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A New Static Field Solver with Open Boundary Conditions in the 3D-CAD-System MAFIA*

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A NEW STATIC FIELD SOLVER WITH OPEN BOUNDARY CONDITIONS IN THE 3D-CAD-SYSTEM MAFIA

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Abstract: Numerically solving MAXWELL's equations involves calculation in a finite volume enclosing the structure of interest. Using simple DIRICHLET - or NEUMANN-boundary conditions causes inaccuracies or demands excessively large meshes. For a static problem, which can be reduced to a scalar potential problem, described by POISSON's equation, one can formulate more accurate boundary conditions. A multipole expansion of the well-known solutions of the POISSON equation can be used to yield better boundary values from the neighbouring inner potentials. This modified formulation is used in solving electro- and magnetostatic problems with the newly-added solver of the 3D-CAD-system MAFIA, which solves MAXWELL's equations for a very broad range of applications.

Structure of the Codes

MAFIA [1] is a set of codes intended for use in computer-aided design of three-dimensional magnets, rf structures, electrostatic devices, and structures, where transient effects are important. The electro- and magnetostatic solver S3 is an addition to this set of codes, whose broad range of applications in solving MAXWELL's equations in the frequency - and time domain is now enlarged by the capability of solving static problems.

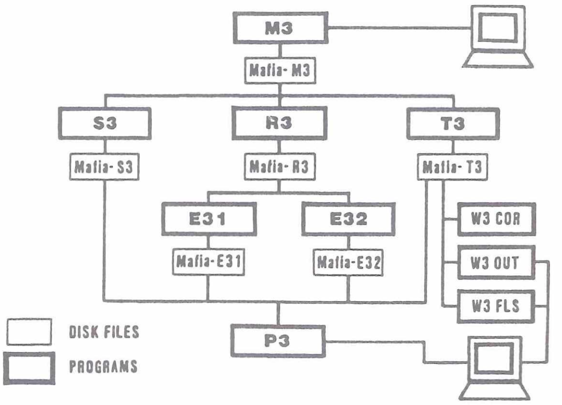

Fig.1 The MAFIA system with its interrelationships

Figure 1 illustrates the structure of MAFIA including the static solver.

- All codes use M3 to generate a mesh which describes the physical problem. It produces a file containing all mesh and material distribution data, but no material properties.
- In the frequency domain R3 sets up the matrix system by using the data from M3 and adding the material properties and boundary conditions. E3X is a package of eigenvalue-solvers for this matrix system.
- The static code S3 also consists of two parts. One part sets up the reduced system for the potentials, incorporating the boundary conditions, material distribution and in the magnetostatic case the current distribution. The second part incorporates the open boundary conditions and solves the resulting system with a SOR-method and a multigrid method. The solver determines potentials, fields and in the electrostatic case the charge distribution on metal surfaces.
- In the time domain T3 solves MAXWELL's equations using a leapfrog scheme for time stepping an initial boundary value problem.
- P3 is a postprocessor for all three domains. It is a tool for interpretation of the solutions by plots of fields, contour lines and evaluation of additional results such as energy, forces, integrals etc.

The General Method

The solution of MAXWELL's equations is done by the Finite Integration Technique (FIT) [2]. This algorithm solves the equations in a first order approximation, where line integrals or surface integrals are replaced by mean field values times step length or areas. The allocation is done following YEE (Figure 2) [3]. That is, the electric field components are allocated at the midpoint of the line connecting two grid-points and the magnetic flux vectors are allocated at the center of the surfaces of the mesh cells perpendicular to these surfaces. This allocation has the advantage that only continuous quantities occur, even when each cell is filled with a different material.

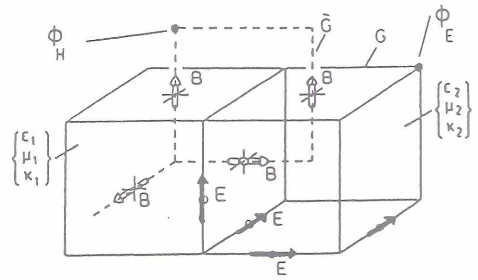

Fig. 2 Allocation of unknown field components and potentials on the grid

With this algorithm MAXWELL's equations reduce to a set of matrix equations, where all operators ('curl', 'div', line integration, surface integration) are represented by a set of sparse and banded matrices, partly defined on the grid and partly defined on the dual grid, where $\vec{E}$ and $\vec{B}$ interchange roles (broken lines in Figure 2).

