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A new submodelling technique for multi-scale finite element computation of electromagnetic fields: application in bioelectromagnetism

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Abstract. Complex multi-scale Finite Element (FE) analyses always involve high number of elements and therefore require very long time of computations. This is caused by the fact, that considered effects on smaller scales have greater influences on the whole model and larger scales. Thus, mesh density should be as high as required by the smallest scale factor. New submodelling routine has been developed to sufficiently decrease the time of computation without loss of accuracy for the whole solution. The presented approach allows manipulation of different mesh sizes on different scales and, therefore total optimization of mesh density on each scale and transfer results automatically between the meshes corresponding to respective scales of the whole model. Unlike classical submodelling routine, the new technique operates with not only transfer of boundary conditions but also with volume results and transfer of forces (current density load in case of electromagnetism), which allows the solution of full Maxwell's equations in FE space. The approach was successfully implemented for electromagnetic solution in the forward problem of Magnetic Field Tomography (MFT) based on Magnetoencephalography (MEG), where the scale of one neuron was considered as the smallest and the scale of whole-brain model as the largest. The time of computation was reduced about 100 times, with the initial requirements of direct computations without submodelling routine of 10 million elements.

1. Introduction

During the last decade considerable interests in large-scale multiphysics analyses were shown in different areas of research [1-4]. Due to increased computational power real-time calculations became possible. At the same time a large number of variuous true-scale analyses appeared to be performed. Nanotechnology and composite material science were the first fields where complex multi-scale FE simulations were used. Then electronics involved such analysis in research and development of various devices. Nowadays almost any R&D process requires these analyses to be performed. However, true-scale simulations still require a lot of computational resources; sometimes this becomes critical to the question of actual possibility for these analyses to run at all.

The term multi-scale refers to problems, where dimensions of different features needed to be considered during simulation of objects are significantly different.

Bioelectromagnetism [5], together with some areas of microelectronics is a very scale-sensitive field of research in computational electromagnetics. The size of one current source can be significant for a given solution; however this size could be on a nanometre scale (e.g. one neuron, one conductive route, or one transistor), with the size of the whole structure being modelled is in centimetres or more (human head, PCB).

Submodelling is the common approach which is successfully used in computational mechanics [6] in order to reduce the time of computation with almost no loss of accuracy of the solution. Currently existing technique involves the improvement of the solution, for example stress concentration values at the points of interest and works only in one direction, from the large scale (coarse model) to the lowest scale (stress concentrator). Our new approach is designed in order to be implemented in electromagnetic problems where the solution must be improved not only at the points of interest but also in full computational domain.

2. Description of Direct Submodelling Routine

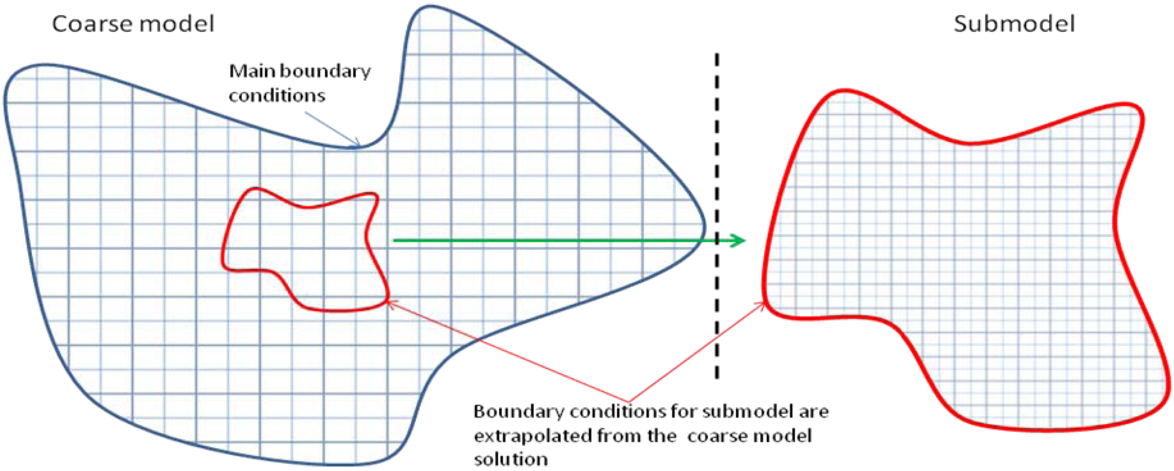

Figure 1. Direct Submodelling Routine (SR)

Well-known existing submodelling routines [6] consist of two major steps which can be seen in Figure 1 and it can be described as follows:

2.1. Solution of the coarse problem

First the coarse model is analyzed with appropriate boundary conditions. During the solution normal mesh convergence analysis must be performed and minimal FE mesh density must be chosen in order to satisfy the required accuracy for the coarse solution. The results must be checked in the area outside the external boundaries of the submodel.

