Fast Frequency and Material Properties Sweeps for Quasi-Static Problems

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We introduce a novel technique that speeds up the computation of a frequency sweep or some parametric change of material properties—assumed uniform over the entire domain—around a nominal value in electroquasi-static problem or magnetoquasi-static problem. In place of using the usual practice of solving the complex systems arising at each frequency and at each material parameter value independently, our technique requires only one factorization of a real, symmetric, and positive definite matrix. The solution at each frequency and each value of material parameter is, then, found with a few back-substitutions only. The obtained speedup is sensible and the implementation is straightforward, showing the usefulness of the proposed technique in practical applications.

Index Terms— **Electroquasi-statics (EQS), finite elements, finite integration technique (FIT), frequency sweep, hybrid direct and iterative solver, magnetoquasi-statics (MQS), real value preconditioner, shifted complex symmetric systems.**

I. Introduction

THE NEED of frequency sweeps arises frequently in electroquasi-static (EQS) or magnetoquasi-static (MQS) problems. We just mention the prediction of the frequency course of impedance in impedance spectroscopy [1] or the transmembrane potential in electroporation [2] and the multi-frequency nondestructive testing based on eddy currents [3]. In addition to the variation of frequency, it is also required in many applications to parametrically change the material properties, for example the electrical permittivity in EQS problems and the electrical conductivity in MQS problems.

The most common approach to operate these sweeps is to perform one independent simulation for each frequency and material property. With iterative linear solvers only, one may use the solution of the previous frequency as a starting point for the new one. But this solution is not available when using direct solvers that are particularly robust and efficient for solving MQS problems on parallel computers. For example, the direct solver Intel MKL PARDISO is suitable for shared memory parallel computers because of its OpenMP-based implementation. Yet, these problems can be solved also on massive parallel computers by using a message passing interface (MPI) distributed direct solver like MUMPS [4].

A number of techniques to solve shifted complex symmetric systems have been introduced in literature, see for example [5]. We just mention the method proposed in [6] based on shifted Krylov subspaces. It exploits the fact that Krylov subspace induced by the shifted matrix does not depend on the shifts. Therefore, one may execute the Lanczos steps for one of the systems and obtain the iterates for all the others.

In this paper, we introduce an alternative approach that exploits the efficient real-valued (RV) iterative method for solving complex symmetric linear systems proposed in [7], see also [8]. The RV method, described in detail in Section II, can be thought as a hybrid between a direct and an iterative solver, trying to preserve the best of the two worlds.

The RV method has been already used in computational electromagnetics to solve EQS problems, see [9]. Yet, algebraic multigrid solvers as AGMG [10] are very efficient in solving EQS problems and the usefulness of the RV method for this application is not clear. To the best of our knowledge, the RV method has not been used as a solver for MQS problems. Therefore, the first aim of this paper is to evaluate the usefulness of the RV technique in solving single MQS problems.

Then, we introduce a novel technique to speed up the computation of parametric sweeps. The advantages of this technique are that it requires only one factorization for all simulations and the matrix that needs to be factorized is real, symmetric, and positive definite. The solution for each simulation is, then, found by a few back-substitutions of this real matrix. This yields to a sensible reduction in the overall computational time required by the sweep.

This paper is structured as follows. In Section II, we briefly describe the RV method for solving complex symmetric systems [7], discussing its implementation and expected performances. Section III introduces the main idea of this paper, i.e., how to hack the RV algorithm to reuse the factorized real matrix for more than one frequency. Section IV presents the numerical results on a number of benchmark problems to show both the usefulness of the RV method and the proposed technique for computing fast sweeps. Finally, the conclusions are drawn in Section V.

II. RV Solver for Complex Symmetric Systems

The idea proposed in this paper is based on the RV algorithm for solving complex symmetric systems [7], which is recalled in what follows. Let us consider a symmetric complex matrix where the real part $\mathbf{R}$ and imaginary part $\mathbf{S}$ are symmetric positive semidefinite and at least one of $\mathbf{R}$ and $\mathbf{S}$ is symmetric positive definite (SPD).

