Excerpt from the Proceedings of the 2011 COMSOL Conference in Stuttgart

Benchmark of COMSOL vs. ROXIE Codes for the Calculation of a Particle Accelerator Quadrupole

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Abstract: The field quality requirements of most particle accelerator magnets are very tight and, therefore, very precise simulations are needed to accurately calculate these devices. CERN's ROXIE [1] code is widely used as a reference software to calculate normal conducting and superconducting magnets for particle accelerator applications. ROXIE uses the full vector potential coupled to the BEM-FEM method to develop the magnetostatic calculations, so it does not require meshing neither the coil nor the air region of the model. However, COMSOL Magnetic Fields Interface uses the magnetic vector potential FEM and requires meshing both the coil and the air regions. The comparison of both codes in terms of precision, memory requirements and time of solution is presented in this paper. The parameterized model of a typical resistive quadrupole has been used for the comparison. The quadrupole iron is very saturated and therefore its solution requires many non-linear iterations. The precision of the solution is calculated by applying the FFT to the magnetic field data.

Keywords: particle accelerator, quadrupole, field quality, FEM codes, benchmark.

1. Introduction

The magnets are used in particle accelerators to deflect, focus or correct the beam of particles along the accelerator trajectory [2]. They can be classified depending on the shape of the magnetic field that they produce: dipoles, quadrupoles, sextupoles, octupoles, etc. Although the field of magnets can be ramped (it can be variable in time), most of the magnets are calculated as magnetostatic devices. Therefore, the Maxwell equations for magnetic fields are reduced to:

$$\vec{\nabla} \times \vec{H} = \vec{J}_s \tag{1}$$

$$\vec{\nabla} \cdot \vec{B} = 0 \tag{2}$$

The design and optimization of most particle accelerator magnets is dominated by the requirements of an extremely uniform field, in the order of 10^{-4} parts of the field magnitude. The precise position of the coils, the conductors in coils and the iron pole profile (for iron dominated magnets) are the typical geometrical aspects that need to be precisely simulated for the field calculation.

Several numerical methods are used by the different FEM codes for simulating magnetostatic fields in the presence of currents and non-linear magnetic materials (soft iron). ROXIE (Routine for the Optimization of magnet X-sections, Inverse field calculation and coil End design) [1] is a CERN code widely used for calculating many of the particle accelerator magnets all around the world. In this document, only COMSOL and ROXIE codes will be compared. Other software solutions like ANSYS® can solve magnetostatic problems using several numerical methods like general, difference and reduced scalar potential, vector potential and edge-based vector potential. COMSOL 4.2 can use the full vector potential or the reduced vector potential methods (reduced + background field) and ROXIE mainly uses the full vector potential BEM-FEM method (currents + magnetization).

A model of a quadrupole magnet is developed in this paper in order to benchmark both COMSOL and ROXIE codes in terms of precision, memory requirements and time of solution. The shape of an ideal quadrupolar field is presented in Figure 1.

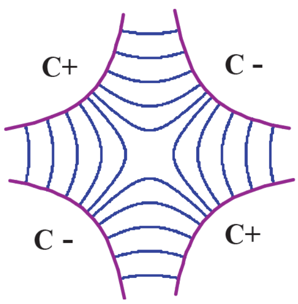

Figure 1. Quadrupolar field shape

The lines of constant scalar potential (in purple) define the iron pole shape. The lines of flux density (in blue) show the focusing effect on charged particles travelling off-axis and perpendicularly to them, according to the magnetic part of the Lorentz equation:

$$\vec{F} = q \cdot (\vec{v} \times \vec{B}) \tag{3}$$

2. Quadrupole specifications

The basic quadrupole design parameters are summarized in Table 1.

Table 1: Initial Specifications of the Quadrupole

Magnitude	Value	Units
Pole tip radius	31.5	mm
Reference radius	21	mm
Maximum gradient (2D)	24	T/m
Iron length	100	mm
Iron yoke width	310	mm
Iron pole width	45.51	mm
Total magnet length (between coil-ends)	208	mm

An optimization process (in 2D and 3D) has been previously developed in ROXIE to obtain the adequate geometry of the quadrupole by maximizing the field quality. This process establishes the current, the coil size, the coil position, the iron shape and the other iron dimensions. The calculated geometry is used to build the magnetic models for benchmarking in ROXIE and in COMSOL.