After the solution is performed all degrees of freedom (DOF) are interpolated on the boundaries of the submodel using element shape functions and then saved.

2.2. Solution of the submodel

The second step is to perform the submodel analysis. This analysis is totally independent of the mesh for the coarse model, therefore the mesh density of the submodel must be chosen according to new accuracy requirements for this particular region. Refined FE mesh could be as dense as it is needed for this solution. The boundary conditions are set up as extrapolated solution values obtained from the coarse model. If the main boundary conditions are applicable to the submodel region they should be transferred to the submodel as well.

In electromagnetic computations this procedure could be used for static problems with external boundary conditions in order to improve the quantities for the required regions of interest, for example for the static volume conduction problems with relatively small inclusions inside the main isotropic domain. However, this approach does not allow operation with problems where the point of interest is outside the object of the lowest scale and this object is significant for the solution, e.g. the current or magnetic field source.

3. New Combined Submodelling Routine (CSR)

This submodelling routine was developed in order to perform electromagnetic analyses for multi-scale problems with the electrical or magnetic sources in the smallest scales. These problems include quasistatic coupled electromagnetic problem formulations with relatively small size of a magnetic dipole, electrical voltage source or electrical current source considered within the computational domain. The schematic diagram of the CSR could be seen in Figure 2. The full process could be considered as a combination of the forward and backward submodelling procedures and can be described using the following steps:

