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MLFMA-accelerated Nyström Method for Ultrasonic Scattering - Numerical Results and Experimental Validation

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Abstract. Full wave scattering models for ultrasonic waves are necessary for the accurate prediction of voltage signals received from complex defects/flaws in practical nondestructive evaluation (NDE) measurements. We propose the high-order Nyström method accelerated by the multilevel fast multipole algorithm (MLFMA) as an improvement to the state-of-the-art full-wave scattering models that are based on boundary integral equations. We present numerical results demonstrating improvements in simulation time and memory requirement. Particularly, we demonstrate the need for higher order geometry and field approximation in modeling NDE measurements. Also, we illustrate the importance of full-wave scattering models using experimental pulse-echo data from a spherical inclusion in a solid, which cannot be modeled accurately by approximation-based scattering models such as the Kirchhoff approximation.

INTRODUCTION

An important aspect of ultrasonic NDE (UNDE) measurement models is how the scattering of ultrasound from flaws/defects is modeled. Semi-analytical scattering models used in UNDE modeling include Kirchhoff approximation (KA) and geometric theory of diffraction (GTD). Although these models are computationally fast and memory-efficient, they do not model the complete physics of scattering. KA cannot accurately predict scattering from defects that are not very large compared to the wavelength of ultrasound and both GTD and KA ignore multiple reflections, which can be a problem if the late arriving signal due to secondary reflections overlaps with the leading edge response. It is therefore, important to consider full-wave scattering models that yield accurate results for the complex yet practical defects that cannot be modeled accurately using the approximation methods.

Progress has been made in developing full-wave scattering models based on hybrid FEM techniques [1]. However, similar progress has not been achieved in developing boundary integral equation techniques, with the main problem being the large simulation time and memory requirement. We applied a boundary integral equation method, called the Nyström method, to model elastic wave scattering from complex defects in 3D [2] and used the multilevel fast multipole algorithm (MLFMA) to reduce computation time and memory requirement. We showed our model to be in good agreement with benchmark data obtained from the World Federation of NDE Centers (WFNDEC) [3]. In this paper, we present numerical results demonstrating improvements in simulation time and memory requirement that can be achieved by our model over other full-wave scattering models that are based on boundary integral equations. As shown previously in [3], both KA and our model agree with experimental data very well in the case of large specular-reflector-like defects at normal incidence. In contrast, significant errors were observed in KA at oblique incidence angles. In this paper, we present further experimental data in validation of our model, particularly for defects that cannot be modeled accurately by KA such as small spherical inclusions.
HIGH ORDER NYSTRÖM METHOD

A brief summary of our scattering model will be presented in this section. We refer the reader to [2, 4] for a more detailed explanation. Consider a defect inside an otherwise infinite unbounded elastic solid. We want to find the displacement and traction fields scattered from the defect when a displacement field \( \mathbf{u}(\mathbf{x}) \) impinges on it. We formulate the problem of finding the scattered fields in terms of the following boundary integral equations [4]:

\[
\frac{1}{2} \mathbf{u}(\mathbf{x}) + \int_{S} dS' \left[ \mathbf{\Sigma}^T_s(\mathbf{x}, \mathbf{x}') \cdot \mathbf{u}(\mathbf{x}') - \mathbf{G}_s(\mathbf{x}, \mathbf{x}') \cdot \mathbf{t}(\mathbf{x}') \right] = \mathbf{u}(\mathbf{x}), \quad \mathbf{x} \in S
\]

\[
\frac{1}{2} \mathbf{t}(\mathbf{x}) + \int_{S} dS' \left[ \mathbf{G}^T_s(\mathbf{x}, \mathbf{x}') \cdot \mathbf{t}(\mathbf{x}') - \mathbf{\Sigma}_s(\mathbf{x}, \mathbf{x}') \cdot \mathbf{u}(\mathbf{x}') \right] = \mathbf{0}, \quad \mathbf{x} \in S
\]

where \( \mathbf{u} \) and \( \mathbf{t} \) are the displacement and traction fields, \( S \) is the surface of the defect, and \( \mathbf{\Sigma}_s \) and \( \mathbf{G}_s \) are the fundamental solutions (Green’s functions) of displacement and traction, respectively, with “+” subscript for the fundamental solution in exterior material and “-” subscript for the fundamental solution in the material of the defect. We solve the system of integral equations formed by Equation (1) and (2) using a high-order Nyström method to obtain the displacement and traction fields on the surface \( S \) from which the scattered fields outside the defect can be obtained via exterior representation formula for the displacement.

