28
7600
25 to 71715

ORNL/CSD/TM-108

UCC-ND

**NUCLEAR
DIVISION**

**UNION
CARBIDE**

**Conversion and Improvement
of the Rutherford Laboratory's
Magnetostatic Computer Code
GFUN3D to the NMFECC CDC 7600**

T. C. Tucker

MASTER

OPERATED BY
UNION CARBIDE CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

CONVERSION AND IMPROVEMENT OF THE RUTHERFORD LABORATORY'S
MAGNETOSTATIC COMPUTER CODE GFUN3D TO THE NMFECC CDC 7600

T. C. Tucker

Sponsor: Y-K. M. Peng

Date Published: June 1980

COMPUTER SCIENCES DIVISION
at
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

NOTICE This document contains information of a preliminary nature.
It is subject to revision or correction and therefore does not represent a
final report.

Union Carbide Corporation, Nuclear Division
Operating the
Oak Ridge Gaseous Diffusion Plant . Paducah Gaseous Diffusion Plant
Oak Ridge Y-12 Plant . Oak Ridge National Laboratory
under Contract No. W-7405-eng-26
for the
DEPARTMENT OF ENERGY

DISCLAIMER

TABLE OF CONTENTS

ACKNOWLEDGMENTS	v
ABSTRACT	1
HISTORY	1
STATUS	2
MECHANICS	3
DIFFERENCES IN GFUN3D ON NMFECC 7600 AND ORNL 360	3
VALIDATION	5
GFUN3D ON THE NMFE NETWORK	6
SUGGESTIONS FOR FUTURE WORK	6
REFERENCES	9
APPENDIX A - GFUN3D NMFE 7600 USER'S GUIDE	11
1. INTRODUCTION	11
2. INTEGRAL EQUATION METHOD	11
3. THE USE OF INTERACTIVE GRAPHICS	11
4. STRUCTURE OF THE GFUN3D PROGRAM	12
5. UNITS	12
6. COMMANDS AND PARAMETERS; TYPES, FORMATS, NOTES	12
6.1. Command Names: List of Commands	12
6.2. DRAW: Enter Element DATA	13
6.2.1. General Comments	13
6.2.2. DRAW Command for Specifying Coils	13
6.2.3. DRAW Command for Specifying Iron	13
6.3. MODI and MOVE: Modify and Move Elements	13
6.4. ERASE: Erase Elements	13
6.5. PECO: Reconstructs Picture	14
6.6. BHDA: Enter B-H Data	14
6.7. GETM: Magnetization Procedure	14
6.8. GETB	16
6.9. MAP	16
6.10. HARM	16
6.11. File Management Commands	16
6.12. TRACK: Tracking of Charged Particles	18
6.13. GETF: Magnetic Forces	18
6.14. INTE: Integration of Field Functions	18

6.15. FIXI	18
6.16. Other Commands	19
7. OFF-LINE GETM	19
8. EXAMPLES	19
9. COMPUTE TIMES	20
10. SUBMITTING THE PROGRAM	22
10.1. Obtaining the Controllee and a Sample Input File	22
10.2. Preparing the Input File	22
10.3. Running GFUN	23
10.4. Running GFMOVEM	25
APPENDIX B - EXAMPLES OF GFUN3D ON THE NMFE CDC 7600	27
APPENDIX C - AN ALTERNATIVE ITERATION TECHNIQUE FOR GFUN3D	29

ACKNOWLEDGMENTS

This version of GFUN3D would not exist if C. W. Trowbridge, C. J. Collie, N. J. Diserens, A. J. Newman, J. Simkin, and A. G. Armstrong had not written the original. We hope that nothing we have done has caused errors for which they might receive unfair blame. We especially appreciate the very kind comments Trowbridge has made about the alternative iteration technique.

The initial conversion of GFUN3D to a CDC 7600 was done before publication of RL-76-029 (A see page 6.10). This version is based upon versions for small problems made at LBL by C. W. Trowbridge and J. Colonias and at LLL by C. W. Trowbridge and S. Sackett. Copies of those codes and plans for expansion to larger problems were made available to us. We are indebted for this simplification of our work.

K. W. Fong of LLL deserves special thanks. He not only discovered and obtained the codes and plans mentioned above, but encouraged and helped throughout the conversion. Further, he wrote a linear equations systems solver subroutine to be used for problems too large for the LCM. It has not been used only because we have not yet needed larger models than LCM can handle.

T. A. Cutler and R. Ferguson of LLL have implemented the beam tracking section of GFUN3D. We thank them for allowing its inclusion in this version and for the many helpful comments they have made.

W. D. Cain of UCC-ND Engineering Division introduced us to

GFUN3D, taught us how to use an IBM/360 version, and encouraged us throughout this work.

Janice V. Hughes has graciously helped us to rectify many mistakes through many draft versions of this report.

Finally, Y-K. M. Peng, R. A. Dory and J. Sheffield of ORNL Fusion Energy Division recognized the need for an NMFE version of GFUN3D and provided support.

Thank you, all.