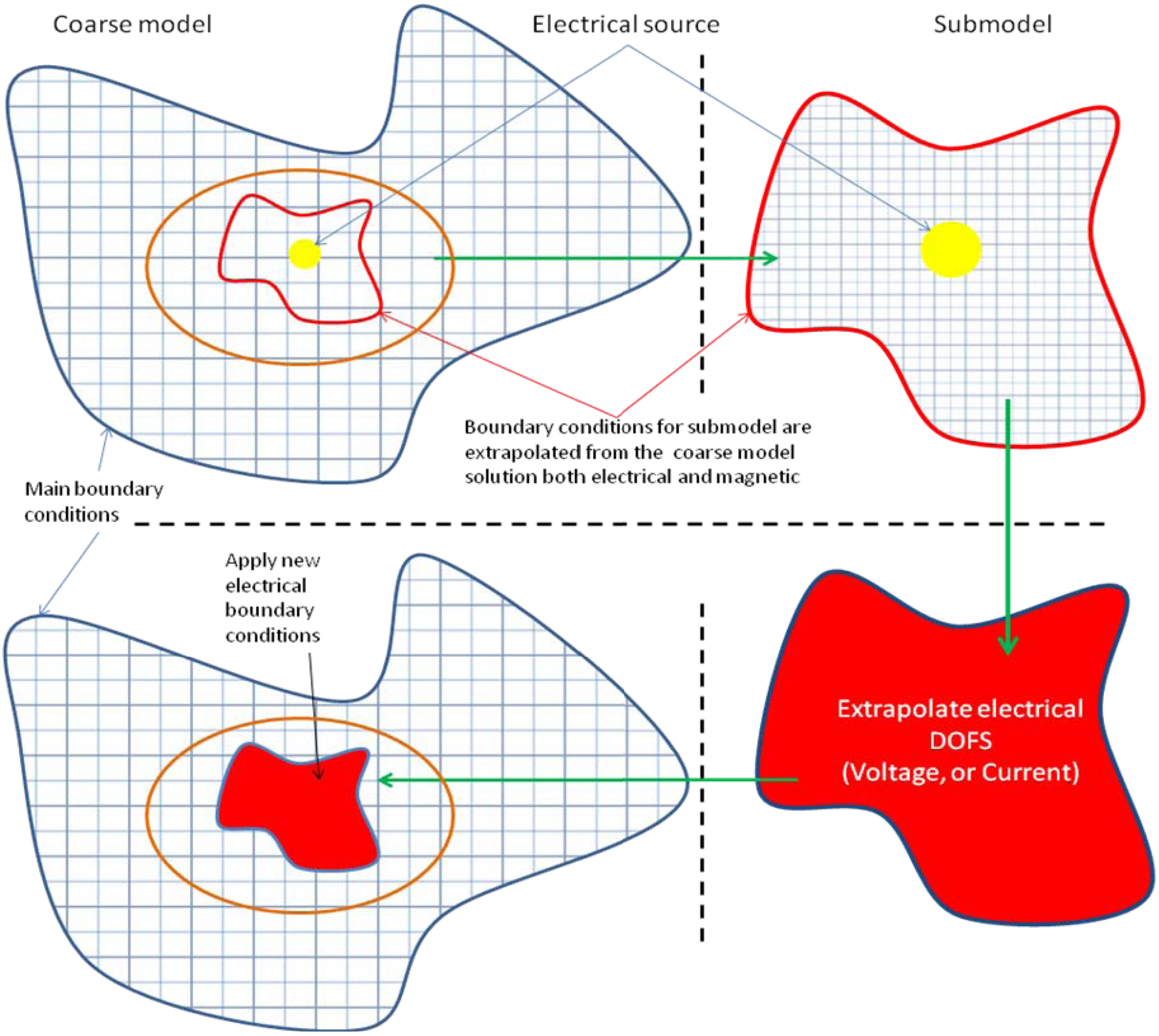

Figure 2. Combined Submodelling Routine (CSR) applicable to electrical source problems.

3.1. Solution of the course model

This step is similar to the first step of normal SR, with the addition that the submodelling region should be taken around electrical or magnetic sources. The interpolation boundaries should be relatively far from the source in order to achieve good approximation for the following submodelling solutions. The interpolation boundary conditions should also include all degrees of freedom of the solution (magnetic and electric).

3.2. Solution of the submodel

The submodel solution is performed and the distribution of electric and magnetic fields is obtained in the entire domain. The next step depends on the sort of source being considered.

3.3. The coarse model volume interpolation

The entire volume solution of the submodel is then interpolated and transferred as a primary source for the coarse model. Only those (electrical or magnetic) degrees of freedom should be transferred into the coarse model of which refer to the primary source. In Figure 2 the electrical source is primary so only the electrical DOFs are transferred into the coarse model. Note that if all DOFs are interpolated back to the coarse model the solution will not change.

3.4. The coarse model solution with improved source

After the interpolation and transferring is performed, the coarse model should be solved with the electric or magnetic field distribution as a primary source instead of the initial source.

The approach presented here could be used for multi-source problems, such as bioelectromagnetic EEG, MEG, or ECG forward analysis. In this case the problem could contain several submodel regions. There are also no restrictions on combination of magnetic and electrical sources in one model.

The CSR allows to analyze multiple scale problems throughout the application to submodel (for example, in case the source is a mixture of a sub-sources). In this case submodelling sub-domain could be also analyzed using CSR.

4. Iterative Submodelling Approach (ICSR)

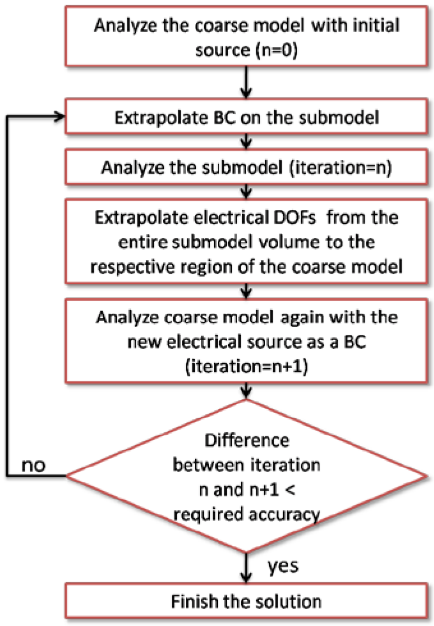

Figure 3. Schematic of the Iterative Combined Submodelling Routine (ICSR).