In practice, the surface \( S \) of the defect cannot be specified exactly except for simple shapes. Therefore, a surface mesh of \( S \), consisting of triangular/quadrilateral patches, is constructed first and then an approximation \( \tilde{S} \) to \( S \) is built via patch-wise parametric interpolation using shape functions. In our implementation, we used triangular patches with interpolation parameters \( \xi_1, \xi_2 \in \mathbb{R}_{>0} \), the set of non-negative real numbers, such that \( \xi_1 + \xi_2 \leq 1 \). The shape functions are polynomials in \( \xi_1 \) and \( \xi_2 \) of degree 1 or 2. We use conformal interpolation so that the surface \( \tilde{S} \) consists of continuous but non-overlapping (curved) triangular elements, with each element on \( \tilde{S} \) mapping to a patch on the surface mesh. Equation (1) and (2) can then be rewritten for the approximation surface \( \tilde{S} \). In the boundary element method (BEM), the displacement and traction fields on the surface \( \tilde{S} \) are approximated using basis functions on each element of \( \tilde{S} \). The unknowns to be determined are the coefficients of the basis functions. In the Nyström method, the displacement and traction fields are approximated via element-wise interpolation with the interpolation nodes located at the quadrature points on each element of \( \tilde{S} \). The unknowns are the values of the displacement and traction at the interpolation/quadrature points. Therefore, in the Nyström method, the integrals in Equation (1) and (2) can be approximated in the following form:

\[
\int_{\tilde{S}} dS' \mathbf{\Sigma}^T_s(\mathbf{x}, \mathbf{x}') \cdot \mathbf{u}(\mathbf{x}') = \sum_{p=1}^{N_s} \sum_{i=1}^{N_p} \int_{\Delta_p} dS' \mathbf{\Sigma}^T_s(\mathbf{x}, \mathbf{x}') \cdot \left[ L_{pj}(\mathbf{x}') u_{pi}^\alpha \mathbf{e}_{\alpha}(\mathbf{x}') \right] \quad \text{sum over } \alpha = 1, 2, 3 \quad \text{and } \mathbf{x} \in \tilde{S}
\]

where \( N_p \) is the total number of elements, \( N_p \) is the number of interpolation points per element, \( \Delta_p \) is the integration domain corresponding to \( p^{th} \) element, \( L_{pj} : \Delta_p \rightarrow \mathbb{R} \) is an interpolation function such that \( L_{pj}(\mathbf{x}_{pj}) = \delta_{ij} \) for all interpolation nodes \( \mathbf{x}_{pj} \) (\( j = 1 \) to \( N_p \)) in the \( p^{th} \) element; \( \mathbf{e}_{\alpha}(\mathbf{x}') \) for \( \alpha = 1, 2, 3 \) are basis vectors at the point \( \mathbf{x}' \) such that \( \mathbf{u}(\mathbf{x}') = u_{pi}^\alpha \mathbf{e}_{\alpha}(\mathbf{x}') \), with sum over \( \alpha \), and \( u_{pi}^\alpha \) are unknowns that need to be determined. The interpolation functions \( L_{pj} \), when written as functions of the interpolation parameters \( \xi_1 \) and \( \xi_2 \), are polynomials of degree 0, 1, 2 or 3.

Equation (1) and (2) can be rewritten by approximating all integrals as shown in Equation (3). This results in two equations that are valid for all \( \mathbf{x} \in \tilde{S} \). Discretization of these equations via Nyström method is performed by collocation at the interpolation/quadrature points. Let \( \mathbf{x}_0 \) be a collocation point. The integral on the right hand side of Equation (3) can be approximated by a quadrature rule when \( \mathbf{x}_0 \) is not close to the patch \( \Delta_p \) as shown below:

\[
\int_{\Delta_p} dS' \mathbf{\Sigma}^T_s(\mathbf{x}_0, \mathbf{x}') \cdot \left[ L_{pj}(\mathbf{x}') u_{pi}^\alpha \mathbf{e}_{\alpha}(\mathbf{x}') \right] = \sum_{j=1}^{N_p} w_j \mathbf{\Sigma}^T_s(\mathbf{x}_0, \mathbf{x}_{pj}) \cdot \left[ L_{pj}(\mathbf{x}_{pj}) u_{pi}^\alpha \mathbf{e}_{\alpha}(\mathbf{x}_{pj}) \right] = w_j \mathbf{\Sigma}^T_s(\mathbf{x}_0, \mathbf{x}_{pj}) \cdot \left[ u_{pi}^\alpha \mathbf{e}_{\alpha}(\mathbf{x}_{pj}) \right]
\]