CONVERSION AND IMPROVEMENT OF THE RUTHERFORD LABORATORY'S MAGNETOSTATIC COMPUTER CODE GFUN3D TO THE NMFECC CDC 7600

T. C. Tucker

ABSTRACT

We report the implementation of a version of the Rutherford Laboratory's magnetostatic computer code GFUN3D on the CDC 7600 at the National Magnetic Fusion Energy Computer Center. We include a new iteration technique which greatly increases the probability of convergence and reduces computation time by about 30% for calculations with nonlinear, ferromagnetic materials. We also discuss the use of GFUN3D on the NMFE network and present suggestions for future work. Appendix A consists of revisions to the GFUN3D User Guide (published by Rutherford Laboratory) which are necessary to use this version. Appendix B contains input and output for some sample calculations. Appendix C is a detailed discussion of the old and new iteration techniques. (Appendices A and B are available in FILEM 27725 .GFUNFILE.)

HISTORY

The GFUN3D magnetostatics computer code¹⁻³ is well known and widely used. One version has been operating on the Computer Sciences Division IBM/360/91 at ORNL since 1976. Long run times, slow turnaround, budget considerations, and limited precision (REAL*4) led to a decision to implement GFUN3D on the NMFECC network. Initial work had been done on versions for a CDC 7600 by C. W. Trowbridge of Rutherford Laboratory with J. Colonias at Lawrence Berkeley Laboratory and S. Sackett at Lawrence Livermore Laboratory. Neither of these versions could handle more than 35-40 iron elements.

K. W. Fong of the NMFECC staff arranged for us to obtain source code for both the LBL and LLL versions, together with notes and plans for more complete versions by Sackett and Colonias. Further discussions with Fong, T. A. Cutler, and others at Livermore led to the

decision to divide the implementation into two sections. Cutler was to implement the beam tracking and graphics sections, while T. C. Tucker, Oak Ridge, was to implement the major computation and data handling sections. Implementation was to be on the CDC 7600 because initial work had been done on it and because the CRAY-I was not in operation at decision time.

STATUS

All of the projected work has not been finished, but a very significant, improved version of GFUN3D is now operable on the NMFECC 7600 (A machine). Use of this code is solicited and encouraged. It is not guaranteed to be error-free, but test runs have shown general agreement with the IBM version at ORNL and the usable examples in the GFUN3D USER GUIDE.

The present NMFECC version of GFUN3D can calculate 170 iron elements in three dimensions or 255 in two. Graphics coding has not been implemented within GFUN3D, but some postprocessing capability exists on the 7600,⁴ and an interactive processor of DRAW and RECO commands exists for the DEC-10 at ORNL.⁵ Nor is this version of GFUN3D interactive. It was decided that an interactive version for input might be appropriate for the input sections, but only with graphics included. Interactive problem-solving with GFUN3D was to be discouraged on the network. Non-interactive time-sharing for short runs and batch submission for longer runs are appropriate for GFUN3D on the NMFECC network.

MECHANICS

The GFUN3D code for the NMFECC CDC 7600 has been implemented using the Los Alamos Scientific Laboratory FTN compiler (LASLFTN). This compiler was chosen over CHATR for its closer resemblance to "standard" FORTRAN, its greater speed in compilation and executable code, and its compatibility with the Livermore Time Sharing System (LTSS). In addition, the Los Alamos Math Library (FTNMTH) available with LASLFTN contains a matrix package designed for large matrices stored in 7600 large core memory (LCM).

The UPDATE code was used to make changes in the GFUN3D source. This means that a record exists of all changes and the order in which they were made. If it is desired, any intermediate version can be recovered.

A three-level, eight-segment overlay loading scheme was devised for GFUN3D on the A machine. This overlay scheme attempts to minimize thrashing of segments, especially for GETM, GETB, and similar time-consuming commands. It also makes it possible to change required core dynamically. Thus, GFUN3D requires 130K (octal) words of SSM and 221K (octal) words of LCM for everything but GETM commands which calculate 32 or more elements in three dimensions (47 or more in two). For larger cases, the additional core used is exactly the minimum needed. GFUN3D can be a good neighbor in time-sharing operation.

DIFFERENCES IN GFUN3D ON NMFECC 7600 AND ORNL 360

There are no basic differences between the GFUN3D implemented on the NMFECC 7600 and that on the ORNL IBM/360. There are differences in detail, however, primarily in input and output formats. Only in the

addition of an alternative iteration scheme, including revised convergence criteria, is there any deviation from the basic GFUN3D algorithm.

There have been a number of changes in information printed and in its format. In all instances, the intent was to present additional information. Any data no longer presented at one particular place are automatically presented at another. For example, the command PRINT originally caused two different descriptions of the iron elements. The first, which was an incomplete description for tetrahedral elements, also included the magnetization vectors, permeability, and susceptibility for the element. The second was a complete description of both prismatic and tetrahedral elements. In this version, the incomplete description has been replaced by the H-field (applied field) for the element and the susceptibility has been deleted. The complete iron description is still present.

An alternative iteration technique has been developed and coded into this version of GFUN3D. The original iteration scheme, which utilizes a relaxation factor, is still the default. The new technique must be requested by stating "CHIF=0" in the GETM command. This technique generally achieves convergence in about one-third fewer iterations than required by the original. The advantage is particularly pronounced when there is a wide range of inducing (H) field over the individual iron elements. Details of this technique are given in Appendix C.

VALIDATION

The NMFE version of GFUN3D has been checked against results of the IBM/360 version at Oak Ridge National Laboratory and four of the examples in RL-76-029/A. Comparison to ORNL IBM/360 calculations shows agreement within tolerances which can be attributed to the differences in machine arithmetic precision, and sometimes with no observable differences.