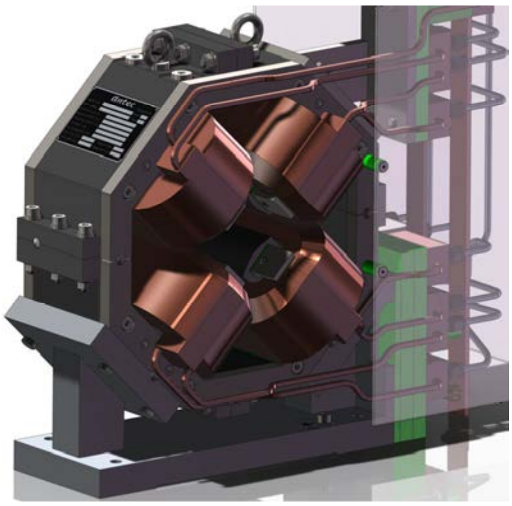

Figure 2. CAD model of the quadrupole

Each coil is wound using 78 turns of 5.5x5.5 mm insulated hollow copper wire. The current on each wire is 143 A, resulting in a total of 11154 A-turn per coil and 4.727 A/mm^2 averaged current density. The detailed coil dimensions for the magnetic model are shown in Figure 3.

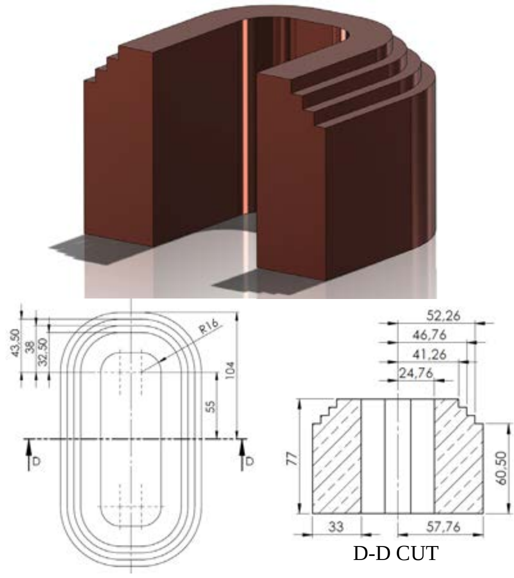

Figure 3. Coil model dimensions (in mm)

The iron dimensions of a quadrant are shown in Figure 4. The pole is the most important part of the geometry for the field quality. It is composed of a hyperbolic profile, $y=r^2/(2x)$, and a tangent straight line starting at 10.3 mm from the pole axis.

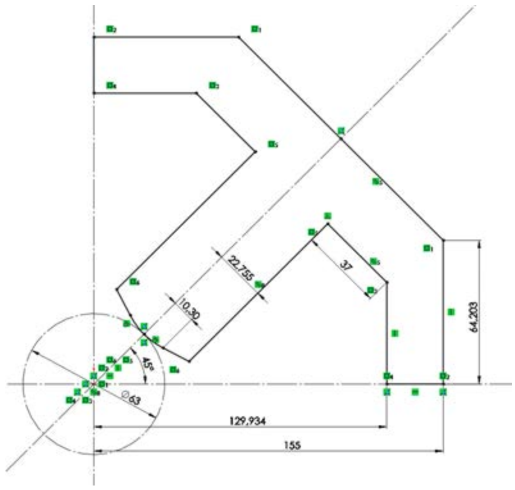

Figure 4. Iron cross-section dimensions (in mm)

3. COMSOL calculations

The previously presented geometry has been parameterized in COMSOL to produce a magnetic model. The Magnetic Fields Interface has been used for the simulation, solving the problem for the full magnetic vector potential. A parametric sweep has been defined to get the solution at some different excitation levels (10% and 100% of current).

3.1. 2D model

The 2D geometry is completely parameterized starting from a few geometrical dimensions. This parameterization is identical to the one used in ROXIE to ensure the same geometrical dimensions on both models.

