3D- MAGNETO- AND ELECTROSTATIC CALCULATIONS USING MAFIA-S3

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Abstract

We report on S3, the static solver in the MAFIA group of codes[1] for numerically solving Maxwell's equations. This code is capable of an improved formulation of boundary conditions when dealing with boundaries towards an unbounded domain. We will demonstrate the resulting improvements in the solution and report on first preliminary applications and their results.

Introduction

As reported [2], the MAFIA group of codes is extended by a solver for electro- and magnetostatic problems. For pre- and post-processing it uses the MAFIA modules M3 and P3 and thus the same approach of FIT-method (Finite Integration Technique)[3] and staggered grid allocation [4] for formulation of the relevant equations. The main emphasis in developing this code has been put on the improved formulation of boundary conditions when the calculation volume is an unbounded domain and on a fast performance (fast $\vec{H}'$-field calculation and a multigrid solver for big problems).

Boundary conditions at open boundaries

The accurate modelling of boundary conditions is an essential part in defining a physical problem described by differential equations. When dealing with a problem in an unbounded domain, this is not always easy to perform. Symmetry planes and materials with confining properties can easily be modelled by Dirichlet- or Neumann boundary conditions. But open boundaries in terms of these boundary conditions are inaccurate and memory consuming. For an analytic approach to the solution of differential equations open boundaries can be moved towards infinity and the vanishing of fields at infinity can be used for correct formulation of boundary conditions.The requirement of a finite calculation volume in numerically solving a problem leads to a half-hearted approach. In defining a huge mesh, open boundaries occur in a large but finite distance from the structure of interest. There the boundary conditions for infinity are imposed.The huge mesh requires a lot of memory, the boundary values imposed are inaccurate and, for the boundary shape does in general not coincide with the shape of isovalue planes, one introduces wrong field shapes also.

We introduced a procedure [2], that uses an analytic approximation for these boundary values and couples them to the equations describing the inner domain. This analytic approximation can easily be obtained from the multipole expansion of the current- or charge-distribution inside the volume of interest.

The description of static problems can be reduced to Poisson's equation [5,8]

$$\int\int_V mgrad\phi \cdot d\vec{A} = Q \tag{1}$$

where $m = \epsilon, \mu$ and $Q = \int\int\int \rho d\vec{V}$ or $Q = \int\int_V \mu\vec{H}' \cdot d\vec{A}$ representing the charge or current distribution. The general solution of Poisson's equation

$$\phi(\vec{r}) = -\frac{1}{m}\int\int\int \frac{Q(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3\vec{r}' \tag{2}$$

expanded in a Taylor series is the aforementioned multipole expansion

$$\phi(\vec{r}) = -\frac{1}{m}\{\frac{q}{r} - \frac{\vec{e}\cdot\vec{d}}{r^2} + \frac{1}{2}\frac{(\vec{e})_l(\vec{e})_k Q_{lk}}{r^3} - ...\} \tag{3}$$

where q represents the total charge, $\vec{d}$ is the dipole moment, Q_{lk} is the quadrupole tensor and $\vec{e}$ is a unit vector. So, using the inner current- or charge-distribution of the problem,

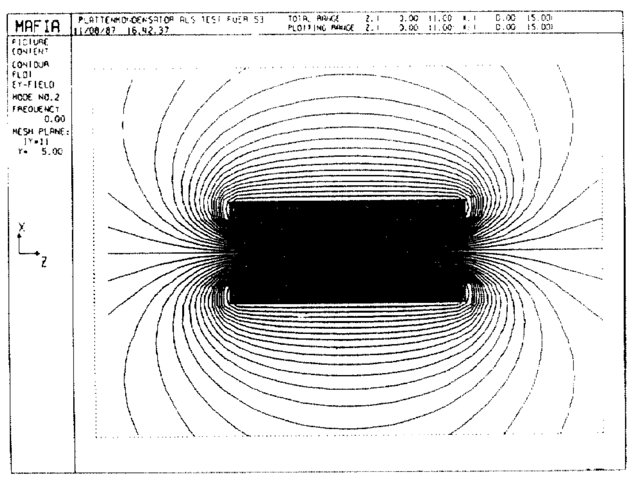

Figure 1a: The parallel plate capacitor calculated with open boundary conditions. Here and in the next figure you see a 2D cut of the 3D calculation showing equipotential lines of the electric potential.