Iterative Combined Submodelling Routine (ICSR) is developed in order to solve full nonlinear or transient coupled electromagnetic problems with the multi-scale effects. As the solution process in case of transient analysis could be nonlinear and/or iterative, the ICSR operates iteratively in each computational step in time domain. The schematic of the ISCR could be seen in Figure 3. The initial step is the same as CSR and then the solution is improved in each iteration until it converges.

This procedure could be also used in a static analysis with mesh convergence criteria to be run in the second step (second box in Figure 3). In this work the performance of ICSR was not tested due to specific areas of application. Transient multi-scale analysis is a relatively new field of research and further investigation is required in order to obtain ICSR parameters and optimize its performance for individual cases. It is believed that for a given particular problem new optimization analyses routine needs to be performed.

Most bioelectric problems are considered quasistatic with a good level of approximation. The frequencies of the signal in biological structures are not higher than 1MHz. So transient effects have no influence on the total solution [5].

5. Results of Simulation and Performance Analysis

In this work the CSR was implemented and tested for solving one of the most complex biomagnetic forward problems. The solution of the forward problem in magnetic field tomography (MFT) based on magnetoencephalography (MEG) constitutes the prime topic of research conducted by the authors.

5.1. Solution of the forward problem in MFT based on MEG

The formulation of the problem can be found in a wide range of literature [7-9]. In short, the forward problem comprises the computation of magnetic field distribution around the human head from known currents in the brain caused by cognitive activity. More precisely this electrical activity is caused by an action potential distribution along the neuronal axon. This effect could be modelled as a voltage difference applied to a small segment of an axon at each time frame [10]. Since action potential propagates with relatively small velocity of 10 m/s, the problem could be considered as quasistatic. Calculations at a given iterative time step can be considered independent of successive time steps and, therefore CSR could be applied in order to significantly reduce computational time.

Here we consider a full realistic 3D finite element model of the human brain described earlier in paper [11]. The parameters of such a model are given in Table 1.

The geometric and physical parameters of the model were obtained from MRI slices resulting from a whole-brain scan. In terms of finite elements, the model considered a complex anisotropic conductor with realistic tissue properties obtained from DTMRI scan of the same subject. A model with fine mesh was considered first in order to validate results of CSR. Around 10m FE elements were chosen for the fine model in order to satisfy the mesh convergence criteria of 1%.

For the coarse model, a relatively low mesh density with around 800k FE elements was used. This satisfies the mesh convergence criteria for the brain model without any neuronal source inside. For the submodel, 300k elements were found to be adequate to satisfy the accuracy requirements.

In Figure 4 and Figure 5 the outline of the brain is shown together with the boundaries of the submodelling region and neuronal source. The neuronal source is considered as an action potential with voltage difference of 50mV. The thickness of the neuronal path is 0.5mm, which is not realistic in order to test the effect of CSR on the solution. It is obvious that the efficiency of the use of CSR is increased with the increase in the difference in scale, so for realistic micron-thickness of neuronal axons the estimated computation time will decrease even further.

5.2. Simulation results and comparison

The computational set-up was made and then the quasistatic Maxwell's equations were solved in the FE domain. The results were obtained for both the fine mesh and the CSR model and then compared.

Figure 6 shows the distribution of magnetic flux density on the detector surface around the head (points of interest for the solution). It can be seen that the coarse model on its own gives less accurate results. However, the application of CSR vastly improves the accuracy and the results are almost the same (maximum error of 5%) as for the fine model.

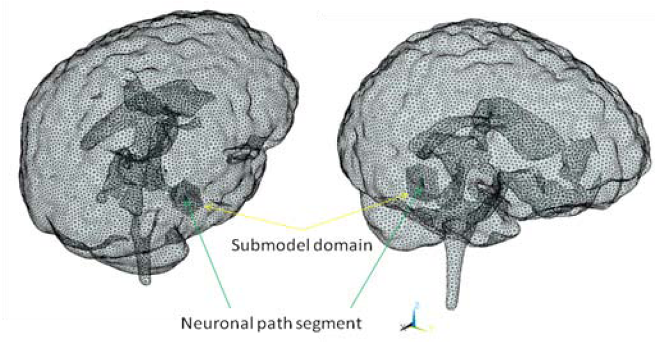

Figure 4. Outline of the brain model showing positions of the submodelling region and the neuronal source.