Only an octant of the quadrupole has been modeled in COMSOL (Figure 5), using a Perfect Magnetic conductor boundary on the X axis. A cubic discretization of the magnetic vector potential has been selected to improve the solution precision of the model, given that the solution time is negligible in 2D. The non-linear behavior of the model is defined by selecting the HB curve of a magnetic material (ARMCO® pure iron). The other two materials are copper and air.

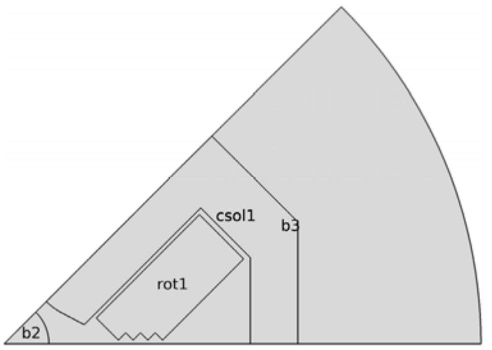

Figure 5. 2D COMSOL model of the quadrupole

A specific air zone (*b2*) has been created in the aperture of the magnet in order to reduce the size of the mesh and to improve the solution. The pole shape also has specific meshing commands to ensure a good discretization. The solution (Figure 6 and Figure 7) has been calculated using the default solver parameters.

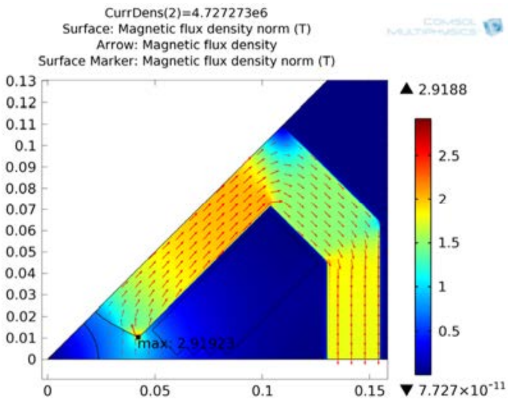

Figure 6. Magnetic flux density in COMSOL

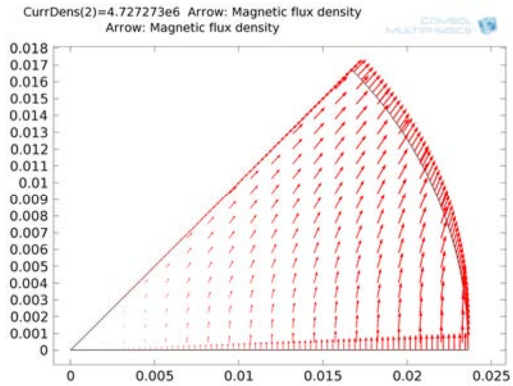

Figure 7. Vector field in the *b2* air zone

A 2D parameterized curve has been defined for the post-processing of fields. This curve defines a 21 mm radius (*rref*) arc centered in the origin of the model. The radius of *b2* zone (Figure 7) is a bit larger to include the *rref* curve. The radial component of the magnetic field, B_r, is calculated on *rref* arc versus the positioning angle (*acos(x/rref)*), being the expression B_r*=(mf.Bx*x/rref) + (mf.By*y/rref)*. The radial field is zero on *X* axis and maximum at 45 degrees for an ideal quadrupolar field. The variation of the radial field is purely sinusoidal for a perfect quadrupolar field. Therefore, a Fourier analysis of these data can be carried out to get the deviations from the ideal sinusoidal shape. These deviations are called the field harmonics and they numerically define the field quality of a given field distribution with high precision.

A MATLAB program has been developed to calculate the Fourier analysis of the COMSOL data. The results obtained for this model are presented in Table 2 up to the harmonic number 18. Higher order harmonics are negligible for this quadrupole.

