Status and Future of the 3D MAFIA Group of Codes*

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ABSTRACT

The group of fully three dimensional computer codes for solving Maxwell's equations for a wide range of applications, MAFIA, is already well established. Extensive comparisons with measurements have demonstrated the accuracy of the computations. A large number of components have been designed for accelerators, such as kicker magnets, non cylindrical cavities, ferrite loaded cavities, vacuum chambers with slots and transitions, etc. The latest additions to the system include a new static solver that can calculate 3D magneto- and electrostatic fields, and a self consistent version of the 2D-BCI that solves the field equations and the equations of motion in parallel. Work on new eddy current modules has started, which will allow treatment of laminated and/or solid iron cores excited by low frequency currents. Based on our experience with the present releases 1 and 2, we have started a complete revision of the whole user interface and data structure, which will make the codes even more user-friendly and flexible.

INTRODUCTION

The acronym MAFIA stands for the solution of MAXwell's equations by the Finite Integration Algorithm. This is the name given to a set of fully three-dimensional codes used in the computer-aided design of accelerators. Rf structures, magnets and electrostatic devices as well as structures in which wake-field effects are of importance can all be calculated. The Finite Integration Technique (FIT) [1,2] produces a first order approximation of Maxwell's equations by replacing the line and surface integrals by mean field values multiplied by path lengths or areas. The algorithm produces a set of matrix equations which can subsequently be solved. The allocation of the field components to the rectangular grid is as shown in Figure 1, with the electric field components allocated at the mid-points of the sides of the rectangular cells and the magnetic field components at the centre of each face. This defines a dual grid where the origin of each dual cell lies at the centre of each original grid cell, and to which

Figure 1: Geometry and Allocation of the Field Components for the FIT Method

the magnetic components are allocated in the same way as the electric components on the regular grid. Thus the transition from one cell to the next involves only continuous components, leading to the fact that Maxwell's equations are always satisfied at the points of allocation, even when different material fillings are involved. In addition, the analytical properties of the matrix operators are preserved on the discrete grid [2], in particular $\text{divcurl} \equiv 0$, $\text{curlgrad} \equiv 0$, which is not necessarily the case for all discretisation methods. Thus the FIT method has an advantage over other methods in that, after the eigenvalues of the problem are calculated, the numerical results can be tested for their physical correctness and any spurious solutions removed automatically.

DESCRIPTION OF THE MAFIA PROGRAMS

- M3 - is the mesh generator used by all programs, which translates the physical problem into mesh data and material distribution data.

Figure 3 shows typical hidden line plots produced by M3.

- S3 - is the three-dimensional static solver for electro- and magneto-static problems.

Figure 4 shows the structure and equipotential lines for the MAFIA emblem, the first and last letters are metal and electrostatically charged and the three central letters are dielectric.

Figure 2: The MAFIA System with its Interrelationships

Figure 3: M3 Plots of Geometry and Mesh for the Jungle Gym Accelerating Structure

Figure 4: Equipotential plot from S3

- R3 and E31 (or E32) - these two codes, run in sequence, solve Maxwell's equations in the frequency domain. R3 sets up the matrices, adding the material properties and the boundary conditions to the mesh data from M3. E31 is the improved, more accurate version of the eigenvalue solver, which solves the matrix equations from R3 and writes the required eigenvectors onto the direct access file. E32 uses advanced multigrid methods and may be used instead of E31 for very large meshes.

Figure 5 shows the structure of a proposed kicker magnet for injection of the proton beam from PETRA into the HERA ring. The magnet is carried on supports by which it can be rotated into the beam line. The computer simulations from the programs M3-R3-E3-P3 showed that the required fields were not economically obtainable by this method and the magnet was not built.

- T3 - solves Maxwell's equations in the time domain.

Figure 6 shows a test example of a single bunch passing through a modified

Figure 5: Structure of a Proposed Kicker Magnet for Injection into HERA

pill box cavity, the wakepotentials were calculated by T3 . The graph shows the three components of the wake potential and the bunch shape.

- TS3 - is a three-dimensional particle-in-cell code, not yet available for public release.
- W3 - will solve Maxwell's equations for eddy currents, not yet available for public release.
- A3 - will solve dynamic-elastic problems such as sound propagation, projected for future release.
- P3 - is the postprocessor for all the codes. Solutions can be displayed graphically, calculations carried out and file manipulations from within the program are possible. Figure 7 shows typical arrow plots of the electric and magnetic fields across the gap of the magnet from figure 5.