The Method for Electro- and Magnetostatics

For the static case there are only two non-trivial equations to solve. A further simplification is that it is not necessary to describe the problem by vector fields or vector potentials. In electrostatics one has to solve

$$\oint \vec{E} \cdot d\vec{s} = 0 \qquad (1)$$

$$\iint_V \varepsilon\vec{E} \cdot d\vec{A} = \iiint \rho dV . \qquad (2)$$

From (1) it follows, that one can replace $\vec{E}$ by

$$\vec{E} = - \text{grad}\, \phi_E \qquad (3)$$

Using a scalar potential fullfills (1) automatically. The matrix formulation [4] of (2) is

$$\boxed{\tilde{S} D_\varepsilon \tilde{D}_A \tilde{S}^t \phi_E = q_e} \qquad (4)$$

where the potentials and charges are allocated at the gridpoints (Figure 2).

In magnetostatics one has to solve

$$\iint_V \mu \vec{H} \cdot d\vec{A} = 0 \qquad (5)$$

$$\oint \vec{H} \cdot d\vec{s} = \iint_A \vec{J} \cdot d\vec{A} \qquad (6)$$

By separating the part from the field with curl

$$\oint \vec{H}_c \cdot d\vec{s} = \iint_A \vec{J} \cdot d\vec{A} \qquad (7)$$

$\vec{H} - \vec{H}_c$ is 'curl-free' and can also be replaced by the gradient of a scalar potential [5]. If one obtains the part of the field with curl from the current distribution e.g. with the BIOT-SAVART law, one ends up with

$$\iint_V \mu \, \mathrm{grad}\, \phi_H \cdot d\vec{A} = \iint_V \mu \vec{H}_c \cdot d\vec{A} \qquad (8)$$

or in matrix formulation

$$\boxed{S D_\mu D_A S^t \phi_H = q_m} \qquad (9)$$

with $$q_m = - S D_\mu D_A h_c \qquad (9a)$$

to solve. In these equations:

- $S(\tilde{S})$ is the matrix operator for 'div' on the grid (dual grid) with dimension $(3N \times N)$.
- D_μ, D_ε are diagonal matrices with dimension $(N \times N)$ describing the material properties for each meshcell including tensorial components.
- $D_A(\tilde{D}_A)$ is the matrix operator for the surface integration on the grid (dual grid) with dimension $(N \times N)$.
- $S^t(\tilde{S}^t)$ is the matrix operator for 'grad' on the grid (dual grid), with dimension $(N \times 3N)$, which comes out to be the transpose of the 'div' operator in the matrix formulation [4].
- ϕ_E, ϕ_H, q_e, q_m are vectors of dimension N, containing the electric and magnetic potentials and the electric and magnetic charges.
- h_c is a vector of dimension 3N containing the part of the magnetic field with curl.
- N is the number of gridpoints of the mesh.

Equations (4) and (9) have an identical structure, if one interprets q_m, resulting from the current distribution, as a set of (unphysical) magnetic charges. Both are POISSON- equations and can be solved by the same procedure.

Up to this point, S3 is very similar to the static code PROFI [6]. The advantages, however, will be the easier handling of input and results, for S3 can use all the features of the MAFIA system. It will also be faster for large problems due to the optional multigrid solver. The most important improvement, however, is the incorporation of open boundary conditions.

