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 electro- or magneto-quasistatic problems. 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 speed up is sensible and the implementation is straightforward, showing the usefulness of the proposed technique in practical applications.

***Index Terms*—magneto-quasistatics, electro-quasistatics, finite elements (FEM), finite integration technique (FIT), frequency sweep, shifted complex symmetric systems**

I. Introduction

THE need of frequency sweeps arise frequently in electro- (EQS) or magneto-quasistatic (MQS) problems. We just mention the frequency course of impedance in impedance spectroscopy or the transmembrane potential in electroporation [1] and the multi-frequency non destructive testing based on eddy currents [2]. Besides the variation of frequency, it is also required in many applications to parametrically change the material properties, for example the electrical permittivity in EQS and the electrical conductivity in MQS. The most common approach to operate the sweep 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 as Intel MKL PARDISO, which usually is the most efficient solution for MQS problems solved on massive parallel computers.

In this paper we introduce an alternative approach which exploits the efficient real valued (RV) iterative method for solving complex symmetric linear systems proposed in [3]. The big advantage of the technique proposed in this paper is 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.

II. RV solver for complex symmetric systems

The idea proposed in this paper is based on the real valued (RV) algorithm for solving complex symmetric systems [3], 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 semi-definite and at least one of $\mathbf{R}$ and $\mathbf{S}$ is symmetric positive definite (SPD). This is the case of the EQS formulation based on the scalar potential and, for example, the gauged MQS formulation based on the reduced magnetic vector potential. Let us write the system as

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

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 solved by using the following recipe:

1) $\mathbf{f} = \mathbf{r} + \mathbf{S}\mathbf{W}^{-1}(\mathbf{s} - \alpha\mathbf{r})$.
2) Solve with a preconditioned conjugate gradient (PCG) iterative solver
$$\mathbf{K}\,\mathbf{x} = \mathbf{f}, \tag{3}$$
where
$$\mathbf{K} = \mathbf{R} - \alpha\mathbf{S} + (\alpha^2 + 1)\mathbf{S}\,\mathbf{W}^{-1}\,\mathbf{S} \tag{4}$$
and $\mathbf{W}$ is the preconditioner.
3) $\mathbf{z} = \mathbf{W}^{-1}\,\left(\alpha\,\mathbf{r} - \mathbf{s} + (1 + \alpha^2)\mathbf{S}\,\mathbf{x}\right)$.
4) $\mathbf{y} = \alpha\mathbf{x} - \mathbf{z}$.

Provided that one computes a factorization of $\mathbf{W}$ 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 [3]. When $\alpha = 1$ and the required residual is 10^{-6}, the upper bound on required iterations is 8.

III. Fast sweep

It appears that the RV method has been exploited in computational electromagnetics only in [4], where it has been used to solve EQS problems. However, systems resulting from EQS problems are nowadays more efficiently solved with available algebraic multigrid codes as AGMG [5].

To the best of our knowledge, we are not aware about papers applying the RV method to MQS problems. Especially, it seems that the idea proposed in this paper, i.e. how to speed-up frequency and some material parameters sweeps, is novel. That is, we are going to show that the RV method can be exploited to solve for all frequencies and all values of material parameters by using only *one* factorization of the real matrix $\mathbf{W}$. To explain the very idea behind the proposed approach, let us consider a MQS problem formulated with the gauged reduced magnetic vector potential [2]. Exactly the same technique may also be used for EQS problems.

A. *Eddy current formulation*

Three regions of the domain $\mathcal{D}$ are identified: the passive conductive region $\mathcal{D}_c$, the nonconductive region $\mathcal{D}_a$, and the source region $\mathcal{D}_s$. 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 [2],

$$(\mathbf{K}_\nu + i\omega \mathbf{M}_\sigma)\, \mathbf{A}_r = -i\omega\, \mathbf{M}_\sigma\, \mathbf{A}_s, \qquad (5)$$

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 [6], [7]. The unknowns $\mathbf{A}_r$ are the circulations of the reduced magnetic vector potential along edges $e \in \mathcal{D}$ due to eddy currents in $\mathcal{D}_c$, only. On the right-hand side, $\mathbf{A}_s$ denotes the circulations of the magnetic vector potential along $e \in \mathcal{D}_c$ produced by current sources in $\mathcal{D}_s$ and zero for edges in $\mathcal{D}_a \bigcup \mathcal{D}_s$. Then, the circulations of the modified magnetic vector potential $\mathbf{A}$ can be found as $\mathbf{A} = \mathbf{A}_r + \mathbf{A}_s$.