All the MAFIA codes for the third release can be used either interactively or in batch. Thus the former input files which were necessary for some of the codes will be replaced by a series of commands, either entered interactively, with a

Figure 6: Wakefield Potentials versus bunch coordinates from T3, for the geometry shown in the insert

help facility to provide explanations where necessary, or read from a command file either interactively or in batch.

PRESENT STATUS

The second release of the MAFIA Programs, comprising M3, R3, E31, E32 and P3, has been distributed to over 75 installations, including MFE in the United States. The programs have already proved their worth through comparison with theoretical calculations and by successful design of accelerator components. For the third release, the existing MAFIA codes are being completely overhauled and new codes added.

NEW FEATURES OF THE PROGRAMS

Some of the new features are listed below:-

- A modular program structure has been adopted.
- A unified, menu-controlled, user interface has been created for all the codes.

Figure 7: Arrow plots of electric(above) and magnetic(below) field, from E3 - P3

- A new command processor has been written.
- The data structure has been changed to accomodate all codes.
- A dynamic memory manager has been added to control both the file and the memory operations necessary for the new structure.
- Many new facilities have been included.

Program Structure

The programs have been restructured and divided into *sections*, each of which represents an independent function of the program, for example, the setting of the mesh or the drawing of an arrow plot.

Each program begins at an *Entry Level* where a menu is displayed that lists all the available commands. One can return to this *entry level* at any time and any *section* may be called from there .

User Interface

The new user interface is guided by menus. Each section prints a menu which lists all the commands available in that section, with their current settings or default values. This reduces the memorisation of command names necessary for running the programs, and displays the status information for the section. All sections have the same basic structure -

menu display
 reading and processing of command lines
 setting of appropriate variables
 optional execution or exit
 (execution may involve calls to additional subroutines)

Control remains with the current section until another section is invoked or the program is terminated.

It is also possible to run the programs without the menu display, which can be slow on some systems. In this mode, the information about the values set for certain commands can still be obtained on request.

Help system - The user interface includes a hierarchical help system to lead the beginning user through the functions of the program.

The help system is matched to the program structure. At the entry level the most basic help is available, addressing the questions -

What does this program do?
 How do I use it?

What should I do next?
Where am I?
How do I get out of this?

These questions are answered by the command *help*. Once this hurdle is passed, help is available for more specific areas, such as types of commands or any named section. A help menu is provided for each section which describes the function of the section, the meaning of the subcommands and gives any necessary instructions on its use. At any stage of the program the command *help* alone will give advice on how to proceed.

Command Processor

All commands are defined with unabbreviated names. This should relieve the user of the task of memorising specific command mnemonics. The command processor is capable of processing shortened versions of these commands; it checks for validity and ambiguity and will accept any unambiguous truncation.

The user has the freedom to enter and leave any section at will and, wherever possible, the order of operations carried out is not predetermined. However, certain sequences are not possible - a file must be opened before it can be read and must be read before anything may be calculated. In order to keep the programs as streamlined as possible, the idea of interactive prompting for missing information was rejected as impractical and time-consuming. Certain necessary checks will be made when the request to execute a section is received and warning messages issued.

A *macro* facility will be included and the command processor will be able to accept predefined macro commands, standing for a string of basic commands. This will enable experienced users to streamline terminal sessions and tailor the program to their particular needs.

Command Structure The commands themselves correspond closely to the structure of the program. For each section of the program there is a *branch* command by which that section is invoked. Each section has its own set of subcommands, its own menu listing these commands with their assigned values or defaults, and its own help menu describing the subcommands.

A certain subset of commands, which are necessary or desirable to have available at any time, have been selected and called *global* commands. Certain global settings are listed on every menu for convenience and a list of global commands can be obtained at will.

Data structure of the direct access file

The structure of the direct access file has been made more flexible and can now be used by all programs. The new file has a transparent structure with a directory, organised like a database. The storage locations of named fields are recorded in the directory and the user has control of the reading and writing of quantities on the file. The directory is stored and updated in memory and written to the file when the program is terminated. Much general information stored on the file, such as the number of mesh points and the boundary conditions, are stored in readable form so that they can be listed on request from inside the program. It will be possible to allocate, open and close direct access files from within the MAFIA programs. The direct access file is designed to be used by all the MAFIA programs, see Figure 8. However, many systems do not support expandable direct access files. While it would be possible to work with one file which is large enough for all the programs, it is unwieldy to do so and often it is not obvious, when M3 is started, how large the final file should be. This is especially true for P3 where many new quantities can be calculated and stored. For this reason, the MAFIA programs are also designed to allocate their own files. Under this regime, see Figure 2, each program uses both an input and an output direct access file. The information stored by the previous program is read, the size of the output file calculated, a new file allocated and the information copied from the old to the new file.

