Surrogate modeling for the solution of electromagnetic inverse problems (grant no. K-105996)

Project closing report (final report)

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1 Introduction

When studying electromagnetic phenomena, the first obvious task is to determine the electromagnetic field knowing exactly the physical configuration, including the sources of the field. This is called the *direct problem* of electromagnetics. By now, sophisticated mathematical models (based on the Maxwell's equations) and powerful numerical simulators (e.g., finite elements, moment methods) are available. Most of the direct problems of practical interest can then be solved with arbitrary precision and the only limitation is then the computational resource.

On the other hand, an electromagnetic *inverse problem* consists in retrieving the physical configuration from the knowledge of the corresponding electromagnetic field. Typical inverse problems are arisen, e.g., in the nondestructive testing of structural components (crack identification of steam generator pipes in nuclear reactors, turbine windings of airplanes, riveted structures, ...) or in material parameter characterization. These tasks are inherently much more difficult than pure direct problems both in theoretical and in numerical terms as well. An inverse problem can be "ill-posed", i.e., can have no solution at all, can have multiple solutions and the solution can be very sensitive to small variations of the input data. Formally, the existence, uniqueness and the stability of the solution might not be guaranteed.

The solution of a single inverse problem usually needs the solution of many direct problems on the configuration modelled (this is called the model-based inversion). Thus the numerical burden of the direct problem solutions can even be multiplied when targeting an inversion task. This has been inspiring the use of *surrogate models* or *metamodels*, which replace the complex direct simulation: they provide approximate results at a much lower computational cost.

Many of the computational challenges of inverse problems (e.g., multiple local minima and the complexity rapidly growing with the number of parameters considered) are inherently present in the optimisation tasks related to electromagnetic device optimisation as well. Thus, surrogate modelling techniques can be applied to optimal design problems, in a way similar to model-based inversion techniques.

A surrogate model often consists in a dataset (database, or training set) of pre-computed direct problem solutions and an interpolation method (e.g., radial basis function, neural network, kriging or some piecewise scheme), based on the stored data. Such data-fit surrogate models are used in two stages: in the first step, the surrogate is generated, using the electromagnetic simulator at hand, and in a second step, interpolated results are found at a much lower computational price.

In this project, the research activities are focused on the generation and application of data-fit surrogate models for electromagnetic optimisation problems, that are related mainly to inverse problems, and secondly, to optimal design problems. Within this framework, not only the algorithms related to the surrogate model but methods for the efficient simulation of the related electromagnetic phenomena are considered as well. In the latter, the aim was to overcome some limitations of standard simulation techniques that strongly influences the performance of the surrogate modelling strategy. To sum up, surrogate modelling has been studied as a whole, strongly embedded in the context of electromagnetic field computation.

This report summarizes the activities that have been done throughout this project.

2 Research activities and results

2.1 Electromagnetic simulations for surrogate modelling

When generating a data-fit surrogate model, a parametric model of the considered electromagnetic phenomenon is defined (or given) first. The surrogate model is aimed to cover a certain domain spanned by the model parameters, i.e., a region-of-interest is specified in the so-called parameter space. For some electromagnetic problems, it might happen that approximations can or practically have to be made at the stage of numerical simulations (e.g., static or quasi-static over time or asymptotic behaviour at large distances). When wide ranges of model parameters are present in the region-of-interest, the standard simulation tools (e.g., commercial software) either apply different approximations within the range of a model parameter or risk of getting numerically unstable. However, the continuity, the asymptotic behaviour and the numerical stability of the results are inevitable for most of the surrogate modelling algorithms, since they usually assume a well-behaved, smooth relationship between the model parameters and the output of the electromagnetic simulation. To this end, special attention has been paid to the development of appropriate simulation tools for the test problems considered for surrogate modelling.

Quasi-static models A very important branch of electromagnetic nondestructive evaluation is the eddy-current testing (ECT) of conducting specimens. Both the direct and inverse problems related to ECT are studied in the frame of this project. Since a low-frequency electromagnetic field is considered in conductive medium, a quasi-static approximation of the Maxwell's equations is used.

A time-harmonic ECT setup is considered in [1]. A rectangular void embedded in a conductive plate models the defect which is to be found based on the impedance variation of an air-cored probe coil scanning above the damaged zone. This classical configuration is commonly simulated by integral formulations, using piecewise constant or linear basis functions for the Method-of-Moments (MoM) technique. However, in [1], a set of globally defined harmonic functions is used for the MoM expansion, resulting in better convergence properties and a smooth variation of the output signal with respect to the variation of the defect parameters.