Comparison to the examples in the GFUN3D USER MANUAL, although more difficult, is also generally satisfactory. In the examples, the presented input and output are not in a one-to-one relation. For instance, in 8.1, the B-H data shown on page 8.2 do not correspond to Figure 8.1.2. If the data in Figure 8.1.2 are used, one can calculate the equivalent of Figure 8.1.3. Further, Figure 8.1.4 belongs to example 8.5.

In Example 8.2, the 7600 version calculates a field about 1% higher than that presented in Figures 8.2.5 - 8.2.8. The reason for this difference is unknown, but the ORNL IBM/360 version calculates a field essentially equal to that from the 7600 version.

Again, in Example 8.3, the 7600 version does not agree with the plotted data in Figures 8.3.2 and 8.3.3 when the input shown are used. But if the permeability is changed from 4669 to 4.669, no observable differences exist.

Comparisons of Example 8.5 to results from the NMFE version are quite good. The plotted data shown in Figures 8.5.3(a) and 9.5.3(b) are reproduced to plot accuracy, and the data shown in Figure 8.1.4 agree to printed accuracy with the interim listing at iteration 21.

No comparisons were made to Examples 8.4 and 8.6. In the case of 8.4, there were no numeric output data. In the case of 8.6, the 200 iron elements exceed the capacity of this version of GFUN3D.

GFUN3D ON THE NMFE NETWORK

This version of GFUN3D is available for all NMFE work. A controllee, modified user's manual, sample calculations, and utility programs are contained in FILEM, user number 27725, directory GFUNFILE.

A potential user must have a copy of the original GFUN3D USER GUIDE, PL-76-029/A. (That document can not be obtained from the implementor of the NMFE version.) File GFUN.MAN contains Appendix A of this report, the changes and differences applicable to the NMFE version. Note that GFUN.MAN contains upper and lower case, so a NETCUT must use option ULC.

SUGGESTIONS FOR FUTURE WORK

Further development of GFUN3D on the NMFE network is expected to be limited. There are, however, three fields which might be considered. The first, and most obvious, is implementation on the Cray-I computer. The second is to introduce coding to eliminate the magnetic eddies (looping) observed in a number of cases. The third is an attempt to include nonisotropic effects in the iron magnetization.

Implementing GFUN3D on the Cray-I is not advisable at this time. There are two basic gains which might be achieved on the Cray. Decreased run time is one. But, GFUN3D does not obviously lend itself to vector calculation, so speed gains would be limited. Further, the 7600 system currently has more time available than the Cray system, and

turnaround is better on the 7600. The second gain from a Cray version of GFUN3D would be the capability of solving larger problems. This gain is smaller than might be anticipated, however, with 275 iron elements an approximate maximum. On the other hand, only minimal recoding would be required to increase the 7600 version from 170 to 190 elements in 3D, and a disk-using matrix solver would make 400 elements possible. (Such a matrix package has been written, but not checked. Its inclusion in the 7600 version would be nontrivial.)

Coding to eliminate the magnetic eddies should be considered. Rutherford has introduced these changes, but does not always use the modified version.⁶ Although the coding changes are minor, additional computation time is not. Even so, the capability of eliminating the incorrect magnetizations should be available to check the results from the present code.

Inclusion of nonisotropic iron magnetization is not recommended at this time. There is insufficient data on actual iron behavior and there is no obvious, simple procedure which GFUN3D might use to approximate it.

REFERENCES

1. GFUN: An Interactive Program as an Aid to Magnet Design, M. J. Newman, C. W. Trowbridge, L. R. Turner, Rutherford Laboratory, Chilton, Didcot, Oxon, OX11 0QX, England, Proceedings of the Fourth International Conference on Magnet Technology, Brookhaven National Laboratory, November 1972.
2. New Developments in the Magnet Design Computer Program GFUN3D, A.G.A.M. Armstrong, C. J. Collie, N. J. Diserens, M. J. Newman, J. Simkin, C. W. Trowbridge, Rutherford Laboratory, Chilton, Didcot, Oxon, OX11 0QX, England, Proceedings of the Fifth International Conference on Magnet Technology, Rome, April 1975.
3. GFUN3D USER GUIDE, A. G. Armstrong, C. J. Collie, N. J. Diserens, M. J. Newman, J. Simkin, C. W. Trowbridge, Rutherford Laboratory, Chilton, Didcot, Oxon, OX11 0QX, England, Report RL-76-029/A, November 1976.
4. Personal Communication, T. A. Cutler and R. Ferguson, Lawrence Livermore Laboratory.
5. Personal Communication, W. D. Cain, Engineering Division, Oak Ridge, Tennessee.
6. Personal Communication, C. W. Trowbridge, Rutherford Laboratory.

APPENDIX A

GFUN3D NMFE 7600 USER'S GUIDE

This User's Guide contains only changes to or differences from the Rutherford Laboratory GFUN3D USER GUIDE (RL-76-029/A). To facilitate use, it follows the format of the original USER GUIDE, and section and page numbers refer to that document. A copy of the latest version of this appendix is in FILEM as 27725 .GFUNFILE GFUN.MAN.