Open Boundary Conditions

The simple boundary conditions one normally imposes cause inaccuracies when DIRICHLET conditions are used. To minimize them, one has to choose a very large mesh to insure that the structure calculated is far enough from the boundaries. For magneto- and electrostatic problems one can choose more accurate conditions with a procedure similar to the recently reported extension of 2D-POISSON [7]. The general form of the solution of POISSON's equation is given by the convolution of the right hand side "charges" with the corresponding GREEN's function. In the 3D case one gets

$$\phi_{E,H}^{(\vec{r})} = - \frac{1}{m} \iiint \frac{\rho_{E,H}(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} d^3 \vec{r}\,' \qquad (10)$$

$$m = \varepsilon \text{ or } \mu$$

This solution can be expanded in a TAYLOR-series, the single contributions of which are known as the multipole moments of the "charge"-distribution. In discrete form the first terms are

$$\phi_{E,H}^{(r)} = - \frac{1}{m} \cdot \sum_{i=1}^{n} \left\{ \frac{q_i}{r} - \frac{\vec{e} \cdot \vec{d}_i}{r^2} + \frac{1}{2} \frac{(\vec{e})_\ell (\vec{e})_k \cdot Q_i^{\ell k}}{r^3} \cdots \right\} .$$

$$m = \varepsilon \text{ or } \mu \qquad (11)$$

If the distances of the charges to the boundaries are not too small, an expansion in the lower moments is appropriate to get an accurate description of the potentials at the boundaries.

The coefficients of the monopole, dipole and higher moments are in general unknown. We investigated two different algorithms to determine them.

1) Substituting the ordinary DIRICHLET-conditions by a local NEUMANN-condition. For each surface meshpoint we use the well-known behaviour of the multipole solution as a function of radius, to determine the local normal derivative.
2) Determining the potential values of the multipole expansion at each point of the grid surfaces and using those as boundary values. This must be done in an iterative process. Starting with the ordinary DIRICHLET-conditions, one determines a first coarse charge distribution. Using this one modifies the boundary conditions accordingly and runs the solver again until the solution, including the boundaries, converges.

The first algorithm has up to now proved to be faster and more easy to handle.

First Results

a) Electrostatics

The SOR-solver can handle problems with common boundary conditions plus open local NEUMANN conditions. The multigrid solver exists already and has only to be adapted to the MAFIA-program structure. The multipole expansion can be chosen with just the monopole contribution or with up to the quadrupole contributions. All test calculations up to now show that in principle the monopole term is sufficient, if one is not dealing with pure dipole or quadrupole distributions.

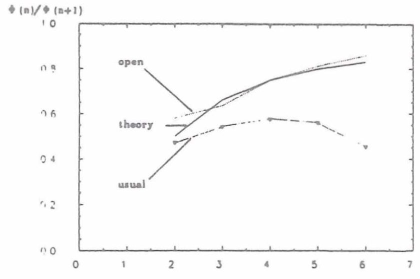

Fig. 3 Behaviour of a pointcharge potential as function of radius. Comparison between analytic (−) and numerically calculated behaviour with (...) and without (∇) open boundaries.

Calculations of simple problems that can be checked analytically indicate that even for fairly small calculation volumes a much better qualitative behaviour of the solutions at large distances can be achieved.

In Fig. 3 one clearly can see the adverse effect of the boundary in the case without open boundary conditions.

The numerical check of the relation $\iint_V \epsilon \vec{E} \cdot d\vec{A} = \iiint \rho dV$ using the calculated solution gives additional information of the solution's quality and of the charge distribution on metal surfaces. There follow some examples of electrostatic calculations, plus a comparison with the usual DIRICHLET-conditions. The plots show a 3D-M3 output of the material distribution and a 2D-cut with equipotential lines created by the postprocessor P3:

1) Parallel plate capacitor

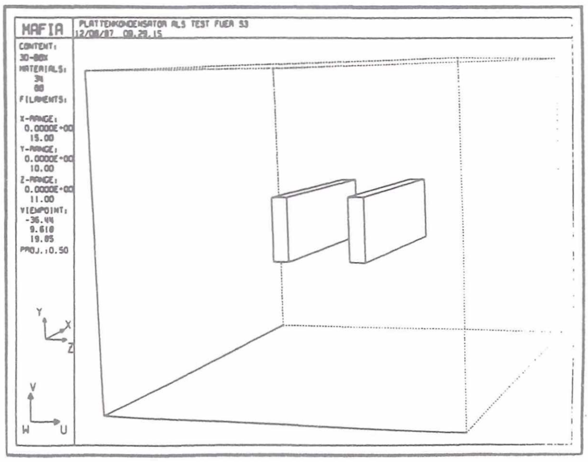

Fig. 4a 3D-material distribution

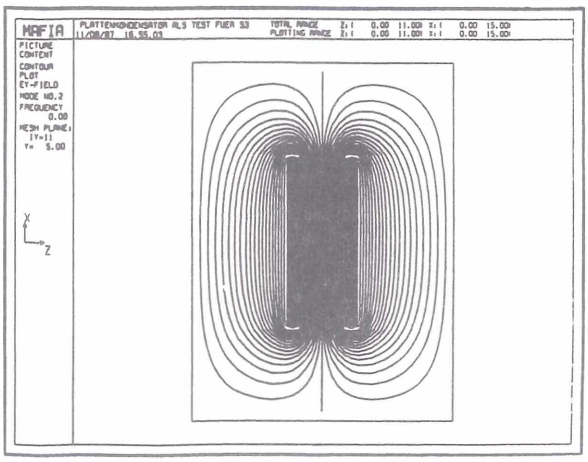

Fig. 4b Equipotential lines with ordinary boundary conditions

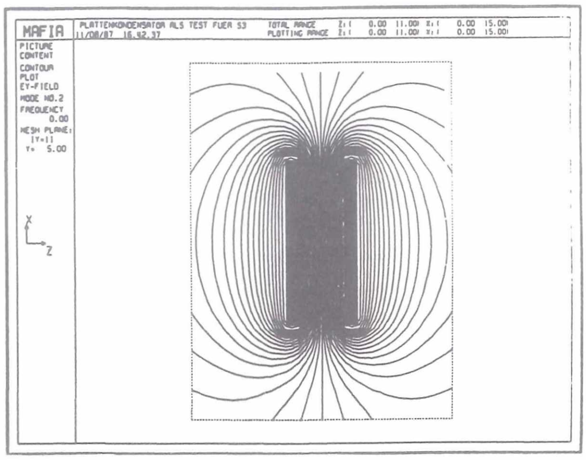

Fig. 4c Equipotential lines with open boundary conditions

2) At DESY a large new p^+-e^- collider named HERA is under construction [8], [9]. One of the two big detectors for high energy physics is ZEUS [9]. This example shows the calculation of a possible design of a muon drift chamber used in this detector.