where \( w_j \) and \( \mathbf{x}_{pj} \), for \( j = 1 \) to \( N_p \), are the quadrature weights and quadrature/interpolation nodes, respectively. When \( \mathbf{x}_0 \) is close to, or is one of the interpolation/quadrature points inside \( \Delta_p \), the integral in Equation (4) cannot be evaluated by a simple quadrature rule because \( \mathbf{\Sigma}^T_s(\mathbf{x}_0, \mathbf{x}') \) is either nearly-singular or singular. In our implementation of

\[200003-2\]
FIGURE 1. (a) RMS error in the scattering amplitude for plane-wave scattering from a spherical cavity inside an elastic solid. (b) Scattered displacement field at $r = 5a$ for plane-wave scattering from a rigid cube inside an elastic solid.

the Nyström method, such integrals are evaluated via singularity subtraction techniques [4]. Our technique of handling non-singular and singular integrals separately is similar to how local corrections are introduced in the Nyström method. Also, our implementation of the locally-corrected Nyström method can be considered as a boundary collocation method with the special characteristic of field interpolation nodes coinciding with the quadrature points.

We accelerate the Nyström method using MLFMA. See [4] for the implementation details. Although the higher-order geometry and field interpolation used in our method increases the complexity of the singular and nearly-singular integral computation, it allows us to achieve convergence with much smaller number of unknowns than that required by the lower order implementations while still maintaining efficiency. Many problems in practical UNDE modeling would remain impossible to tackle via boundary integral equation techniques without higher-order approximations. We will demonstrate this by comparing our method with a lower-order implementation of the MLFMA-accelerated Nyström method [5]. All simulations in this work were performed on a Dell Precision T7500 workstation with two quad-core 2.13 GHz processors and 24 GB memory but using only a single core. No parallel computing was involved. The simulations in [5] were performed on a Dell Precision 690 workstation with two dual-core 3.0 GHz processors and 16 GB RAM but using only a single core.

NUMERICAL RESULTS

Figure 1(a) shows the RMS error in the shear wave scattering amplitude of a spherical cavity inside an elastic solid as a function of the number of field interpolation nodes per shear wavelength. The spherical cavity is of radius $a$ and is located at the origin. The mass density and Lamé constants of the elastic solid are $\rho = 3 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$, respectively. The incident wave is a plane longitudinal-wave with normalized wavenumber $k_p a = \pi / \sqrt{3} \approx 1.813799$ propagating along the positive $z$-axis. The scattering amplitude was calculated at 181 uniformly sampled points between $\theta = 0$ and $\theta = \pi$ and the RMS error was calculated using these samples. The reference solution was calculated analytically via the technique of separation of variables. The RMS error is presented for different orders of field interpolation. In case of zeroth and first order field interpolation, first order geometry interpolation was used, while the results of second order field interpolation were obtained with second order geometry interpolation. From Fig. 1(a), we can see that for an RMS error of 0.01, second order interpolation needs roughly five nodes per shear wavelength, while the zeroth and first order interpolations need more than ten nodes per shear wavelength. As the required accuracy increases, the difference in the number of nodes required by lower and higher order methods increases further.
We will now compare our method with a lower-order implementation of the MLFMA-accelerated Nyström method [5] to show that our method achieves faster convergence without significantly increasing the computation time. Specifically, we will present the CPU time, memory and no. of unknowns required by our method and compare them with those of the lower-order method for three numerical examples presented in [5].

In the first example, we consider scattering from a rigid cube inside an elastic solid. The mass density ($\rho$), Poisson’s ratio ($\nu$) and normalized longitudinal wavenumber ($k_p a$) of the elastic solid are 1 kg/m$^3$, 0.5 and 20, respectively, where $a$ is half of the side length of the cube. The incident wave is assumed to be a plane wave traveling along the positive $z$-axis. The cube is centered at the origin. Since there exists no exact solution for this problem, we set our mesh density small enough to obtain external fields that are visually similar to those presented in [5]. Figure 1(b) shows the displacement at a distance $r = 5a$ from the origin as a function of the elevation angle. Table 1 shows the CPU time, memory usage of both [5] and our method. The size of the cube is around six times the wavelength of the longitudinal wave inside the material. This obstacle-size to wavelength ratio is comparable to that observed in immersion testing measurements towards the higher-end of the frequency band of inspection. The CPU time for the lower-order Nyström method is prohibitively large to be of any practical use and can be reduced by at least 50 times using higher order approximations.