1. INTRODUCTION

The package was modified for the NMFECC CDC 7600 computer by T. C. Tucker of ORNL and T. A. Cutler of LLL. It runs under the LTSS operating system in time-sharing or batch mode, but is not interactive.

2. INTEGRAL EQUATION METHOD

No changes.

3. THE USE OF INTERACTIVE GRAPHICS

No interactive graphics are available for GFUN3D on the NMFE network. Non-interactive postprocessing graphics are being developed at Livermore,⁴ and an interactive preprocessor for checking model definition is being developed on the DEC-10 system at ORNL.⁵

There is a single controller which does the work of both the "on-line (GFUN3D) and the off-line (GETM400)" programs referred to in RL-76-029/A.

4. STRUCTURE OF THE GFUN3D PROGRAM

The GFUN3D program on the NMFECC 7600 is a single code with overlays. It requires a minimum 221000 (octal) words LCM and about 130000 (octal) words of SSM. As the number of iron elements calculated increases above 31 in three dimensions (47 in two), LCM allocation is increased automatically to near the maximum possible at 170 elements in three dimensions or 255 in two.

5. UNITS

No changes.

6. COMMANDS AND PARAMETERS; TYPES, FORMATS, NOTES

6.1. Command Names: List of Commands

Command input generally follows the original version, including the footnotes for offline and CDC versions. The input line contains a maximum of 72 characters, but the last "value" must not use column 72. Only the comma indicating continuation can occupy column 72. Numerical parameters cannot be in floating point (E) format.

The C and S commands (p. 6.1, bottom) are for interactive control. Since this is a non-interactive version, these commands are not implemented and should not be used.

The table of Commands, Functions, and Parameters on pages 6.2 and 6.3 serves as an approximation only. Since graphics are not implemented, any command which plots, displays, etc., will not operate. (This version will accept and ignore any inoperable commands. An error message will not be issued in most cases.) The parameter list for some

commands may not be accurate. In particular, command parameters for the "direct access filing system" differ as discussed below.

6.2. DRAW: Enter Element Data

6.2.1. General Comments

No changes.

6.2.2. DRAW Command for Specifying Coils

On page 6.22, a necessary parameter is omitted from the list for END=6, the circular arc conductor. The omitted parameter is R1, which is erroneously labeled k in Figure 6.2.18.

6.2.3. DRAW Command for Specifying Iron

Two iron SHAPE parameters do not operate as described in RL-76-029/A, p. 6.39. For SHAP=-2, R1=0, the basic pentahedron is subdivided into 4 tetrahedra. For SHAP=-6, R1=0, the pentahedron is subdivided into 6 tetrahedra.

6.3. MODI and MOVE: Modify and Move Elements

No changes.

6.4. ERASE: Erase Elements

No changes.

6.5. RECO: Reconstructs Picture

Inoperative.

6.6. BHDA: Enter B-H Data

The C command for removing the table entry (B-H pair) last stored is not operable. Numerical values of B and H must be in fixed point (F) format. To prevent a divide-by-zero error, each B-value must be greater than the corresponding H-value. (An initial point B=0, H=0 is acceptable.) An "AA" in columns 1 and 2 signals the end of a B-H table.

When using the alternate iteration scheme, if the difference of B and H decreases in successive pairs of entries, saturation is presumed for the higher difference and all succeeding entries are ignored. This means that diamagnetic materials cannot be treated with this procedure.

6.7. GETM: Magnetization Procedure

The GETM procedure can calculate the magnetization for a maximum of 170 iron elements in three dimensions (255 in two). A maximum of 400 iron elements can be entered by DRAW commands. Any iron elements in excess of the 170 which can be calculated must be treated as "fixed" magnets by using the MODI and FIXI commands.

Parameter NITD is not compulsory, as indicated on page 6.3. When data are entered by a READ command, NITD is included. This simplifies restarting an interrupted calculation. However, if a new model is to be specified by changing an old one through MODI, MOVE, etc., NITD=0 should be entered.

The parameter NIT must be greater than NITD. The GETM section will perform a maximum of NIT-NITD iterations.

Parameter MPRI should not be used. The run may abort with an output or range error.

The initial permeability, IMU, need not be specified. With the original iteration scheme a default of 1000 is available. The alternate iteration procedure does not use IMU.

The alternate iteration procedure is invoked by CHIF=0. This procedure generally requires one-third fewer iterations than the original method. Further, it has achieved convergence in all cases tried, including some in which the original failed.

The default value for TOLM is 10^{-6} rather than the 10^{-4} given on page 6.47. A new tolerance has been introduced for relative changes in H, M, and X (susceptibility) of each iron element. The default value for this tolerance is the square root of TOLM, but it may be changed by TOLE=.

The original version of GFUN3D printed an intermediate listing of H and M for each element every 20 iterations, starting with iteration 1. Parameter LFRE has been introduced to control the frequency of this listing. The value for LFRE may be 0 (never list), 1 (always list), or any other positive integer.

The parameter HEXT is used to specify a constant magnetic field in gauss in the Y direction.

6.8. GETB

The default value for parameter COMP is unknown, but it is not "HY" as stated on page 6.48. The field components HX, HY, and HZ are always listed. Similarly, the default value of FINT seems to be variable. Field integrals are sometimes printed and sometimes omitted when no FINT is entered.