Table 2: 2D harmonics for the COMSOL model

Harmonic	Value (T)	Value (pu x10^{-4})
2	**0.5054131686**	**10000**
4	6.161778e-18	1.21915e-13
6	**0.0016098131**	**31.85142914**
8	-3.533460e-18	-6.9912e-14
10	**0.0001160668**	**2.296474041**
12	1.510835e-18	2.98930e-14
14	**-1.840054e-05**	**-0.36406927**
16	-1.311237e-18	-2.5943e-14
18	**-1.683019e-06**	**-0.03329987**

Only the even harmonics are calculated due to the symmetry of the data. The "allowed" harmonics due to the symmetry of the quadrupolar field are 2, 6, 10, 14… and the rest of the results are small numerical errors.

The harmonic number 2 is the main quadrupole field and all the other harmonics are referenced to them in the third column of Table 2. The main figures of these results are the values of the harmonics b6=31.85, b10=2.296 and b14=-0.364, in units of 10^{-4}.

3.2. 3D model

The 3D model has been extruded from the 2D cross section up to the half iron length, afterwards modeling the 3D curved coil ends. Therefore, the symmetry used is 1/16th of the full quadrupole (Figure 8). All the 3D geometry has been parameterized and developed inside COMSOL by using multiple workplanes to extrude the different solids. The air completely surrounds the quadrupole up to an adequate radius (1.5 times the yoke radius) and length, to ensure a good accuracy in the solution (no infinite elements have been used).

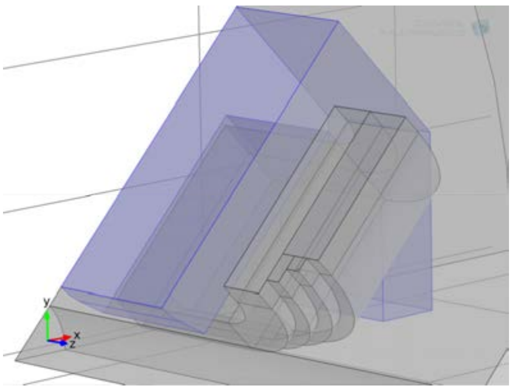

Figure 8. 3D COMSOL model of the quadrupole

The most challenging job for this model is the energization of the coils by only using the Magnetic Fields Interface of COMSOL. The "Electric Currents" and the "Magnetic Fields" interfaces can be combined to achieve a solution while making the coil energization easier (using a multi-turn coil trick). However, the solution precision has been proved not as good as for the "Magnetic Fields Interface" alone, and the solution time is much longer.

Several "External Current Density" definitions have to be independently applied to the geometry according to the straight-curved geometry of the coils. Several parameterized auxiliary coordinate systems are defined for the application of the external current density in each coil part. A rotated cylindrical system is used for the curved parts of the coil, and some rotated Cartesian systems are used for the straight parts.

The model has been solved using three different quality meshes (fine, coarse and coarser, all using quadratic discretization) to compare the precision and the solution time. Special care has been taken to mesh the pole profile and the air zone inside the aperture.

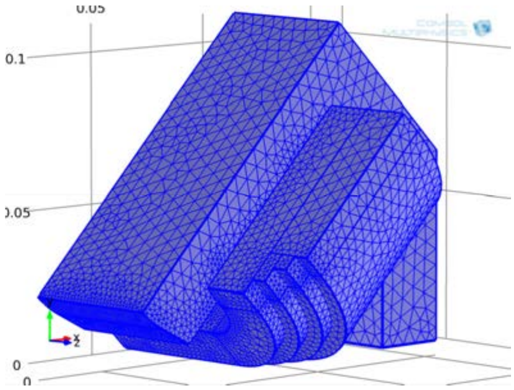

Figure 9. Fine mesh for the yoke and coil

The solver parameters are the default ones, except from the Predictor value in the Parametric option, which is set to constant. This is necessary to avoid an excessive long solution time of the second step (100% of current) due to a bad prediction of the initial conditions. COMSOL 4.2 has been used to solve the models, although they were modeled in the previous version.

Concerning the simulation results, the iron seems very saturated (Figure 10); even more than in the 2D model. This is due to the effect of the coil-ends in a short magnet. However, the peak field (and the auto scaled value in the plot) depends a lot on the plot quality parameters.