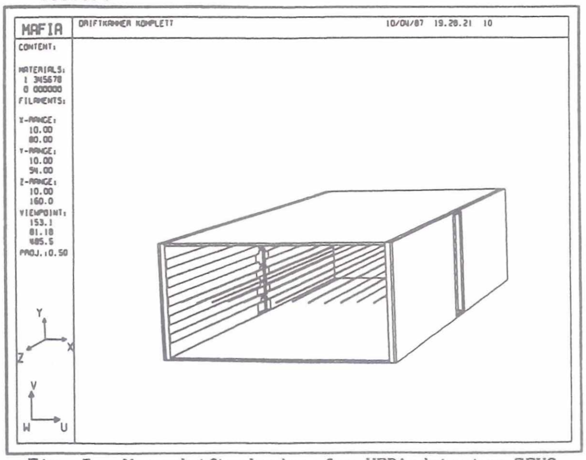

Fig. 5a Muon drift chamber for HERA-detector ZEUS

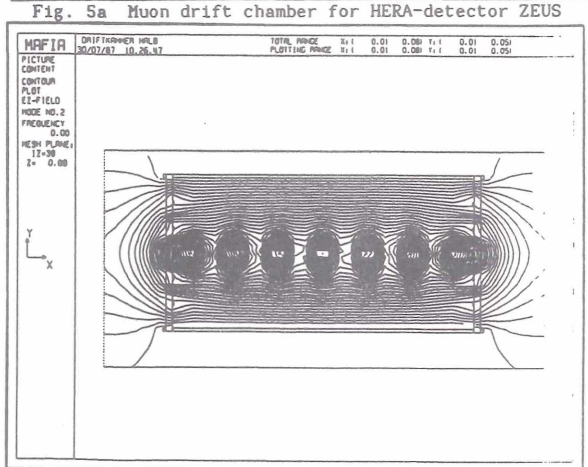

Fig. 5b Equipotential lines of ϕ_E in the symmetry plane of the drift chamber

3) Another increasingly important electrostatic device is the radiofrequency quadrupole (RFQ) [10]. It is used e.g. as a focussing, accelerating and bunching device to get low energetic heavy particles p^+, H^-...) into a linac-structure. This example shows the calculation of potentials in the end region of such an RFQ.

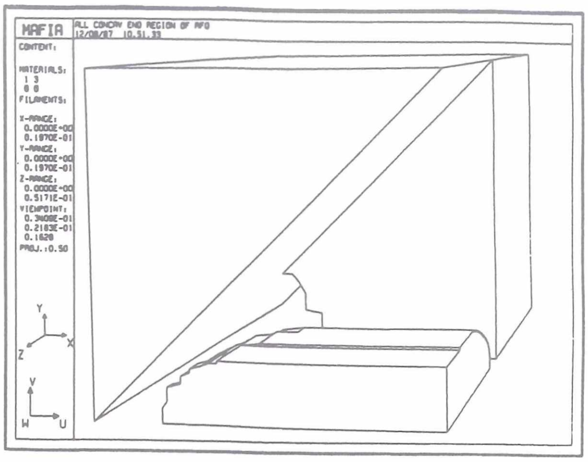

Fig. 6a 3D-plot of one fourth of the end region of an RFQ

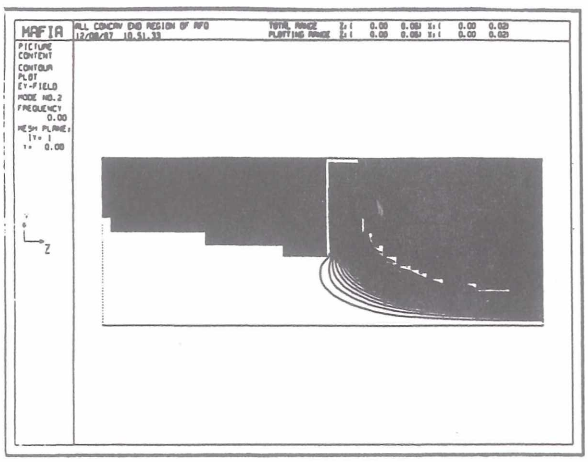

Fig. 6b Equipotential lines of ϕ_F in a cut of one of the symmetry planes

b) Magnetostatics

The magnetostatic solver is undergoing final tests. In a first step we determine the part of the magnetic field with curl due to the current distribution, using the method in PROFI [6], [11] or optionally a modified approach adapted to open boundary conditions. Also the BIOT-SAVART solution is a choice, though more cpu time consuming.

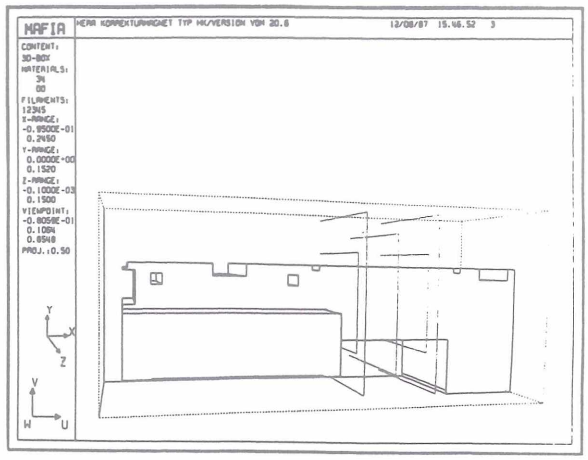

Fig. 7 A typical material input for a magnetostatic calculation including a permeable material and current filaments.

In the second step the description of the 'curl-free' part by a static potential makes it possible to solve magnetostatics problems with the electrostatic solver.

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