Parameters referring to plotting (ARROW, ERASE, etc.) are inoperative.

When a field is to be calculated at polar coordinate grid points, the plane of the polar grid must be specified by "PLANE".

6.9. MAP

Not operative.

6.10. HARM

The GETB command which precedes HARM must include parameter PLANE=XY.

6.11. File Management Commands

GFUN3D on the NMFECC 7600 includes an optional filing system for model definitions and calculations. Use of this system is recommended. It allows saving magnetization data for later analysis, simplifies modifying model definitions, and provides a means of saving the latest iteration if time runs out during a batch run.

Since GFUN3D was designed for an IBM system, it is necessary to know the IBM nomenclature used in this section of RL-76-029/A. In that report, both "dataset" and "direct access filing system" refer to a

large file which corresponds to an LTSS disk file. "File" refers to a smaller collection of data within the "dataset". (An approximate parallel is a file in a LIX library.) To minimize confusion, we use "LTSS disk file" whenever the "dataset" is intended, and "file" whenever the smaller subset is meant.

The LTSS disk file must be defined and initialized before it can be used by GFUN3D. This can be done easily by obtaining a controllee from FILEM by

RDS 27725 .GFUNFILE SETFILE

and preparing a one-line input file named SETUPI. The file SETUPI must contain the desired name of your LTSS disk file left-adjusted in columns 1-8. If a size other than one million octal (262144 decimal) words is desired, that size is entered as a decimal number, right-adjusted in columns 11-20. (Omitting this number results in the default.) For example, to make a file named MYDATA which contains 256 segments of 512 words, SETUPI contains

	0	1	1
Col.	1234567890	1234567890	
	MYDATA	131072	

Then running SETFILE will define and initialize MYDATA, and also produce an output listing, SETUP0. This output file should consist of one line of text, about a dozen positive integers, three negative integers, and many zeroes. If SETUP0 looks like this, the LTSS disk file is ready to use.

Command "LIST" has been completely changed. Parameter "DSN" has no effect since there is a single LTSS disk file. Parameter "ID" has been replaced by an optional parameter "FL". If LIST is requested with no parameter, the entire directory will be listed. Including

"FL=value", where "value" is a string of one to four characters, lists all file names which start with that character string.

Commands READ and DELE require special entry of a file name when a generation number is included. In particular, 5 to 8 characters must occur between "FL=" and the "," preceding the generation number. Trailing blanks are acceptable. For example

```
READ FL=JOE,4
```

will fail, but

```
READ FL=JOEbb,4 (where b represents a space)
```

will retrieve JOE, generation 4.

6.12. TRACK: Tracking of Charged Particles

Reference to "C" and "S" commands under the "PRINT" parameter should be removed.

The "BEAM" command is inoperative.

6.13. GETF: Magnetic Forces

No changes.

6.14. INTE: Integration of Field Functions

Inoperative.

6.15. FIXI

No changes.

6.16. Other Commands

There are four commands listed on pages 6.2 and 6.3 which are mentioned nowhere else in RL-76-029/A. These commands are discussed here.

FRAM is basically a graphics command, but GFUN3D refuses to run under some conditions unless this command has been issued. A simple FRAM as the second line is sufficient.

PRINT causes a detailed printing of the model including the description of coils; the corners, centroid, magnetization, and permeability of iron elements; and the B-H tables supplied. It is invoked automatically after every READ command.

CLEAR reinitializes the GFUN3D code. It allows stacking problems within a single controllee run.

END terminates a run.

7. OFF-LINE GETM

There is no separate "off-line" code.

8. EXAMPLES

We have calculated four of the six examples given in RL-76-029/A. Example 8.4 was not done because only graphic output is shown in that report. Example 8.6 has 200 iron elements, exceeding the capacity of our version. Two of these examples have also been modified to illustrate the alternative convergence scheme.

In comparing results from these calculations to those presented in RL-76-029/A, some care must be exercised. In the first place, all figures shown in that report do not result from the input data given,

but are illustrative of a particular type of output. For example, the B-H data shown as input for Example 8.1 includes pairs (0,0), (10000,6.99), (12000,9), etc. In Figure 8.1.2, however, the listing adds the pair (8000,4.57) to the table. If this point is added to the input, then the results shown in Figure 8.1.3 are achieved (within machine precision). Further, Figure 8.1.4 actually comes from a run of Example 8.5.

A second caution about comparing to RL-76-029/A results concerns the scales on some graphs. The self-scaling algorithm used works correctly insofar as it includes all data points and little else. Unfortunately, the subdivisions are not always nice increments (1, 2, or 5 times a power of 10 is a nice increment), the number of minor subdivisions per major subdivision is variable (Figure 8.3.2 has 7 minor/major on one axis), and the labels are often properly rounded but deceptive (.006 and .008 both rounded to .01).

The input, output, and limited comments about the examples are presented in Appendix B. A more detailed discussion of the comparisons is in the body of this report.

9. COMPUTE TIMES

Execution time for GFUN varies widely with the problem. The most significant portions of the code for timing purposes are calculation of the magnetic field of the conductors at each iron element, definition of the matrix of interaction between iron elements, solution of the matrix equation, and calculation and analysis of the resultant field for the model. Data input and use of the LTSS disc file system usually requires less than 5 seconds.

