE ' /
8T 'FOR THE FUSION ENERGY PROGRAM AT OAK RIDGE^" BY P.W.GAFFNEY ' /
// 2T '2.   ^"THE KEY WORD INDEX OF NUMERICAL SOFTWARE^" BY M.T.HEATH'
// 5T '*** END OF NASTI REPORT ***' END.
SECTION FINAL.
REPORT END.
```

Figure 5. (contd.)

NASTI.TYP

NASTI.TYP provides the same information as NASTI.FIL. However, NASTI.TYP types this information at the user's terminal. Therefore, the differences between the two files is that in NASTI.TYP all of the print statements are replaced with type statements and the statement INIT 1 NASTI.OUT is removed. Because of these similarities we do not give the listing of NASTI.TYP.

APPENDIX B. Abbreviations Used in NASTI

Abbreviation	Meaning and Information
ACH.LLL	Alan C. Hindmarsh, Lawrence Livermore Laboratory.
FMM	"Computer Methods for Mathematical Computations" by G. E. Forsythe, M. Malcolm and C. B. Moler. Published by Prentice-Hall.
HARWELL	Harwell Subroutine Library.
IMSL	International Mathematical and Statistical Libraries.
LINPACK	A collection of subroutines for solving linear systems. LINPACK was developed at Argonne National Laboratory, the University of California at San Diego, the University of Maryland, and the University of New Mexico.
MINPACK1	A subroutine package for optimization. The package is being constructed at the Argonne National Laboratory by B. S. Garbow, K. E. Hillstrom and J. J. More.
NAG	Numerical Algorithms Group Subroutine Library.
NCAR	National Center for Atmospheric Research.
QUADPACK	A subroutine package for numerical integration. The package is being constructed in a joint project by the "Technische Universitat Wien" (H. J. Stetter and C. W. Uberhuber, Vienna, Austria) and the "Katholieke Universiteit Leuven" (R. Piessens and E. de Doncker, Leuven, Belgium).
S.G.	"Computer Solution of Ordinary Differential Equations" by L. F. Shampine and M. K. Gordon published by W. H. Freeman and Company.
S.S.	"Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations," by P. Swarztrauber and R. Sweet, NCAR Technical Note/IA-109.
TOMS	ACM Transactions on Mathematical Software.

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