**TABLE 1.** CPU time and memory usage for scattering from rigid cube.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference [5]</th>
<th>Present method</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time (hr.)</td>
<td>64.1</td>
<td>1.03</td>
</tr>
<tr>
<td>Memory (GB)</td>
<td>-</td>
<td>5.8</td>
</tr>
<tr>
<td>No. of unknowns</td>
<td>343,224</td>
<td>31,104</td>
</tr>
<tr>
<td>MLFMA levels</td>
<td>5</td>
<td>4</td>
</tr>
</tbody>
</table>

The second example is that of scattering of a longitudinal plane-wave from a rigid sphere inside an elastic solid. The mass density ($\rho$), Poisson’s ratio ($\nu$) and normalized longitudinal wavenumber ($k_p a$) of the solid are 1 kg/m$^3$, 0.1 and 20, respectively, where $a$ is the radius of the sphere. The incident wave is assumed to travel along the positive $z$-axis. Since only the absolute values of the displacement at a radial distance of 5$a$ are shown in [5], we set our mesh density such that our solution matches the exact analytical solution at least as closely as in [5]. The results are presented in Fig. 2(a). The displacement is normalized with respect to the radius of the sphere and $\theta$ is the polar angle. Figure 2(b) shows the error in our solution with respect to the exact analytical solution. The error is normalized with respect to the maximum value of the displacement over all $\theta$. Table 2 shows the CPU time and memory requirement of our method and [5]. The higher-order Nyström method performs 40 times faster than the lower-order method.

**TABLE 2.** CPU time and memory usage for scattering from rigid sphere.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference [5]</th>
<th>Present method</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time (hr.)</td>
<td>50.7</td>
<td>1.23</td>
</tr>
<tr>
<td>Memory (GB)</td>
<td>-</td>
<td>2.9</td>
</tr>
<tr>
<td>No. of unknowns</td>
<td>317,196</td>
<td>23,040</td>
</tr>
<tr>
<td>MLFMA levels</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

Finally, we consider the problem of scattering from an elastic sphere embedded inside an elastic solid. The incident wave is a longitudinal plane-wave traveling along the positive $z$-axis. The mass density ($\rho$), longitudinal wave speed ($c_p$) and shear wave speed ($c_s$) of the host medium are 1 kg/m$^3$, 0.95 m/s and 0.63 m/s, respectively, and those of the embedded sphere are 2 kg/m$^3$, 0.77 m/s and 0.5 m/s, respectively. The surface displacement along a principal cut is shown in Fig. 3(a) and the CPU time and memory usage are given in Table 3. In our MLFMA implementation, we used three levels for the trees corresponding to the Green’s functions of the host medium and four levels for those corresponding to the Green’s functions of the scattering medium. As in the case of the previous examples, significant reduction in the number of unknowns and simulation time can be achieved by the higher-order method.
FIGURE 2. (a) Radial and polar components of the scattered displacement field at \( r = 5a \) as a function of the elevation angle for plane-wave scattering from a rigid sphere. The results from the MLFMA-accelerated Nyström method are compared with the exact analytical solution. (b) Error in the radial and polar components of the displacement field normalized with respect to the maximum value of the corresponding components over all elevation angles.

TABLE 3. CPU time and memory usage for scattering from elastic sphere.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference [5]</th>
<th>Present method</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time (hr.)</td>
<td>55.9</td>
<td>2.67</td>
</tr>
<tr>
<td>Memory (GB)</td>
<td>12</td>
<td>1.3</td>
</tr>
<tr>
<td>No. of unknowns</td>
<td>237,600</td>
<td>11,520</td>
</tr>
<tr>
<td>MLFMA levels</td>
<td>5</td>
<td>3, 4</td>
</tr>
</tbody>
</table>

EXPERIMENTAL VALIDATION FOR SPHERICAL INCLUSIONS

Model predictions of the Nyström method and KA have been compared with experimental data for benchmark problems proposed by the WFNDEC [3]. In some of these benchmark problems, KA showed similar accuracy as the Nyström method. For oblique incidence on crack-like flaws, however, the Nyström method was demonstrated to be significantly better than the KA in terms of the modeling accuracy. The benchmark problems mentioned above are limited to the detection of void-like defects. For such defects, KA is fairly accurate in predicting the scattered fields in the direction of specular reflection as demonstrated in [3]. However, when considering inclusion-type defects, where one material is embedded inside the other, KA will lose accuracy unless secondary reflections are taken into account. The loss of accuracy of KA is even more severe when the secondary reflections overlap with the leading-edge response from the defect.