The time needed to define the matrix can be estimated by

$$t_d = 7 \times 10^{-4} n_t^{2.11} 2^r$$

where

t_d = time for matrix definition, seconds,

n_t = total number of iron elements in model,

r = number of iron symmetry reflecting planes.

For example, 50 iron elements with no symmetry planes require about 2.7 seconds, but 140 iron elements with 2 reflecting planes require about 95 seconds.

No simple estimating equation for the conductor field has been determined. The time should be proportional to the number of iron elements, the number of conductors, and the appropriate symmetry factors. The type of conductor model, however, appears to be most important, and no correlation has become apparent. Times observed for calculating the current field have ranged from virtually none to more than 40% of the matrix definition time.

The time required for matrix solution for one iteration can be estimated by

$$t_i = 7.4 \times 10^{-6} n_c^{2.90}$$

where

t_i = time for one iteration, seconds,

and

n_c = number of "free" iron elements.

Notice that the number of iron elements in the model (n_t) may be greater than the number of "free" elements (n_c) being calculated. Approximate execution times are 0.63 seconds per iteration for 50 free elements and 21 seconds for 167. The number of iterations required is

quite variable, but one should estimate enough time for the maximum specified.

Again, there is no simple formula for time needed to calculate the magnetic field for the model or to do an harmonic analysis or particle tracking calculation. It is best to save the magnetization on the LTSS disc file using "WRITE" and then do the calculations. Then, if insufficient time has been allowed for the field calculations, the magnetization need not be recalculated.

Overall execution time may run from less than 30 seconds for 50 iron elements and a single solenoid conductor to 30 minutes or more for 170 iron elements with multiple, variously shaped conductors.

10. SUBMITTING THE PROGRAM

10.1. Obtaining the Controllee and a Sample Input File

The GFUN3D controllee, named GFUN, and a sample input file, GFUNIN, are obtained in FILEM by

```
RDS 27725 .GFUNFILE GFUN GFUNIN
```

This controllee will be updated as changes or corrections are made.

Use the HOW command in FILEM to check the date the controllee was last changed.

10.2. Preparing the Input File

Input for the GFUN controllee must be in a file named GFUNIN. The first line of this file must contain the name of the LTSS disc file for the GFUN3D filing system in columns 1-8 (see Section 6.11) or be blank. Any other first line may cause an abnormal end. The second line may or

may not need to be a FRAM command. There is a possibility that some variables initialized by FRAM may sometimes be needed even though graphics are not implemented. In any case, FRAM does no harm, and its presence on the second line is recommended. The order in the remaining input lines is restricted only in that a model must first be defined and then magnetized before field calculations can be made. The last line of the input file GFUNIN should always be the END command.

A sample GFUNIN is available as mentioned in the preceding section. It is suitable for a sample run requiring about 15 to 20 seconds cpu.

10.3. Running GFUN

The NMFECC 7600 version of GFUN3D can be run in batch or timesharing (but noninteractive) mode. In either case the code generates and destroys certain disc files, which the user may ignore. The names are chosen to be unique, thus they cannot affect any other files. However, an output file named GFUNOUT is also written. It is essential that the user have no file which is to be kept named GFUNOUT because that old file will be destroyed when GFUN is started.

In timesharing mode, one prepares the input file GFUNIN, enters

GFUN / t v

from the keyboard, and when the code finishes, does something with GFUNOUT. Note that GFUNIN and GFUNOUT are special names, and hence only one controllee can be run at any time by a single user.

In batch mode, it is recommended that the controllee always be read from 27725 .GFUNFILE. This assures the latest version. Multiple batch runs naturally require multiple input files, so remember to

change the name to GFUNIN before executing GFUN. The first batch operation after GFUN should be a FILEM replace of the GFUN3D filing system LTSS disc file. If an iteration runs out of time, the last iteration will be written to the LTSS disc file (see Sec. 6.11); but, if that file is not written to FILEM, it will be lost when batch cleans up.

There are two sources of potential trouble for the standard, printed output from GFUN3D batch runs. This output appears as a family of files starting with GFUNOUT. One must ensure that all members of the family are used. If this output is to be kept in FILEM, one must ensure it does not conflict with some other set. The simplest solution is to include the following COSMOS instructions:

```
*FILEM RDS .GFUNFILE COMPACT
```

```
*COMPACT GFUNOUT NEWNAME
```

This will replace all members of the GFUNOUT family by a single file called NEWNAME.

Another problem in batch runs arises from the possible parallel execution of two or more GFUN jobs. If the two jobs write into the same LTSS disk file, the second job's replacing the file in FILEM will overwrite the output from the first. The solution is to use multiple LTSS disk files for batch runs which may run simultaneously. Such files do not need to be very large. An interactive utility program, GFMOVE, has been written to facilitate the necessary data manipulation. Given two LTSS disk files, GFMOVE can copy a problem file from one LTSS disk file to another, list the contents, and delete specified files. Thus many small LTSS disk files can be used for a number of batch runs and the results transferred to a master for

permanent storage. Instructions for GFMOVE are in the following section.