Another type of ECT applies motion-induced eddy-currents, usually realized by the measurement of lift and drag Lorentz forces acting on a small permanent magnet moving near the examined conductive specimen. The material degradations change the eddy-current distribution and so the Lorentz force as well. Our studies are not related to the whole experimental setup but they focus on some special simulation aspect of such motion-induced electromagnetic fields. As discussed in [2], the electromagnetic field is usually decomposed to an incident term (due to the magnet's remanence) and a reaction term (due to the eddy-currents induced). The latter can be neglected under some assumptions on the speed and the material parameters, however, more precise models have to incorporate the reaction term, too. The work [2] points out the difference between the two models.

Some computational issues related to motion-induced eddy-currents are discussed in [3]. In that paper, it is pointed out that the relative motion of the medium and the magnet can be modelled by introducing a special anisotropic material parameter. This can facilitate the simulation of such configurations when using the finite element method. Although neither [2] nor [3] focuses on a particular ECT setup, thus, we have not used these modelling tools for the surrogate-based solution of inverse problems, both are considered as useful contributions in the field and worth for further studies related to ECT nondestructive testing.

Full-wave models Besides the low frequency electromagnetic problems, applications involving wave phenomena are also targeted in this project. Nowadays, the design and optimisation of Frequency Selective Surfaces (FSS) is getting more and more attention. First, a numerically very efficient simulation environment has been developed for the FSSs, based on an integral formulation and the MoM. The main idea is reported in [4]: an impedance-type boundary condition is introduced to model the metallic part of the FSS. This idea has then been improved in order to extend the frequency range in which the formalism is applicable; results are reported in [5]. We believe that its computational efficiency makes the method worth to be implemented as a forward solver in design optimization algorithms.

Another very up-to-date high-frequency (near optical) application has been studied and reported in [6]: an electromagnetic cloaking device made with composite materials and operating in the range of near-infrared light is presented. The transformation optics is used to design the invisibility cloak, consisting of 15 concentric rings of different anisotropic two-phase metal-dielectric composites. The simulation of the concealment produced by the multilayer nanocomposite is performed by using the finite element method. The optimal design of the geometry and the material parameters rises a very complicated optimisation problem that has been solved by a differential evolution-based algorithm. Due to the large number of device parameters, finally the optimisation task could not be treated in the frame of the deterministic methods we have developed, thus, a stochastic algorithm had to be applied — i.e., this work is a bit aside of the original research plan.

As mentioned in the introduction, a crucial point of the surrogate modelling is the availability of a reliable electromagnetic model with continuous outputs over a wide range of input parameters. Standard simulation techniques are available for different frequency ranges, using different formulations, however, the smooth fitting of the results when changing to one model to another is inevitable when generating a surrogate model with smooth interpolants (e.g., kriging), or solving an inverse problem based on the model. This challenge is in the focus of our work [7], where a potential formulation for wave problems is developed that ensures numerical stability at both the high and the low frequency limits as well.

During this project, we have experienced a rapid growth of the interest in wireless power transfer (WPT) applications. In parallel with the main research direction of the present project, we have started some studies on the electromagnetic simulation of magnetically coupled WPT. Although we have not reached yet the stage of surrogate modelling for these models, the results are partially connected to this project since efficient simulation tools have been developed with attention to the subsequent use in design optimisation algorithms. Let us highlight that the resonant behaviour of such WPT systems needs special considerations in both the simulation and the optimisation point of view. Herein we refer to our paper [8] in which the self-resonance phenomenon of air-cored coils are studied by means of a newly developed integral formulation. Such coils form the transmitter and receiver units of resonant WPT systems.

Model choice and coupled models For some problems of practical interest –including WPT applications– models of different precision and computational complexity are commonly used. In such cases, one has to either choose the "best" model for the purposes targeted or couple the models for the best performance. The test problems we have considered in this domain are mainly related to WPT and they fit partially into the main research direction of the present project. However, we are convinced that these problems have some features that make them particularly interesting from the viewpoint of surrogate modelling (e.g., the resonant behaviour, the multi-scale geometry and high number of geometrical parameters). In the near future, the developed models will be incorporated to surrogate-based device optimisation algorithms. Without going into details, herein we just refer to our further WPT-related works: a full WPT chain is analysed with full-wave and circuit models in [9], whereas [10] and [11] report new finite element and integral equation schemes for the analysis of WPT systems with full-wave and quasi-static formulation.

Another example for the coupled use of different electromagnetic models for a large-scale problem is discussed in [12] where a cable shielding is examined by means of a quasi-static and a full-wave formulation.

2.2 Sampling strategies, databases, interpolation

In this section, the algorithms directly related to the data-fit surrogate models and their applications are briefly presented, with references to our published results.

All methods discussed herein are applied to the direct and inverse problems of electromagnetic nondestructive evaluation. In all cases, a parametric defect model is defined with N defect parameters, i.e., the parameter space is N dimensional. The output data (that can be measured in a real configuration or numerically simulated by electromagnetic field computation) consist in a set of scalar values related to the probe actually used. In the eddy-current testing examples, the probe is a small air-cored coil driven by time-harmonic current and the output data consist in its complex impedance variations at M pre-defined probe locations.

