Efficient Jacobian Matrix Determination for H^2 Representations of Nonlinear Electrostatic Surface Integral Equations

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***Abstract*—In this paper, a nonlinear electrostatic surface integral equation is presented that is suitable for predicting corrosion-related fields. Nonlinear behavior arises due to electrochemical reactions at polarized surfaces. Hierarchical H^2 matrices are used to compress the discretized integral equation for the fast solution of large problems. A technique based on randomized linear algebra is discussed for the efficient computation of the Jacobian matrix required at each iteration of a nonlinear solution.**

Keywords—corrosion-related fields, hierarchical matrices, nonlinear integral equation, randomized linear algebra.

I. INTRODUCTION

The prediction of corrosion-related fields is an important problem in various areas such as ships in marine environments. Knowledge of the corrosion-related fields is useful in the design of various systems to mitigate corrosion. Due to the electrochemical reactions that may occur at polarized conducting surfaces in an electrolyte, the electromagnetic integral equations that describe the relevant physics are often nonlinear, and Newton-Raphson techniques are commonly used in the solution of these nonlinear problems. However, for large problems, the Jacobian matrix that arises in the Newton-Raphson solution of a nonlinear integral equation can be expensive to compute in terms of memory and time. The determination of the Jacobian matrix becomes even more challenging when using fast methods since the system matrices are not fully computed but are represented in a compressed form.

In this paper, the basic electrostatic surface integral equation [1] for predicting corrosion-related (CR) fields is presented. For large problems, the integral equation discretization is compressed using Hierarchical (H^2) matrices [2]. An overview is then provided of the appropriate Jacobian matrix that arises in the nonlinear solution. Finally, an efficient method for determining the Jacobian matrix using randomized linear algebra [3] is discussed.

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II. THEORY

A. Nonlinear Integral Equation

Consider an unbounded electrolytic region V with a homogeneous conductivity σ. The region V is bound by a surface $\Gamma = \Gamma_\infty \cup \Gamma_b$ where Γ_∞ is an unbounded surface and Γ_b is a bound surface. The electrostatic potential in the electrolytic region V is:

$$\Phi(\mathbf{r}) + \oint_\Gamma \Phi(\mathbf{r}')\hat{\mathbf{n}}'\cdot\nabla' G(\mathbf{r},\mathbf{r}')\,d\Gamma' = \oint_\Gamma G(\mathbf{r},\mathbf{r}')\hat{\mathbf{n}}'\cdot\nabla'\Phi(\mathbf{r}')\,d\Gamma', \tag{1}$$

where $\mathbf{r}\in V$, $\hat{\mathbf{n}}$ is the unit normal to Γ oriented out of V, and $G = 1/\left(4\pi|\mathbf{r}-\mathbf{r}'|\right)$ is the static Green's function. Restriction of $\mathbf{r}\in\Gamma_b$ leads to the integral equation:

$$\frac{1}{2}\Phi(\mathbf{r}) + \oint_{\Gamma_b} \Phi(\mathbf{r}')\hat{\mathbf{n}}'\cdot\nabla' G(\mathbf{r},\mathbf{r}')\,d\Gamma' - \Phi_\infty = \oint_{\Gamma_b} G(\mathbf{r},\mathbf{r}')\hat{\mathbf{n}}'\cdot\nabla'\Phi(\mathbf{r}')\,d\Gamma', \quad \mathbf{r}\in\Gamma_b, \tag{2}$$

where $\Phi_\infty = -\oint_{\Gamma_\infty} \Phi(\mathbf{r}')\hat{\mathbf{n}}'\cdot\nabla' G(\mathbf{r},\mathbf{r}')\,d\Gamma'$ is a possible constant potential offset that must be determined as part of the nonlinear solution. The nonlinear problem admits a one-dimensional null space that is eliminated by requiring that the total flux through the bound surface be zero:

$$0 = \oint_{\Gamma_b} \hat{\mathbf{n}}'\cdot\nabla'\Phi(\mathbf{r}')\,d\Gamma' \ . \tag{3}$$

A pure Neumann problem is assumed, and the normal flux on Γ_b is specified as $\hat{\mathbf{n}}\cdot\nabla\Phi(\mathbf{r}) = f(\Phi)$. For insulating surfaces, $f(\Phi) = 0$, and, for non-insulating surfaces, $f(\Phi)\neq 0$. If on any part of Γ_b, $f'(\Phi)\neq 0$, then that portion of the surface is polarized, and the integral equation is nonlinear. For polarized