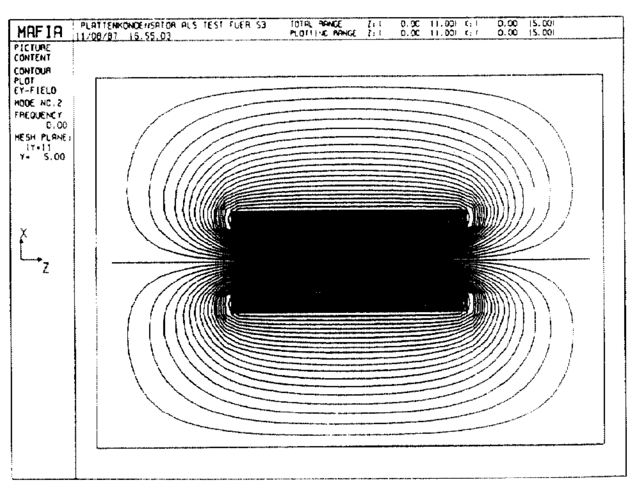

Figure 1b: The parallel plate capacitor calculated with ordinary Dirichlet boundary conditions.

each boundary point can be described with arbitrary accuracy, depending on the number of multipoles taken into account. This can be done in locally calculating ϕ at the open boundaries.Or, using that (3) is only r-dependent, $\partial\phi/\partial n$ can be calculated.Both methods have been programmed.The latter allows an easier iteration scheme but might cause mathematical problems in applications with Neumann conditions at all boundaries. There will be further testing which method is the best. In electrostatics, tests up to now seem to indicate that the quadrupole as highest multipole contribution is sufficient for most applications, for higher multipoles vanish rapidly towards the boundaries.In magnetostatics higher order multipoles might be important.

Prove of principle

With a fairly simple three dimensional parallel plate capacitor the power of this formulation of open boundaries can easily be demonstrated. We made calculations on a farily small mesh, comparing a run with open boundary conditions to one with ordinary Dirichlet conditions.Figure 1a shows that the solution seems not to be influenced by the boundaries, while in figure 1b you see the fieldshaping influence of the Dirichlet boundary. Another fairly easy way to demonstrate the improvements is, comparing the potentials of a problem calculated analytically to the solutions calculated numerically using both approaches for the open boundary conditions. Figure 2 shows the comparison of the qualitative behaviour of a pointcharge potential calculated in the three different ways.

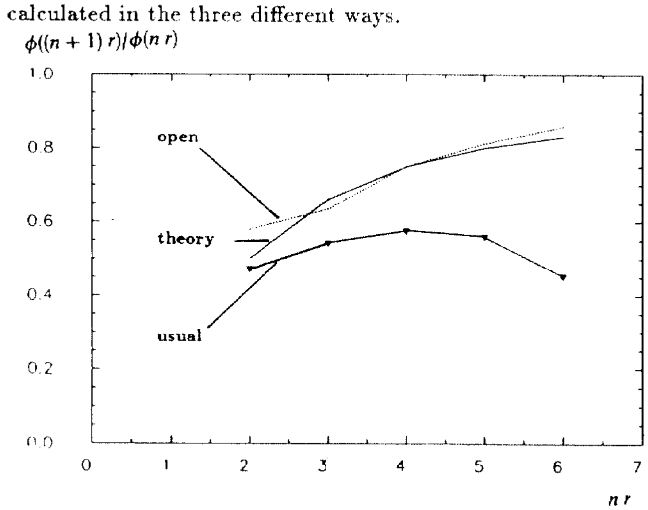

Figure 2: Qualitative behaviour of the pointcharge potential. Here the ratios of potential values at equidistant steps r are plotted. They should behave like n/(n+1).The comparison for analytically(-) and numerically calculated results with(...) and without(▼) open boundaries are plotted.

First applications in electrostatics

First applications here show that it is necessary to put the code in a form that allows calculations with a big number of meshpoints. A lot of information users want to deduce from field calculations depends very senitive on the field accuracy. In collaboration with the ZEUS detector group we calculated the electric fields for the forward/rear driftchamber of this detector(figure 3)[11]. ZEUS is one of the two high energy physics experiments at the new DESY p^+, e^- collider HERA [6,7]. The aim of a numerical modelling of this chamber was a parameter study to find an optimal set of potential values for the field shaping strips to get a homogenuous electric field in the drift region, which should cover most of the chamber.[12] And to get a realistic idea of the chamber's gas amplification, determined by the electric field close to the wire surfaces. Most of the modelling has been done with a PROFI [8,12] 2D approach due to memory problems. But the testchamber, used for calibration, has a geometry that requires a 3D calculation and due to a dielectric window there are open boundaries to be modelled accurately. These changes in the testchamber construction compared to the chamber used in the detector later might be important to judge the quality of the calibration done with this chamber. For to know the gas amplification with an accuracy of 1 %, one needs to know the electric field with an accuracy of about 0.05 %. To achieve accuracies in this order of magnitude demands a very fine and well behaved mesh. Which requires a lot of memory in itself, memory you do not want to

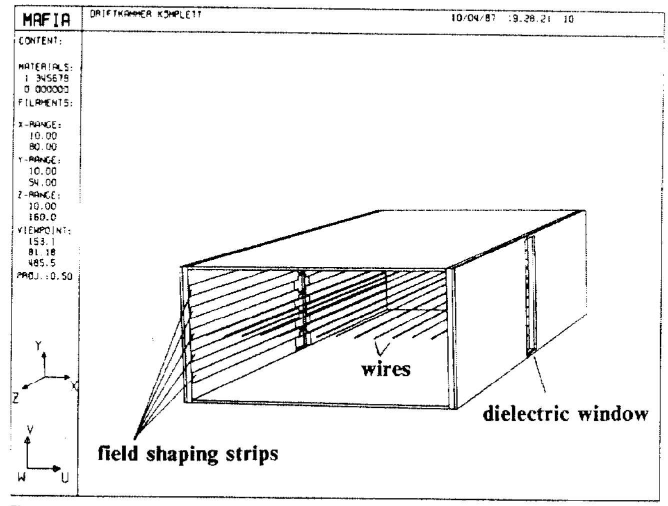

Figure 3: The FTD/RTD driftchamber of the ZEUS detector.This is the design of the test chamber used for laser calibration of the chamber's gas amplification.The driftchamber will be used as trigger for other detector components and due to a high resolution (100 μ) will be important for path reconstruction.