B. *Main idea*

If we consider a frequency ω, we instantiate the RV method with $\mathbf{R} = \mathbf{K}_\nu$ and $\mathbf{S} = \omega \mathbf{M}_\sigma$. So, to exploit the RV method, one should compute a factorization of $\mathbf{W} = \mathbf{K}_\nu + \alpha\, \omega\, \mathbf{M}_\sigma$. 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 $\mathbf{W} = \mathbf{K}_\nu + \alpha\, \omega\, \mathbf{M}_\sigma = \mathbf{K}_\nu + \hat{\alpha}\, \hat{\omega}\, \mathbf{M}_\sigma$ holds. If we set $\alpha = 1$, we have that $\hat{\alpha} = \omega/\hat{\omega}$ and $\hat{\mathbf{S}} = \hat{\omega}\mathbf{M}_\sigma$.

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. Let us suppose that the conductivity is scaled by the real number k. We can chose $\hat{\alpha}$ such that $\mathbf{W} = \mathbf{K}_\nu + \alpha\, \omega\, \mathbf{M}_\sigma = \mathbf{K}_\nu + \hat{\alpha}\, \omega\, k\, \mathbf{M}_\sigma$ holds. If we again set $\alpha = 1$, we have that $\hat{\alpha} = 1/k$ and $\hat{\mathbf{S}} = \omega k \mathbf{M}_\sigma$.

IV. Numerical Experiments

A benchmark comprising a coil above a conducting plate is considered, see Fig. 1 and [7]. 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. The central frequency is assumed 1kHz.

First, we note that the RV method is useful even if only one simulation at a fixed frequency is needed. In fact, the direct solver PARDISO for complex symmetric matrices takes 65 seconds for the frequency of 1kHz, whereas the RV method takes 39 seconds (23 for the factorization of $\mathbf{W}$ plus 16 for the

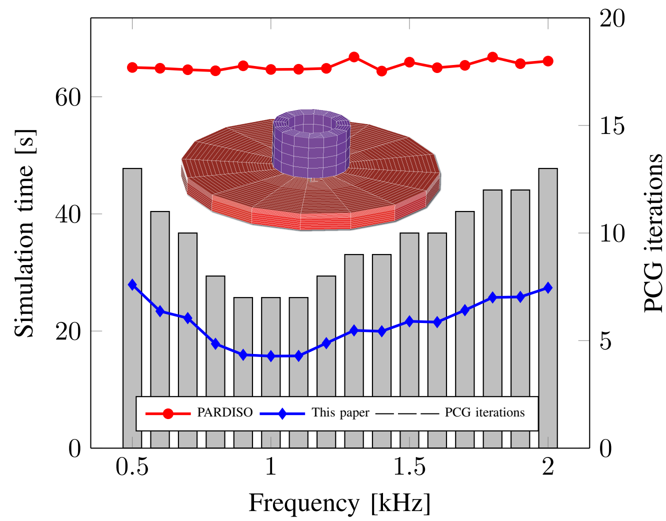

Fig. 1. Lines represent the time in seconds required to solve the eddy current problem at each frequency point. The histogram represents the number of PCG iterations required. With the chosen frequency range, $0.5 \leq \hat{\alpha} \leq 2$.

PCG iterations stopped as soon as the relative residual gone below 10^{-6}).

When a frequency sweep of 16 points between 500Hz and 2KHz is needed, the standard technique takes a total time of 1044 seconds. The technique proposed in this paper requires a first preprocessing comprising the factorization of $\mathbf{W}$ which takes about 23 seconds. Then, the solution at each frequency requires from 15 to 24 seconds, depending how far the frequency is from 1kHz, see Fig. 1. The stopping criterion used is a relative residual below 10^{-6} for all frequencies. In Fig. 1, the histogram represents the required PCG iterations for each frequency. The total time for the sweep is 365 seconds, with a speedup factor of about 3 with respect to PARDISO.

Of course, 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, in order 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.

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