Let us write the resulting system as

$$(\mathbf{R} + i\,\mathbf{S})(\mathbf{x} + i\,\mathbf{y}) = \mathbf{r} + i\,\mathbf{s} \tag{1}$$

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and let us define the real matrix $\mathbf{W}$ as

$$\mathbf{W} = \mathbf{R} + \alpha\,\mathbf{S} \tag{2}$$

where $\alpha > 0$ is a real number such that $\mathbf{W}$ is SPD. The system may be written as an RV system whose number of unknowns is twice as big as (1)

$$\begin{bmatrix} \mathbf{R} & -\mathbf{S} \\ \mathbf{S} & \mathbf{R} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{r} \\ \mathbf{s} \end{bmatrix}. \tag{3}$$

Let us now subtract the first equation of (4) multiplied by α to the second one. We get the system

$$\mathbf{R}\,\mathbf{x} - \mathbf{S}\,\mathbf{y} = \mathbf{r}(\mathbf{S} - \alpha\mathbf{R})\,\mathbf{x} + (\mathbf{R} + \alpha\mathbf{S})\,\mathbf{y} = \mathbf{s} - \alpha\mathbf{r}. \tag{4}$$

We can compute $\mathbf{y}$ from the second of (4)

$$\mathbf{y} = \mathbf{W}^{-1}(\alpha\mathbf{R} - \mathbf{S})\,\mathbf{x} + \mathbf{W}^{-1}(\mathbf{s} - \alpha\mathbf{r}) \tag{5}$$

and substitute it in the first of (4) getting

$$\mathbf{R}\,\mathbf{x} - \mathbf{S}\mathbf{W}^{-1}(\alpha\mathbf{R} - \mathbf{S})\,\mathbf{x} = \mathbf{r} + \mathbf{S}\mathbf{W}^{-1}(\mathbf{s} - \alpha\mathbf{r}). \tag{6}$$

By substituting

$$\alpha\mathbf{R} - \mathbf{S} = \alpha(\mathbf{R} + \alpha\mathbf{S}) - (1 + \alpha^2)\mathbf{S}$$

in (6), we get a linear system whose solution provides $\mathbf{x}$

$$\mathbf{K}\,\mathbf{x} = \mathbf{r} - \mathbf{S}\mathbf{W}^{-1}(\mathbf{s} - \alpha\mathbf{r}) \tag{7}$$

where we defined $\mathbf{K}$ as

$$\mathbf{K} = \mathbf{R} - \alpha\mathbf{S} + (\alpha^2 + 1)\mathbf{S}\,\mathbf{W}^{-1}\,\mathbf{S}. \tag{8}$$

Thus, the complex system may be solved over the real numbers using the following recipe [7].

1) First, compute the right-hand side

$$\mathbf{f} = \mathbf{r} + \mathbf{S}\mathbf{W}^{-1}(\mathbf{s} - \alpha\mathbf{r}). \tag{9}$$

2) Second, solve with a preconditioned conjugate gradient (PCG) or other iterative solvers the linear system

$$\mathbf{K}\,\mathbf{x} = \mathbf{f}. \tag{10}$$

The important point is to use $\mathbf{W}$ as preconditioner in the PCG solver. We also remark that $\mathbf{x}$ is the real part of the desired complex-valued solution, so the algorithm can be terminated, here, if the imaginary part of the solution is not needed.

3) Compute the array $\mathbf{z}$ as

$$\mathbf{z} = \mathbf{W}^{-1}(\alpha\mathbf{r} - \mathbf{s} + (1 + \alpha^2)\mathbf{S}\mathbf{x}). \tag{11}$$

4) Finally, find the imaginary part of the complex-valued solution with

$$\mathbf{y} = \alpha\mathbf{x} - \mathbf{z}. \tag{12}$$

Provided that one computes a factorization of the real SPD matrix $\mathbf{W}$ first, steps 1, 3, and 4 require just two back-substitutions. Solving step 2 requires also a few back-substitutions, since it is proved that the condition number of the preconditioned system is bounded above by 2 when, without knowing any estimate for the eigenvalues of the matrices, one simply sets $\alpha = 1$, see [7]. To give an idea, when $\alpha = 1$ and the required relative residual is 10^{-6}, the upper bound on required iterations is 8.