Mesh-based database Prior to the present project, our research team has introduced the concept of the N-dimensional mesh database. The nodes of the mesh define the parameters of the prototype-defects ("samples"), to which the output data are stored in the database. By appropriate adaptive generation of the N-dimensional mesh, a considerable improvement in the interpolation performance of the database is gained over the standard regular sampling.

During this project, a new adaptive mesh-generation technique has been developed [13] that incorporates the sensitivity information of the underlying electromagnetic problem. The sensitivity information consists in the first partial derivatives of the output values with respect to the N defect parameters. Omitting the details, briefly, this technique is able to heuristically minimise the average interpolation error by an appropriate choice of the samples, using piecewise linear interpolation. The method is found to be efficient via the eddy-current testing examples in [13].

Output space filling database Another type of algorithm for the database generation is the output space filling which has been in principle developed prior to this project. Briefly, this strategy aims at constructing a set of prototype defects such that the corresponding output data samples uniformly fill the space spanned by all conceivable outputs. This means that the distance –in a given norm– between the output data samples is controlled during the adaptive sampling process.

In the frame of this project, a very robust implementation of this output space filling strategy has been developed. The algorithm has been connected with the CIVA simulation software [14] in cooperation with our international partner[1]. CIVA can simulate the output signal corresponding to various types of defects in a wide range of eddy-current testing configurations. Based on the databases generated by this newly developed combination of tools, the inverse problem of defect characterisation has been targeted. We have proposed to use piecewise linear interpolation, based on the samples in the database, to approximate the measured output data at unsampled defect parameters. Beyond providing robustness, this interpolation considerably speeds up the solution of the inverse problem since the general optimisation problem boils down to a couple of quadratic optimisation problems that can be efficiently solved by standard techniques. The method is discussed in detail in [15].

Using the developed efficient method for inversion, studies have been performed for the characterisation of the uncertainty of the solution [15]. Even simple Monte-Carlo sampling techniques can be used within reasonable computation time thanks to the speed of the new inversion scheme, up to 6 defect parameters. These studies justify our expectations about the uncertainties, based on the physical nature of the phenomena (e.g., small flaws near large ones are hard-to-characterise, etc.), moreover, they seem to be a robust tool for the characterisation of the confidence that one can have in the solution.

Sparse grid database A serious limitation of both the mesh-based and the output space filling strategy is the "curse-of-dimensionality" with respect to the number of parameters N. This means that the size of the database and the complexity of the interpolation grows in an exponential order with N, making the surrogate model intractable for problems having N more that approximately 6.

This bottleneck inspired the research on "sparse grid" databases. Sparse grids are known to overcome the curse-of-dimensionality to some extent. They apply a hierarchical set of basis functions in each dimension of the problem and a sparse tensor product is defined to generate the set of N-dimensional basis functions. For smooth functions to be interpolated (which smoothness can usually be assumed for the response of electromagnetic models), the loss of interpolation accuracy of sparse grids compared to full grids is far less that the gain in the reduction of sample number needed.

Our first results on sparse grid surrogate models used for inversion in eddy-current testing have been reported in [16]. This work has been performed in collaboration with the CEA. Besides the eddy-current testing examples, another nondestructive testing method –the magnetic flux leakage technique– is included in the very recent work [17], to demonstrate the performance of sparse grid surrogate models. In this work, 9 defect parameters are considered –which could not be achieved with the methods previously used–, moreover, an adaptive strategy for the generation of the sparse grid database is proposed, further reducing the number of direct simulations needed in the database generation.

3 Conclusions, utilization and publication of the results

During this project, a large variety of aspects have been concerned related to surrogate modelling for the solution of electromagnetic inverse and optimisation problems. To sum up, our activities can roughly be categorised to three main classes: (i) definition and analysis of direct problems by means of electromagnetic simulation, with special emphasis of the needs of surrogate modelling, when incorporating these models; (ii) development of various sampling strategies and interpolation methods to efficiently construct surrogate models; and (iii) use of the surrogate models for inversion, with attention to the performance in terms of precision and simplicity, along with studies on the effects of measurement noise.

[1] CEA: Commisariat à l'énergie atomique et aux énergies alternatives, France

Part of the results are utilized in industrial environment, too. This is realised by our co-operation with CEA, the developer of the CIVA simulation software [14]. Some algorithms related to the output space filling, the sparse grid database and the optimisation-based inversion will be implemented in CIVA, in the frame of a separate contract between the CEA and our Department. This clearly justifies the utility of these research results out of the academic sector, too. In conclusion, the work that has been performed in the frame of this three-year project fulfills all aspects targeted in the workplan.

The results obtained in this project are well-published, this is why the present report is brief and it refers to our articles instead. 16 communications have been published (including some accepted for publication, appearing later on), among which 10 is in recognized international journal with impact factor, and many others are in proceedings of international conferences.

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