10.4. Running GFMOVE

An interactive program has been written for manipulating LTSS disk files for the GFUN direct access filing system. The controller GFMOVE can be obtained by

```
FILE RDS 27725 .GFUNFILE GFMOVE .
```

The commands for GFMOVE are analogous or identical to the GFUN3D file management commands (Sect. 6.11). GFMOVE can operate on one or two LTSS disk files at once. These files and their use are specified by the following commands:

```
FROM DS=filename1
```

```
INTO DS=filename2
```

The commands READ, WRITE, and DELETE operate upon the grammatically correct file. They READ or DELETE FROM, but WRITE INTO. Commands LIST and ROOMAC operate on both files; but, if only one is specified, the code does not object.

One runs GFMOVE by entering

```
GFMOVE / t v
```

and responding to the prompt with a command. The usual END command will terminate the run.

Two further commands have been implemented in GFMOVE. The first of these is

```
COPY FL=name, gen .
```

This results in a READ of name, gen FROM filename1 followed by a WRITE of name INTO filename2. Note well, however, that the generation number

may be changed. (The last paragraph of Sec. 6.11, concerning the number of characters in name, applies here also.) The command

MOVE FL=name, gen

causes the READ and WRITE of COPY, followed by a DELETE of name, gen FROM filename1.

Commands COPY and MOVE are convenient, but name is unchanged. If one wishes to change the name of a set of data, then READ and WRITE are the appropriate commands.

The LTSS disk files in use can be changed at any time by issuing a FROM or INTO. The only restriction is that a single LTSS disk file cannot be opened for both.

APPENDIX 9

EXAMPLES OF GFUN3D ON THE NMFE CDC 7600

This appendix is published as a microfiche which is enclosed at the back of the report.

The examples in this appendix are also available in FILEM as, for example, 27725 .GFUNFILE EXAMPLE8.1. The complete list of names can be obtained by LST 27725 .GFUNFILE ALWITH. EXAM.

APPENDIX C

AN ALTERNATIVE ITERATION TECHNIQUE FOR GFUN3D

We have developed an alternative iteration technique for GFUN3D on the NMFE 7600. The original technique is often slow, sometimes fails to converge, and has incorrectly indicated convergence on occasion. The new technique generally needs one-third fewer iterations and has always converged, even on cases for which the original method fails.

The basic equation of GFUN3D is

$$H_k = C_k + \sum_j G_{jk} M_j \quad (1)$$

where

H_k is the total magnetic intensity at point k ,

C_k is the magnetic intensity at k caused by currents and fixed fields,

M_j is the constant magnetization throughout iron element j .

and

$G_{jk} M_j$ is the magnetic intensity at k caused by element j .

(Variables H_k , C_k , and M_j are m -dimensional vectors and G_{jk} is an $m \times m$ matrix, but it is sufficient to consider them as scalars for this discussion.) However, iron magnetization, M , is a function of the applied magnetic intensity, H , and may be expressed by

$$M = \chi \cdot H \quad (2)$$

where χ is the iron susceptibility, not generally a constant. In GFUN3D, if point k in (1) is interpreted as a representative point for iron element k , then (1) and (2) lead to

$$\sum_{j \neq k} G_{jk} M_j + (G_{kk} - 1/\chi_k) M_k = -C_k \quad (3)$$

Thus, with a known susceptibility for each iron element, calculation of the magnetizations is a linear problem. If susceptibility is not

known, GFUN3D assumes a value for each element and solves for the magnetizations, iterating with successive assumptions until some convergence for consistency criterion is satisfied. The procedure for choosing the successive values for χ and the convergence criterion make up the iteration technique.

In the original GFUN3D, the iteration technique consists of the following steps:

1. Assume a single susceptibility, $\chi_{k,0}$, for all elements (notice that a second subscript now denotes the iteration number.)
2. Solve the system of equations (3) for $M_{k,i}$ using $\chi_{k,i-1}$.
3. Calculate the total field $H_{t,i}$ at some test point t .
4. If $|H_{t,i} - H_{t,i-1}| \leq \epsilon_t H_{t,i}$ where ϵ_t is a specified tolerance, presume convergence and stop iteration. Otherwise, proceed to step 5. $\chi_{k,i}^* = M(H_{k,i})/H_{k,i}$.
5. Calculate $H_{k,i} = M_{k,i}/\chi_{k,i-1}$.
6. Find $M(H_{k,i})$ from tabular input data giving $B = M+H$ as a function of H , and define

$$\chi_{k,i}^* = M(H_{k,i})/H_{k,i}.$$

7. Determine $\chi_{k,i}$ from

$$\chi_{k,i} = w\chi_{k,i}^* + (1-w)\chi_{k,i-1},$$

where w is the relaxation factor (input parameter CHIF), and iterate from step 2.

This technique can fail completely when $w > 1$ and $\chi_{k,i}^* < (w-1)\chi_{k,i-1}/w$. The result is a negative susceptibility, an impossibility for ferromagnetic materials. The iteration can sometimes recover from such a situation, but often cannot. Again, the single point convergence test in step 4 can be and has been passed accidentally with susceptibilities and magnetizations nowhere close to true solution values. Finally, the χ^* determined in step 6 often approaches the

solution asymptotically (especially for iron elements near saturation), causing a slow rate of convergence.

There are a number of ways to avoid false convergence after the fact. (First, of course, it must be recognized. This is not always trivial.) Changing the initial susceptibility by specifying a different input value for IMU may work. Choosing a different test point is another way. Unfortunately, the only method of assuring convergence with the original technique is to choose a relaxation factor no greater than 1. This choice necessarily limits the rate of asymptotic approach and slows convergence. Thus, two of the problems have opposing solutions.