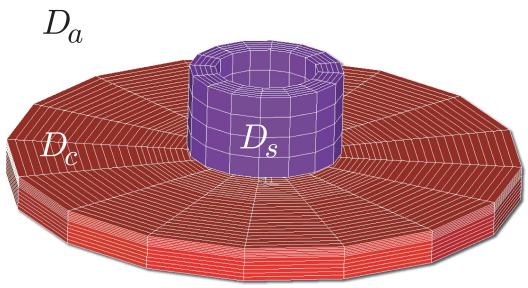

Fig. 1. Computational domain D is partitioned into a passive conductive region D_c, a nonconductive region D_a, and a source region D_s.

A. Solving EQS and MQS Problems

The hypothesis that the RV technique requires is fulfilled by formulating the EQS problem with the scalar potential and the MQS problems, for example, with the gauged reduced magnetic vector potential formulation A_r. In such a case, in fact, at least the real part of the system matrix is SPD, whereas the imaginary part may be positive semidefinite. We focus on the A_r MQS formulation because it avoids the explicit meshing of the source regions in such a way that the same mesh may be used for many different coil positions.

Other eddy current formulations may not fulfill the aforementioned assumptions required on $\mathbf{R}$ and $\mathbf{S}$, as for example, the A-V formulation, which is usually more efficient than the A formulation, when iterative solvers are used [11]. Nevertheless, in [7, Remark 1] it is shown how to weaken the assumptions of the RV method to just require a nonsingular $\mathbf{R} + \alpha\mathbf{S}$.

III. Fast Sweeps

This section shows how the RV method can be exploited to solve for all frequencies and all the values of material parameters using only one factorization of the real matrix $\mathbf{W}$.

To explain the very idea behind the proposed approach, let us consider an MQS problem formulated with the gauged reduced magnetic vector potential [3]. Exactly the same technique may also be used for EQS problems.

A. Eddy Current Formulation

Three regions of the domain D are identified: 1) the passive conductive region D_c; 2) the nonconductive region D_a; and 3) the source region D_s (see Fig. 1). By combining discrete Ampère's and Faraday's laws with the discrete counterpart of constitutive laws, a symmetric complex linear system of equations is obtained [3]

$$(\mathbf{K}_\nu + i\omega\mathbf{M}_\sigma)\,\mathbf{A}_r = -i\omega\mathbf{M}_\sigma\,\mathbf{A}_s \tag{13}$$

where ω is the angular frequency. The construction of $\mathbf{K}_\nu$ and $\mathbf{M}_\sigma$ for a mesh composed by star-shaped polyhedral elements is addressed in [12] and [13].

The unknowns $\mathbf{A}_r$ are the circulations of the reduced magnetic vector potential along edges $e \in D$ due to eddy currents in D_c, only. On the right-hand side, $\mathbf{A}_s$ denotes the circulations of the magnetic vector potential along $e \in D_c$ produced by current sources in D_s and zero for edges in $D_a \bigcup D_s$. Then, the circulations of the modified magnetic vector potential $\mathbf{A}$ can be found as $\mathbf{A} = \mathbf{A}_r + \mathbf{A}_s$.

B. Frequency Sweep

If we consider a frequency ω, we instantiate the RV method with

$$\mathbf{R} = \mathbf{K}_\nu \quad \text{and} \quad \mathbf{S} = \omega \mathbf{M}_\sigma . \tag{14}$$