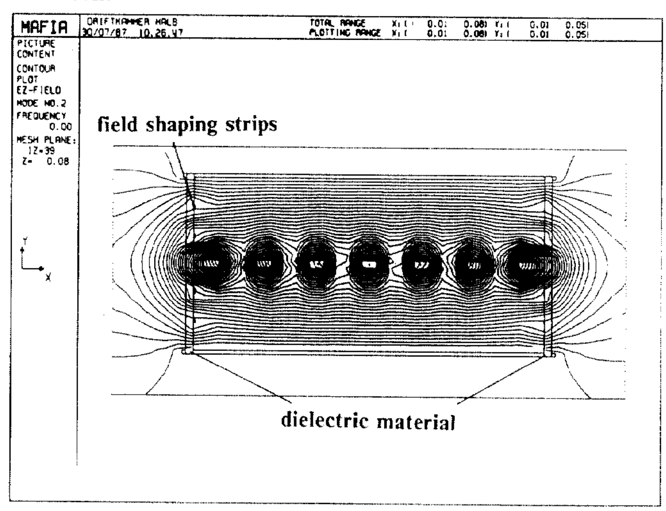

Figure 4: Equipotential lines in a cut through the dielectric window.One can see the influence of the window on the solution even in this preliminary run with a coarse mesh.

use on the modelling of open boundaries instead, as codes with the ordinary way to treat open boundaries would require.
Our 3D calculations performed quite well for the homogenuous part of the chamber.Also the influence of the dielectric window on the gas amplification could be demonstrated qualitatively with the cost of a few extra meshplanes. Only close to the wires the mesh could not be defined fine enough, due to memory problems.For this reason a better simulation of lines of constant potential, simulating thin wires, has been introduced in addition to the standard MAFIA-preprocessor input and has to be tested now.
This example required a huge mesh(140.000 mesh points), high accuracy, full 3D treatment and open boundary conditions.On an IBM 3084 it took about 30 minutes of cpu-time with the SOR solver to obtain these results.They indicate that with a few improvements that are easy to incorporate, S3 is a useful tool for designing electrostatic devices.

Magnetostatics

In codes that numerically solve Maxwell's equations for magnetostatics, it is a common technique to reduce the problem -like in electrostatics- to one described by Poisson's equation for a scalar potential. This is done by splitting the magnetic field into two parts [9]. One part is $\vec{H}'$ that in a pure mathematical sense represents all contributions of the constant currents $\vec{J}$.This means $\vec{H}'$ is a solution of

$$\oint \vec{H}' \cdot d\vec{s} = \int\int_V \vec{J} \cdot d\vec{A} \qquad (4)$$

This is in general not a sourcefree physical field.So it has to be corrected by a second part that comes up for the sources introduced

$$\int\int_V \vec{H}' \cdot d\vec{A} = -\int\int_V (\vec{H} - \vec{H}') \cdot d\vec{A} \qquad (5)$$

with

$$\oint (\vec{H} - \vec{H}') \cdot d\vec{s} = 0 \qquad (6)$$

For all current contributions are already represented by $\vec{H}'$, $(\vec{H} - \vec{H}')$ can be described by a scalar potential ϕ_H and the sum of both $\vec{H}' - grad\phi_H$ is the physical field that solves both of Maxwell's equations simultanuously.So the magnetostatic problem is reduced to a direct solution for $\vec{H}'$ given by the currents and by an iterative solution for ϕ_H,where the same procedure as in electrostatics can be used. The fact that $\vec{H}'$ only has to fulfill the mathematical requirements of (4) gives a lot of freedom for its construction . Even so some procedures used in distributed codes need a tricky strategy to do this construction. We use a new and simple procedure developed at KfA Juelich [10] that guarantees an easy performance independent of the type of problem and boundary conditions. This easy procedure even allows to choose $\vec{H}'$ in a way that makes its contributions small in permeable materials and so reduces the problem of cancellation errors compared to other procedures. First preliminary runs for magnetostatics indicate that the new procedure for $\vec{H}'$ is as easy to handle as the mathematical theory states.First applications, accuracy tests and cpu time comparisons are just starting.

Final remarks

Up to a few improvements and additions to be made, the S3 module has been put together.Compared to other codes improvements have been made in the treatment of open boundaries, in the calculation of the part of the magnetic field described by the "curl"-equation alone and as a fast solver a multigrid solver has been added as optional choice. Now a phase of testing and comparing with measurements and other established codes begins.

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