Trowbridge² has recognized the flaws in the original iteration technique. He proposed a secant method for accelerating convergence. Difficulties in implementation and higher priorities for other work left the secant method in the proposal stage.

We met all three convergence problems in calculating ISX magnetization using GFUN3D. We wanted a new iteration procedure which would assure convergence of each iron element as well as the external field. We wished to avoid initial guesses and user intervention, usually an after-the-fact correction. We believed that the iteration history should contain information which could be used to accelerate convergence. Starting from these desires and beliefs, we made a number of experimental changes in the GFUN3D iteration.

Standard techniques for accelerating convergence, e.g. Aitken's δ^2 process, did not work. Attempts to automate the choice of relaxation factor failed. But a number of procedures were found which

worked well under certain circumstances. A selective combination of these makes up the new iteration technique.

The new iteration technique consists of the following steps:

1. Find the entry in the input B-H table with maximum difference B minus H. This is taken as the saturation point. (Note that this presumption eliminates diamagnetic materials.)
2. Calculate $H_{k,0}$ at each element assuming susceptibility $\chi_k = 0$, and determine the corresponding $M_{k,0}$ from the input data using linear interpolation. Assume initial, individual susceptibilities

$$\chi_{k,0} = M_{k,0}/H_{k,0}$$

3. Solve the system of Eqs. (3) for $M_{k,1}$ using $\chi_{k,i-1}$. Calculate $H_{k,i} = M_{k,i}/\chi_{k,i-1}$.

4. Find the "near point", (HN_k, MN_k) , which minimizes

$$\left(\frac{HN_k}{H_{k,i}} - 1 \right)^2 + \left(\frac{MN_k}{M_{k,i}} - 1 \right)^2$$

for each iron element.

5. Find all intersections (HI_k, MI_k) of the line through $(H_{k,i}, M_{k,i})$ and $(H_{k,i-1}, M_{k,i-1})$ and the curve defined by linear interpolation of the input table.
6. If any (HI_k, MI_k) points interpolate $(H_{k,i}, M_{k,i}) - (H_{k,i-1}, M_{k,i-1})$ use the measure in step 4 to find the nearest $(HI_k^{\#}, MI_k^{\#})$. Then the new estimate for susceptibility is $\chi_{k,1} = MI_k^{\#}/HI_k^{\#}$. Proceed to step 9.

7. If any (HI_k, MI_k) points exist such that

$$0 < \frac{(H_{k,i} - HI_k)}{(H_{k,i} - HN_k)} < r$$

and

$$\frac{|M_{k,i} - MI_k|}{|M_{k,i} - MN_k|} < r$$

where r is an arbitrary constant, choose the nearest as (HI_k^*, MI_k^*) . Set $\chi_{k,i} = MI_k^*/HI_k^*$ and proceed to step 9.

8. If $\chi_{k,i}$ is not set in step 6 or 7, then $\chi_{k,i} = MN_k/HN_k$.

9. Calculate the total field $H_{t,i}$ at some test point t .

10. If $|H_{t,i} - H_{t,i-1}| \leq \epsilon_t \cdot H_{t,i}$,

$$|H_{k,i} - H_{k,i-1}| \leq \epsilon_e \cdot H_{k,i},$$

$$|M_{k,i} - M_{k,i-1}| \leq \epsilon_e \cdot M_{k,i},$$

and

$$|\chi_{k,i} - \chi_{k,i-1}| \leq \epsilon_e \cdot \chi_{k,i}$$

for all iron elements, where ϵ_t and ϵ_e are specified tolerances, presume convergence and stop iteration. If any of the tests is failed, iterate from step 3.

The assumption of a saturation point in step 1 simplifies data input and provides a means for avoiding incorrect magnetization for H fields larger than expected. Step 2 eliminates initial guesses of iron permeability and provides individual values for each iron element. The near point evaluation of steps 4 and 8 finds a susceptibility very

close to that which is found by the original technique as an iron element approaches saturation. When an element is in the high susceptibility portion of the curve, the near point selection essentially inverts the original scheme by finding H as a function of M . This works well because the $1/X$ term of Eq. 3 becomes negligible. In the region of the knee, the near point makes a smooth transition.

Steps 5, 6, and 7 essentially perform "regula falsi" when possible and otherwise use Newton's method with a first difference approximation to the derivative. The arbitrary constant, r , in step 7 is intended to prevent gross changes which perturb other elements too much. In our initial runs, r was set at 2. Since convergence has been achieved rapidly with this value, no tuning has been attempted. The other restriction of step 7 (that $H_{k,i} - H_{I_k}$ have the same sign as $H_{k,i} - H_{N_k}$) was found to be essential.

The tests of step 10 assure that all iron elements are converged. All of H , M , and X must be checked because there are regions of the magnetization curve in which any one may be virtually constant while the other two change. We have set $\epsilon_e = \sqrt{\epsilon_t}$ as a default. Limited experiments have shown little to be gained in speed or accuracy by using a different value.

Using this technique in the NMFE CDC 7600 version of GFUN3D increases the time per iteration by less than 5%, but generally cuts the number of iterations by about one-third. The net gain is a decrease in iteration time on the order of 20%. More important is that this technique has always converged.