Thus, to exploit the RV method, one should compute a factorization of

$$\mathbf{W} = \mathbf{K}_\nu + \alpha\, \omega\, \mathbf{M}_\sigma . \tag{15}$$

The novel idea is that if we need to simulate at a different frequency $\hat{\omega}$ we can reuse $\mathbf{W}$ and its factorization. This is because we can chose an $\hat{\alpha}$ such that

$$\mathbf{W} = \mathbf{K}_\nu + \alpha\, \omega\, \mathbf{M}_\sigma = \mathbf{K}_\nu + \hat{\alpha}\, \hat{\omega}\, \mathbf{M}_\sigma \tag{16}$$

holds. If we set $\alpha = 1$, we have that

$$\hat{\alpha} = \omega / \hat{\omega} \tag{17}$$

and

$$\hat{\mathbf{S}} = \hat{\omega} \mathbf{M}_\sigma . \tag{18}$$

C. Material Parameter Sweep

Clearly, this idea can be easily translated to produce a fast solution also when a parametric study of some material property is needed (for example, changes of the electric permittivity ε in EQS or conductivity σ in MQS), provided that the change in material property is uniform over the entire domain. That is, let us suppose that the conductivity is scaled by the real number k. We can chose $\hat{\alpha}$ such that

$$\mathbf{W} = \mathbf{K}_\nu + \alpha\, \omega\, \mathbf{M}_\sigma = \mathbf{K}_\nu + \hat{\alpha}\, \omega\, k\, \mathbf{M}_\sigma \tag{19}$$

holds. If we again set $\alpha = 1$, we have that

$$\hat{\alpha} = 1/k \tag{20}$$

and

$$\hat{\mathbf{S}} = \omega k \mathbf{M}_\sigma . \tag{21}$$

IV. Numerical Experiments

A benchmark comprising a coil above a conducting plate is considered (see Fig. 1) [13]. The geometry is discretized with an hexahedral mesh consisting of 270 125 nodes, 265 360 elements, and 805 464 edges. The number of resulting unknowns is 529 182.

All simulations have been performed on a laptop with 16 GB of RAM and an Intel i7-3720QM @ 2.60 GHz quad core CPU.

All complex symmetric systems are solved using the OpenMP-based direct solver Intel MKL PARDISO suitable for shared memory parallel computers. Of course, these problems can be solved also on massive parallel computers using an MPI distributed direct solver, such as MUMPS [4].

The Cholesky factorization of the matrix $\mathbf{W}$ in the RV method has also been performed in parallel by the PARDISO solver. The remaining parts of the RV method have been parallelized with the optimized OpenMP-based basic linear algebra subprograms (BLAS) routines included in the Intel MKL library.

We also remark that an implementation of the RV method for massive parallel computers is straightforward, since many optimized MPI implementations of the Cholesky factorization and BLAS routines exist.

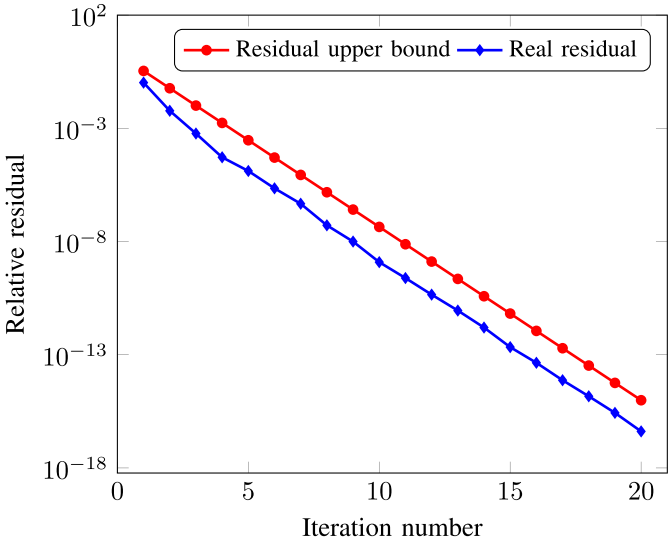

Fig. 2. Relative residual at the various PCG iterations. Comparison with the theoretical upper bound of residual for each iteration and real relative residuals.

A. Efficiency of RV Method for a Single Simulation

The frequency of the sinusoidal current in the source coil is assumed 1 kHz. The direct solver PARDISO for complex symmetric matrices takes 65 s for the frequency of 1 kHz, whereas the RV method takes 39 s (23 for the factorization of $\mathbf{W}$ plus 16 for the PCG iterations stopped as soon as the relative residual gone below 10^{-6}). We can conclude that the RV method is useful even if only one simulation of an MQS problem at a given frequency or material parameter is needed.