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surfaces, $f(\Phi)$ is called a *polarization curve*. For a nonlinear problem, the locally-corrected-Nyström discretized integral equation is [4]:

$$[H]\bar{\Phi} = [G]\, f(\bar{\Phi}) \,, \tag{4}$$

where $[H]$ and $[G]$ are the discretized forms of the left and right (of the equal sign) parts of (2) and (3), respectively, and $\left[\bar{\Phi}\right]_j = \Phi(\mathbf{r}_j)$ where $\mathbf{r}_j$ is the *j*th quadrature point in the Nyström discretization. Note that for a linear problem, $f(\bar{\Phi})$ in (4) does not depend on $\bar{\Phi}$ and is known everywhere *a priori*; hence, $[G]\, f$ reduces to a single excitation vector.

Application of the Newton-Raphson method to (4) gives the update equation at the *k*th iteration as:

$$\bar{\Phi}_{k+1} = \bar{\Phi}_k - [J_k]^{-1} \bar{F}(\Phi_k) \,, \tag{5}$$

where the residual $\bar{F}$ is:

$$F(\bar{\Phi}) = [G]\, f(\bar{\Phi}) - [H]\bar{\Phi} \,, \tag{6}$$

and the Jacobian matrix is:

$$[J_k] = [G]\,\mathrm{diag}\left[\, f'(\bar{\Phi}_k)\right] - [H] \,. \tag{7}$$

Here, $\mathrm{diag}\left[\, f'(\bar{\Phi}_k)\right]$ is a diagonal matrix whose diagonal entries are taken from the vector $f'(\bar{\Phi}_k)$.

B. Efficient Jacobian Matrix Determination

When the matrices $[G]$ and $[H]$ in (7) are represented as dense matrices, the determination of $[J_k]$ is straight-forward. Furthermore, when only a small portion of the bound surface is polarized, an efficient update using the Schur complement has been presented [4]. On the other hand, if $[G]$ and $[H]$ are represented in a compressed form, the operations in (7) are more difficult since it is desired that all intermediate operations and the final $[J_k]$ remain in compressed form. In this work, $[G]$ and $[H]$ are represented using Hierarchical H^2 matrices [2], and, so, $[J_k]$ should also be represented in H^2 form. Efficient computation of (7) requires being able 1) to compute $[G]\,\mathrm{diag}\left[\, f'(\bar{\Phi}_k)\right]$ directly with the result in an H^2 representation and 2) to subtract two H^2-represented matrices directly with the result in an H^2 representation.

In general, the required operations fall into the general form:

$$[C] = [A]\,\mathrm{diag}(\bar{a}) \pm [B]\,\mathrm{diag}(\bar{b}) \,, \tag{8}$$

where $\mathrm{diag}(\bar{x})$ indicates a diagonal matrix constructed from the vector $\bar{x}$ and $[A]$, $[B]$, and $[C]$ are H^2 matrices. It is further assumed that all H^2 matrices are built using the same tree structure. The necessary algorithm to implement (8) is constructed by noting that H^2 matrices are usually formed by compressing sub-blocks of the matrix using techniques such as the Adaptive Cross Approximation (ACA) to efficiently sample rows and columns of the sub-block and then compressing the sub-block ACA approximation using an SVD [5]. Direct use of the ACA+SVD method to sample the rows and columns of the $[A]\,\mathrm{diag}(\bar{a}) \pm [B]\,\mathrm{diag}(\bar{b})$ would be inefficient, although it does produce the desired H^2 representation of $[C]$.

Randomized linear algebra methods, on the other hand, provide a simple method to generate the SVD compressed sub-blocks in the H^2 representation without resorting to the row and column sampling required in an ACA technique. For example, an efficient randomized sampling method to generate the SVD of a matrix is detailed in [3]. Such methods enable the construction of controllably accurate outer-product representations of the sub-matrices of (8) through left and right multiplication with sets of random vectors. Because the matrices in (8) are represented using H^2 data structures, the required matrix-vector products encountered when using random projection methods (RPMs) can be rapidly evaluated.

Hence, randomized projection methods can be used to construct the H^2 representation of $[C]$ in (8). For an efficient and accurate method, the re-use of random matrix-vector product data at different levels of the nested H^2 data structure as well as rank and convergence estimation for the blocks of $[C]$ are necessary. Finally, random projection methods can be modularly fitted within an existing software framework that constructs the original H^2 representations of $[A]$ and $[B]$ using ACA-based methods.

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