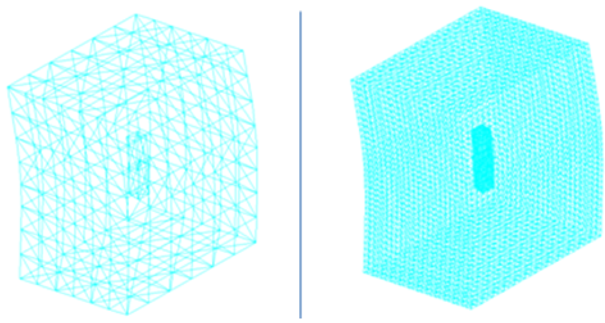

Figure 5. Comparison of meshes for submodelling region and the neuronal source: coarse model (left) and submodel (right).

Table 1. Parameters of FE models and solution.

Parameter	Value/description
Geometry of the model	Realistic geometry obtained from MRI scan
Material Properties	Realistic anisotropic tensor conductivity distribution obtained from DTMRI scan; permeability of the air
Solution	Quasistatic, single step coupled electromagnetic problem (magnetic vector potential **A** and electric potential V)
Neuronal source	Part of neuronal axon with voltage difference of 50 mV applied to ends of a segment; thickness of the axon is 0.5 mm
Number of elements	Fine model – 10m Coarse model – 800k Submodel – 300k

Figure 7 shows and improvement of current density distribution in the solution with the application of CSR. This distribution has been found to be the main reason for adequate magnetic field computation and it has been computed more accurately using the submodelling technique which results in the improvement on the solution obtained by the coarse model.

The magnetic flux density isosurfaces (Figure 8) also show less accurate spatial magnetic field distribution in the coarse model, which has been improved in the CSR model (note the difference in the top configuration of the isosurface).

Average resulting CSR error for this case was calculated using the equation:

$$e = \frac{\sum_{\Omega}\left(\frac{B_i^{fine} - B_i^{CSR}}{B_i^{fine}}\right)}{N}, \tag{1}$$

where B_i^{fine} and B_i^{CSR} are the values of magnetic field flux density at the nodes on the detector surface Ω, and N is the total number of nodes on this surface. Overall, comparison results are summarized in Table 2, where solution times of for both the fine and CSR models are presented.

6. Conclusions

The Combined Submodelling Routine (CSR) and Iterative Combined Submodelling Routine (ICSR) were developed for multi-scale problems in order to reduce the computational time with minimum loss solution accuracy.

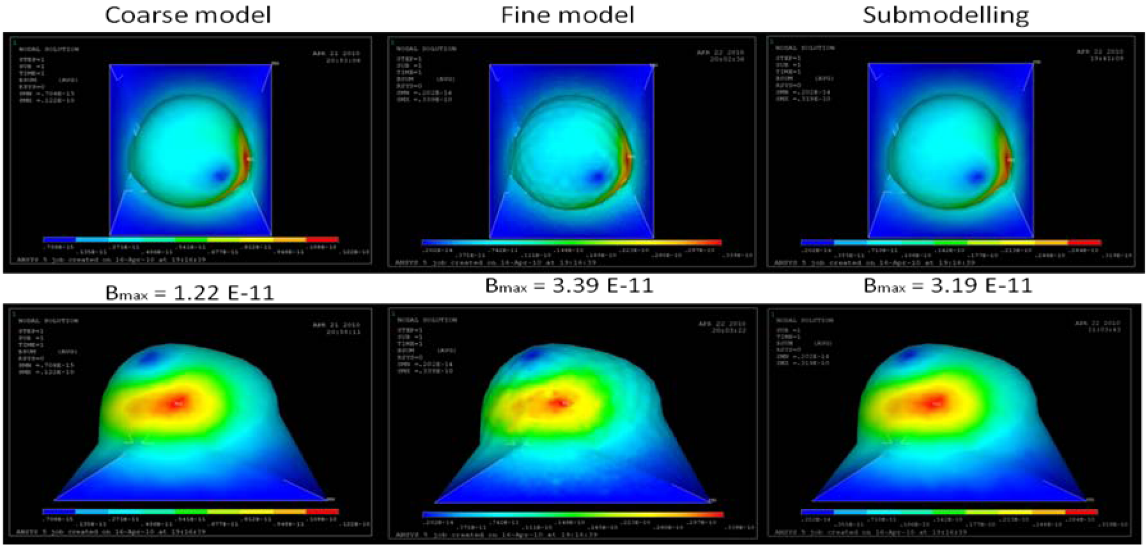

Figure 6. Results of simulation: comparison among results from initial coarse model (left), fine model (middle), and CSR solution (right). Rows represent top and side views respectively.