Fig. 2 shows the number of iterations required for lower relative residuals. In Fig. 2, we show also the theoretical upper bound of required iterations for a given relative residual as predicted in [7]

$$\mathrm{itn}_{\max} \leq \frac{1}{2\ln\left(1+\sqrt{2}\right)} \ln\frac{2}{\epsilon}$$

where $\mathrm{itn}_{\max}$ is the maximum number of iterations and ϵ is the required relative residual.

B. Efficiency for a Frequency Sweep

For nondestructive testing applications, a frequency sweep of 16 points between 500 Hz and 2 kHz is needed. The standard technique of solving each problem independently takes a total time of 1044 s. This correspond to roughly 65 s for each frequency step.

The technique proposed in this paper requires a first preprocessing comprising the factorization of $\mathbf{W}$, which takes ~23 s. Then, the solution at each frequency requires from 15 to 24 s, depending how far the frequency is from 1 kHz (see Fig. 3).

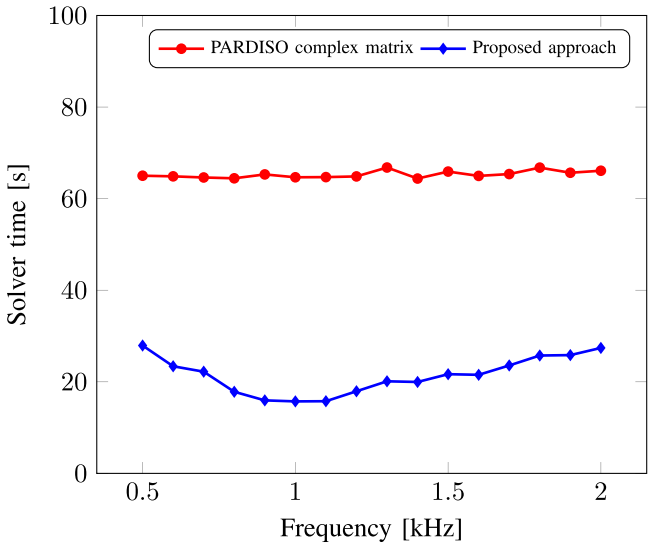

Fig. 3. Lines: time in seconds required to solve the eddy current problem at each frequency point with PARDISO and with the proposed technique based on the RV method.

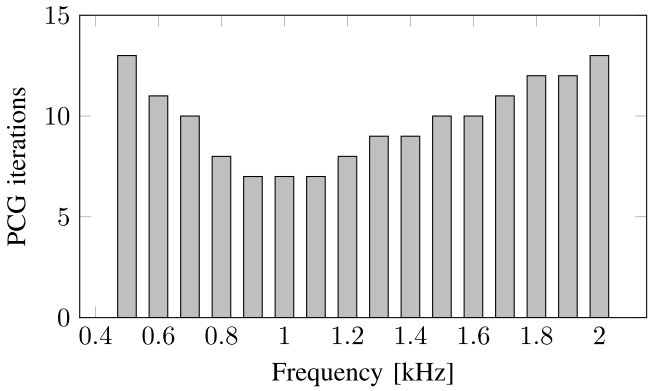

Fig. 4. Histogram represents the number of PCG iterations required. With the chosen frequency range, $0.5 \leq \hat{\alpha} \leq 2$.

The stopping criterion used in the PCG is a relative residual below 10^{-6} for all frequencies. In Fig. 4, the histogram represents the required PCG iterations for each frequency. The total time for the sweep turned out to be 365 s, with a speedup factor of $\sim$3 with respect to PARDISO for complex-valued systems.

V. Discussion

We remark that when the parameter variation is large and consequently $\hat{\alpha}$ differs sensibly from the unity, it is convenient to factorize again matrix $\mathbf{W}$ considering a different frequency. Moreover, to be more efficient over a wide number and range of frequencies, this technique should be coupled together with other standard model order reduction strategies as, for example, [14] and [15].

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