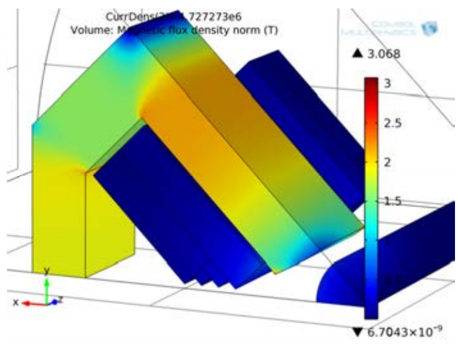

Figure 10. 3D magnetic flux density plot

The 3D harmonic analysis is very similar to the 2D model, but averaging the results on each transverse slice of the quadrupole for Z between 0 to 0.2 m. The 2D harmonic slices are calculated for Z=1 mm increments (201 harmonic analyses). A “Parameterized Surface” has been defined to calculate the field data in all the slices at a time. All the simulations have been developed in a 2 processor Intel Xeon E5620 @ 2.4 GHz (eight physical cores) with 24 GiB RAM.

The harmonic results for the fine mesh model are presented in Table 3 (at 100% of current). The solution time of this model was about 9.9 hours, and it used about 10 GiB of memory. For the coarse mesh model (Table 4), the solution time was about 3.4 hours, and it used about 5.4 GiB of memory. And finally, for the coarser mesh model (Table 5), the solution time was about 1.5 hours, and it used about 2.8 GiB of memory. All the results are very similar, which indicates that the mesh can be even coarser to increase the solution speed. Anyway, no more meshes have been simulated in order to find the precision vs. speed limit.

Table 3: 3D averaged harmonics in COMSOL for the fine mesh model (about 1x10^6 elements)

Harmonic	Value (T)	Value (pu x10^{-4})
2	**0.1402814757**	**10000**
4	1.590892e-18	1.13407e-13
6	**-4.004679e-05**	**-2.8547458**
8	-7.870655e-19	-5.6106e-14
10	**3.064928e-05**	**2.18484208**
12	3.120971e-19	2.22479e-14
14	**-4.547662e-06**	**-0.32418127**
16	1.578601e-19	1.12530e-14
18	**-5.770789e-07**	**-0.04113721**

Table 4: 3D averaged harmonics in COMSOL for the coarse mesh model (about 5.5x10^5 elements)

Harmonic	Value (T)	Value (pu x10^{-4})
2	**0.1402774138**	**10000**
4	1.557294e-18	1.11015e-13
6	**-4.072698e-05**	**-2.90331724**
8	-7.568610e-19	-5.3954e-14
10	**3.104489e-05**	**2.213107485**
12	3.606539e-19	2.57100e-14
14	**-4.504128e-06**	**-0.32108721**
16	1.708735e-19	1.21811e-14
18	**-5.019539e-07**	**-0.03578294**

Table 5: 3D averaged harmonics in COMSOL for the coarser mesh model (about 2.7x10^5 elements)

Harmonic	Value (T)	Value (pu x10^{-4})
2	**0.1402796821**	**10000**
4	1.581666e-18	1.12750e-13
6	**-4.078396e-05**	**-2.90733211**
8	-7.254137e-19	-5.1711e-14
10	**3.126175e-05**	**2.22853041**
12	3.591395e-19	2.56016e-14
14	**-4.482339e-06**	**-0.31952879**
16	1.580071e-19	1.12637e-14
18	**3.082246e-07**	**0.021972152**

The effective length is a characteristic distance that indicates the length of the magnet as if it had no coil-end effects, i.e. having a constant transverse field that abruptly falls at the ends. For a quadrupole:

$$l_{eff} = \left(\frac{1}{B_{r0}}\right) \cdot \int_{-\infty}^{\infty} B_r(z) \cdot dz \qquad (4)$$

where B_r is the radial field at the reference radius (*rref*), i.e. $sqrt(B_x^2+B_y^2)$. The result is 0.13213 m for all the COMSOL models.

4. ROXIE calculations

COMSOL applies a total vector potential FEM formulation, where the current density $\boldsymbol{J_s}$ appears on the right hand side of the differential equation. The consequence of this is that the relatively complicated shape of many coils has to be modeled in the mesh, in addition to the also complicated air volumes.