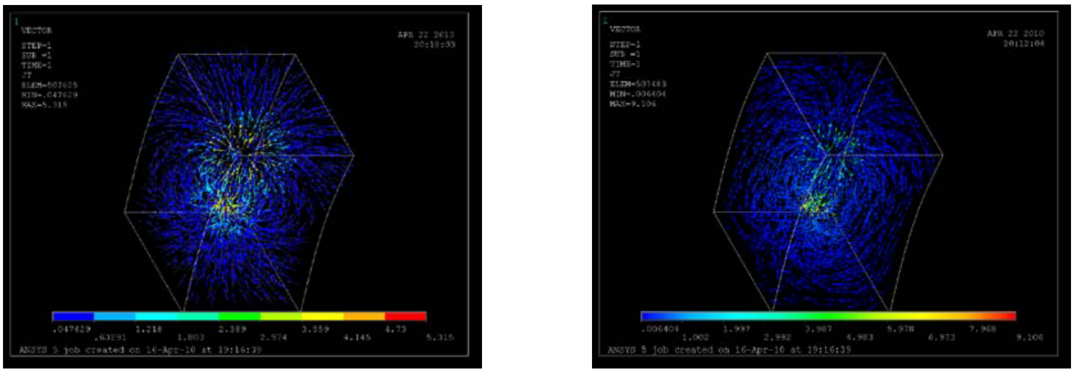

Figure 7. Current density distribution inside the submodelling region of the coarse model. Direct coarse model solution (left), and solution after application of CSR (right).

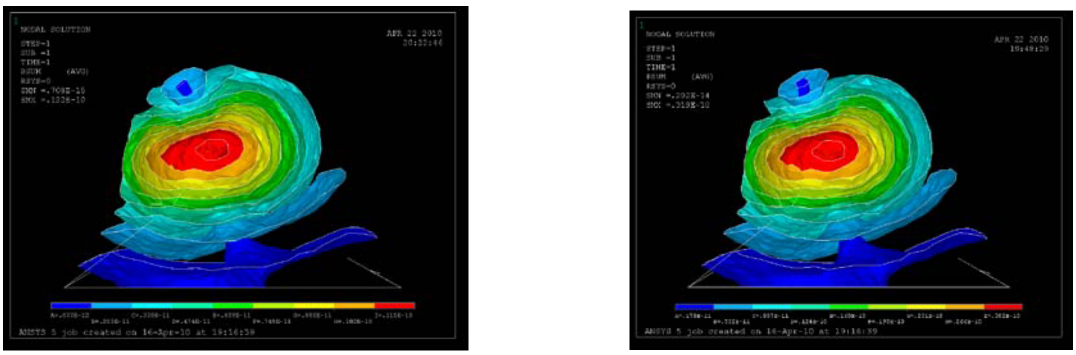

Figure 8. Magnetic flux density isosurface plots for coarse model (left) and with submodelling approach (right).

These routines can have a wide range of application, especially in bioelectromagnetic problems where in many cases it is important to consider multiple scales. The CSR was tested for the solution of the forward problem in MFT based on MEG. Comparison of results between the solutions from initial fine FE model with appropriate mesh density required for direct analysis and CSR applied to the same problem highlighted the ability of CSR to significantly reduce computational time (approximately 100 times) with almost no loss of solution accuracy. Average error of the CSR solution has been found to be 0.3% for the chosen size of submodelling region.

Further analyses carried out show that CSR can decrease computational time even more for those cases where the difference between geometric dimensions is higher.

Future investigation is planned in order to evaluate errors and optimal parameters for ICSR which is also applicable to transient and nonlinear electromagnetic multi-scale problems, for example in microelectronics.

Table 2. Comparison between fine model and CSR solutions.

Parameter	Fine model	CSR model
Number of elements	10m	0.8m (coarse) + 0.3m (submodel)
Maximum magnetic flux density	3.39×10^{-11} T	3.19×10^{-11} T
Maximum error of the CSR solution	5%	
Average error of the CSR solution computed by equation (1), *e*	**0.3%**	
Solution time	168 hours	1.5 hours

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