Dynamic Memory Manager

One of the restrictions of three dimensional mesh codes in general is the number of mesh points which can be handled on any particular system. The more mesh points available, the greater the accuracy obtainable in the approximation of the structure. One of the aims of the new file structure and memory manager is to provide the maximum flexibility in the use of available memory. A combination of selective loading of quantities from the file and of selective deletion in memory of whatever is not needed for a particular operation, can make optimum use of the space available. Thus, in the post-processor, it will be possible to load a specific quantity from the file, or even to define a range and load only a part of that quantity if the field is very large. Then a calculation can be carried out and the results stored and lastly deleted from memory, freeing the space for further use. A load section is provided, where the functions of the memory manager can be invoked. Here one can load a quantity from one file, write something to another file, rename a quantity, or delete a field in memory or on a file; however caution is advised - any precious file should be copied before processing begins. If this has not been done the file can still be copied from within the program. Only the command 'delete all' will give you a warning message and a second chance.

Figure 8: The Flow of Data between the the Programs and the Direct Access File

Sequential Files

The following sequential files are provided, all of which may be opened or closed by name from within the program and switched on or off at any time :

- Command file - Commands may be read from this file instead of from the terminal.
- Log file - When this file is open, all the commands entered will be written onto it. This is a useful method of creating a command file for future use as well as of recording the progress of a session. The commands used during a session are also automatically recorded on the direct access file when the program is terminated. This is to aid in the diagnostic work of following up on user-reported problems which are often not otherwise exactly reproducible.
- Print files - Two print files are provided, one of which is usually the interactive terminal. Output to the interactive terminal may also be turned off by a global command.
- Plot files - Similarly, there are two plot files. Graphic output may be directed to either, the graphic terminal or a metafile for later display. Global commands switch output on or off to these files.

There is also a section where the contents of any of these files can be listed. In this way a command file can be used several times to make a set of arrow and contour plots for the same geometrical values, or more than one command file may be used in a session to perform various tasks. The listing facility even enables an old command file to be opened to check its contents before using it. Also a logfile could be renamed as a command file, closed, and then reopened to repeat a complicated series of commands.

Other New Features of the Post-Processor, P3

Mathematical Operations - The original concept of the post processor was to provide the calculation of physical quantities of interest for accelerator design, each of which was separately programmed. This proved to be very inflexible and many users found that further calculations were necessary to adapt these quantities to their needs. Now these quantities will still be available but they

will be programmed at the level of the individual mathematical operations and combined by means of internal macros. This facility will also be made available to the user. It will be possible, for example, to load a field from one direct access file, load the corresponding field from a file with the same mesh but slightly different geometry, difference the two and display the result graphically or perform further calculations as needed. This can be a very powerful tool in the design of accelerators and will enable the codes to be used more creatively. However this freedom also brings certain dangers and the full responsibility for the physical correctness and interpretation of the results lies with the user.

Windows - A zoom is available for all graphic output and calculations can be performed for a limited mesh window if desired. There is also a window section where the user has the possibility of presetting different windows for calculations or plots and for one, two or three dimensions. These windows are normally coupled so that changing one changes all the others but can be kept separate if required.

Range - A range is a limited set of values for which a quantity has been calculated or stored. The range section can set a reduced mesh or time range when a quantity is written to the file either in a previous program or in the post-processor. These ranges are recorded on the file and automatically checked whenever quantities are read.

Calculations - One, two and three dimensional integrals will be available, and calculations for impedance, charge and forces will be added.

AVAILABILITY

The MAFIA codes are written in Fortran 77 and currently run on IBM 3081, CRAY, VAX, Amdahl, Cyber and Apollo computers. The distribution centre for the codes is DESY, and the codes are available without charge to all non-profit organisations. For information contact T. Weiland at DESY.

CONCLUSION

Many new features will be added to the MAFIA group of codes. The additional programs will extend the scope of the codes while the new command processor, the conscious file manipulations and the additional calculations that will be possible, will be the features affecting users most directly. However the underlying restructuring of the programs themselves enables a much more efficient management of the support of the codes and is flexible enough to accommodate virtually any future extensions. The newest release of the MAFIA codes will be more user friendly than before, while the new flexibility will allow users to adapt it to their own particular needs.

References

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