In ROXIE, the boundary-element method allows to split the vector potential $\boldsymbol{A}$ in two parts $\boldsymbol{A}=\boldsymbol{A_s}+\boldsymbol{A_r}$ where $\boldsymbol{A_r}$ is the vector potential due to the magnetization and $\boldsymbol{A_s}$ is the source potential of the free currents computed from Biot-Savart law. The source field is calculated by approximating the coils by line currents located at a determined conductor position in the coil. The coil does not have to be represented by the finite element mesh because it is part of the BEM domain.

ROXIE also contains the BEMFEM program [3]. The BEM-FEM method decomposes the physical problem into a BEM part, which represents the surrounding space as well as exciting currents, and a FEM part which contains the magnetic material. BEM is coupled to a full vector-potential FEM. Thus, the BEM-FEM coupling method does not require any meshing of the air region.

4.1. 2D model

The parameterized geometry has been defined in ROXIE using points, lines and areas. Quarter symmetry has been used for the 2D model because ROXIE does not allow using octant symmetry for the quadrupolar boundary conditions. However, this is not an issue for the 2D model, although a small mesh asymmetry can generate small “impossible” harmonics in the solution (b4, b8…). The coils are defined in several blocks and modeled as sets of a number of current lines coincident to the number of conductors of each block.

The iron mesh density is not as fine as in the COMSOL model, but ROXIE uses 8-node quad elements and curvilinear boundary elements for the iron profiles (circles, hyperbolas, etc.). This improves the mesh efficiency using a lower number of elements.

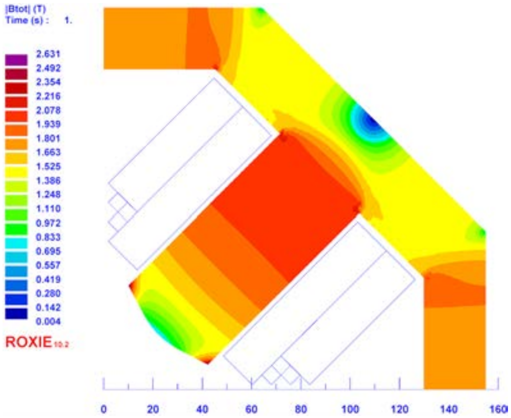

Figure 11. 2D magnetic flux density in the iron

The 2D ROXIE harmonic results are presented in Table 6. ROXIE automatically calculates the harmonics of the solution in the post-processing and thus, it is not necessary to use an external program.

Table 6: 2D harmonics for the ROXIE model

Harmonic	Value (T)	Value (pu x10^{-4})
2	**0.505586**	**10000**
4	4.1054e-07	0.00812
6	**0.0016**	**31.92239**
8	6.2187e-08	0.00123
10	**1.1584e-04**	**2.29122**
12	8.0894e-09	0.00016
14	**-1.8397e-05**	**-0.36388**
16	-1.5168e-09	-0.00003
18	**-1.6791e-06**	**-0.03321**

However, if the field data is exported from ROXIE and the harmonics are calculated using MATLAB, the results have been proved identical. Like in the previous COMSOL results, the main figures of the Table 6 are the values of the harmonics b6=31.92, b10=2.291 and b14=-0.3639, in units of 10^{-4}.

4.2. 3D model

The 3D model is easily defined in ROXIE starting from the 2D cross section. Symmetry of 1/8th has been used for the iron yoke (Figure 12). The coils and the surrounding air are outside the FEM domain and hence no symmetry is required.

Only one iron mesh quality has been used for the solution of ROXIE. The 3D mesh is defined in ROXIE as a number of elements in longitudinal (*Z*) cuts of the model, extruded from the 2D mesh. Ten longitudinal elements for the half iron (50 mm length) have been used. That produces a 3D mesh much more coarse than the coarser COMSOL model. Indeed, the number of elements used for the iron mesh in ROXIE are only 3060 (20-node hexahedral elements) with a total of 14971 problem nodes. In COMSOL, 43k elements are used in the iron of the coarser model (86k for comparison purposes due to the symmetry).