To investigate this, we obtained pulse-echo immersion testing measurement data for detecting a polystyrene sphere embedded inside Buehler’s TransOptic™ material. Similar experiments have already been performed [6], but results from KA were not considered in [6]. Also, we use a more accurate beam model in this paper. Figure 4(a) shows a schematic of the experimental setup for detecting a polystyrene sphere of diameter 600 \( \mu m \) embedded inside a specimen made of Buehler’s TransOptic™ material. Both the TransOptic™ block and the transducer are immersed in water. The transducer is 0.5 inch in diameter and is spherically focused with a geometric focal length of 4.657 inches, which was determined experimentally. The simulation model assumes that the transducer acts like a piston. The front surface of the TransOptic™ block is large enough that it can be can be approximated with an infinite surface while computing the displacement fields incident at the flaw due to the transducer. A pulser/receiver fires the transducer and
receives the pulse-echo from the defect.

We refer the reader to [3] for a detailed explanation of our measurement model. The material parameters relevant to the modeling were obtained using methods similar to those in [7, Ch. 9], and are given in Table 4. We obtained the material properties of polystyrene from [6]. Figure 4(b) shows the pulse-echo waveforms predicted by the Nyström method and KA along with the measured waveform. The two distinct pulses observed in the measurement occur due to reflections from the front and the back surfaces of the polystyrene sphere. The first pulse, also called as the leading-edge response, can be accurately predicted by KA as seen in the figure. The fields that penetrate into the sphere reflect from its back surface causing the second pulse. This pulse does not exist for spherical cavity-like defects as such cavities are impenetrable due to high acoustic-impedance contrast with respect to the specimen under test. For inclusion-type defects, however, the later-time response includes this pulse, which can have greater peak amplitude than the leading edge response for certain shapes of the defect. As the KA does not consider secondary reflections, it cannot predict the second pulse as seen in Fig. 4(b). On the other hand, the Nyström method, being a full-wave model, accurately predicts the second pulse. This difference between KA and full-wave models such as the Nyström method is very important while modeling inclusion-type defects that are small enough to allow significant overlap between the leading edge response and the response from secondary reflections, since such an overlap can cause large error in the peak-amplitude predicted by KA.

CONCLUSIONS

The high-order Nyström method is an improvement to the state-of-the-art elastic scattering models based on boundary integral equations for scattering. Because of the higher order geometry and field approximation, the number of unknowns required for achieving accurate scattering solutions is much smaller than that required by lower-order methods, and this improvement can be achieved without a significant overhead in computing the near-field matrix elements as demonstrated by several numerical examples. Both full-wave scattering models such as the proposed Nyström method and the KA can accurately predict the leading-edge scattering response from inclusion-type defects embedded in elastic solids. However, as demonstrated here, only the full-wave models can fully capture the later-time scattering response occurring from secondary reflections.
FIGURE 4. (a) Schematic of the immersion testing measurement setup for detecting a 600 µm diameter polystyrene sphere embedded inside a specimen made of Buehler’s TransOptic™ material. (b) Pulse-echo waveforms predicted by the Nyström method and KA compared with the measured waveform.

TABLE 4. Material parameters used in modeling the experiment shown in Fig. 4(a).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-wave speed in water (m/s)</td>
<td>1489.6</td>
</tr>
<tr>
<td>Density of water (kg/m$^3$)</td>
<td>1000</td>
</tr>
<tr>
<td>Attenuation in water (Np/m) ($f$ in MHz)</td>
<td>0.02479 $f^2$</td>
</tr>
<tr>
<td>P-wave speed in block (m/s)</td>
<td>2669.7</td>
</tr>
<tr>
<td>S-wave speed in block (m/s)</td>
<td>1340</td>
</tr>
<tr>
<td>Density of block (kg/m$^3$)</td>
<td>1171</td>
</tr>
<tr>
<td>P-wave attenuation in block (Np/m) ($f$ in MHz)</td>
<td>10.346 $f^{0.946}$</td>
</tr>
<tr>
<td>P-wave speed in polystyrene (m/s)</td>
<td>2400</td>
</tr>
<tr>
<td>S-wave speed in polystyrene (m/s)</td>
<td>1280</td>
</tr>
<tr>
<td>Density of polystyrene (kg/m$^3$)</td>
<td>1060</td>
</tr>
</tbody>
</table>
ACKNOWLEDGMENTS

The authors would like to thank Dr. Frank Margetan and Prof. Lester Schmerr for valuable advice in preparing the specimen for model validation, and Dan Barnard, Dr. Robert Grandin and Seval Oren for their help in performing the measurements.

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