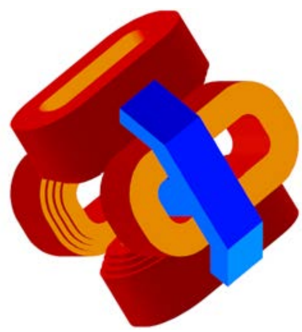

Figure 12. 3D model in ROXIE

The 3D harmonic results are presented in Table 7 (at 100% of current). To compare codes in the same circumstances, 201 2D harmonic analyses have been averaged to calculate the 3D harmonics. The solution time of this model (including the post-processing) was 4.9 hours. It is noticeable that the Newton-Raphson iterations converge in only 15 minutes, but the calculation of the fields in the aperture (data grid for the harmonic analyses, 3D line data for plots, etc.) need a much longer processing time in the BEM-FEM code. Every point evaluation in the BEM domain requires two numerical integrals over the BEM-domain boundary. In addition, ROXIE is not a multithreaded application and it cannot use the multiple cores of the machine. The maximum used memory is about 1.7 GiB in post-processing.

Table 7: 3D averaged harmonics in ROXIE

Harmonic	Value (T)	Value (pu $x10^{-4}$)
2	**0.1401099**	**10000**
4	-9.5345e-07	-0.06805
6	**-3.8093e-05**	**-2.71876**
8	-7.1456e-09	-0.00051
10	**2.9500e-05**	**2.10551**
12	1.0508e-08	0.00075
14	**-4.4482e-06**	**-0.31748**
16	-1.2610e-09	-0.00009
18	**-3.4747e-07**	**-0.02480**

The effective length calculated from ROXIE solution is 0.13209 m.

5. Results comparison

The B_y component of the magnetic flux density along the quadrupole length is plotted in Figure 13 for both codes. The *Z* coordinate is swept between 0 and 0.2 m while *X*=21 mm and *Y*=0.

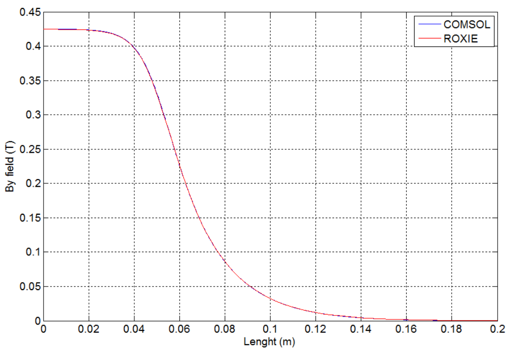

Figure 13. Magnetic field comparison along *Z*

A good agreement between ROXIE and COMSOL is observed in Figure 13. The maximum difference of the B_y component along *Z* is 8.95e-04 T (about 0.21 % of the maximum field). However, this difference is very constant and therefore it does not necessarily affect to the field shape (harmonic analysis), but it should affect to the integrated fields (effective length). Indeed, the harmonic components of the field are amazingly similar in both codes, even when the coarser COMSOL mesh is used (Table 8). ROXIE is much slower than COMSOL to obtain the huge amount of results in this comparison.

Table 8: Summary of the main results

	Value	COMSOL	ROXIE
2D	b6	31.8514 pu	31.92239 pu
	b10	2.29647 pu	2.29122 pu
	b14	-0.36407 pu	-0.36388 pu
3D	b6	-2.90733 pu	-2.71876 pu
	b10	2.22853 pu	2.10551 pu
	b14	-0.31952 pu	-0.31748 pu
	l_{eff}	0.13213 m	0.13209 m
	mem.	2.8 GiB	1.7 GiB
	time	1.5 h	4.9 h (15 min)

6. Conclusions

There is a great agreement in the field harmonic contents between the results of COMSOL and ROXIE codes, even when they are using totally different methods and very high precision is expected (one part in 10^4). The small disagreement in the absolute field results could be due to the very different iron meshes, but anyway it must be further studied.

If a high number of data points are to be calculated in the post-processing, ROXIE is much slower than COMSOL.

Nevertheless, ROXIE is still unbeatable in the calculation of 3D superconducting cosine theta magnets (in fact, it is its main purpose). These magnets use very complex multi-turn coils that are extremely difficult to model and mesh in a FEM code. In addition, the keystoning of the cables and the grading of the current density are also very difficult to implement in multipurpose FEM codes.

7. References

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