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Combined shape-material sensitivity approach for elastic-wave identification of penetrable obstacles

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Abstract. This study deals with elastic-wave identification of heterogeneities (inclusions) in an otherwise homogeneous “reference” solid from limited-aperture measurements taken on its surface. On adopting the boundary integral equation (BIE) framework for elastodynamic scattering, the inverse query is cast as a minimization problem involving experimental observations and their simulations for a trial inclusion defined through its boundary, elastic moduli, and mass density. Expressions for the shape and material sensitivities of the misfit functional are obtained via the adjoint field approach and direct differentiation of the governing BIE's, respectively. A constrained nonlinear optimization framework based on the direct BIE method and an augmented Lagrangian is implemented. Numerical results for the reconstruction of an ellipsoidal defect in a semi-infinite solid show the effectiveness of the proposed shape-material sensitivity formulation, which constitutes an essential computational component.

1. Introduction
Elastic-wave sensing of penetrable (i.e. deformable) heterogeneities in a solid matrix is a long-standing problem in mechanics with applications to e.g. nondestructive material testing and medical diagnosis. This investigation focuses on the mapping of objects buried in a known reference solid, from only a limited number of remote measurements. In such instances, boundary integral equation (BIE) formulations [3, 5] provide a direct mathematical link between the observed waveforms and the geometry and material characteristics of a hidden object.

Although inverse scattering in general has been the subject of intensive mathematical and computational research [4, 15], only limited efforts have so far been devoted to the wave-based reconstruction of homogeneous elastic inclusions. Two-dimensional BIE formulations of the inclusion identification problem were proposed in [9] (elastostatics) and [16] (elastodynamics). Volume integral equations of the Lippmann-Schwinger type are used in e.g. [13]. Mathematical studies on the issue of identifiability can be found in e.g. [8]. More recently, approximate identification methods based on the small-inclusion asymptotics were proposed in e.g. [1, 6] for preliminary “scanning” of solid bodies.

The focus of this investigation is the development of a computational platform for the 3D identification of penetrable elastic inclusions via an elastodynamic BIE framework. For identification purposes, the inverse problem is reduced to the minimization of a cost functional representing the misfit between experimental observations (values of displacements at sensor locations) and their simulations for an assumed inclusion configuration. For computational efficiency of gradient-based search techniques, the shape sensitivity of the featured cost functional
is evaluated via an adjoint field approach, generalizing upon previous work on inverse scattering of acoustic waves [2] and elastic-wave void identification [7], while its material sensitivity is derived using a direct differentiation approach. Both types of sensitivity are implemented and integrated into an optimization algorithm based on the augmented-Lagrangian approach [10].

2. Direct and inverse scattering by elastic inclusions

The reference homogeneous solid \( \Omega \), containing an unknown bonded inclusion \( \hat{\Omega}^{true} \) with boundary \( \Gamma^{true} \), is probed by elastic waves. The reference medium, whose external boundary (available for testing) is denoted by \( S \), is characterized by its elastic tensor \( C \) and mass density \( \rho \); the corresponding characteristics of the inclusion are denoted as \( \hat{C}^{true}, \hat{\rho}^{true} \).

To identify the hidden defect in terms of its geometry \( \hat{\Omega}^{true} \) and material characteristics \( \hat{C}^{true}, \hat{\rho}^{true} \), time-harmonic excitations are applied in the form of prescribed surface \( g \) force densities over \( S \). For brevity, the implicit time-harmonic factor \( \exp(i\omega t) \) where \( \omega \) denotes the angular frequency of excitation is omitted hereon. Letting \( \hat{\Omega} \) denote a trial inclusion bounded densities over available for testing) is denoted by \( \hat{\Omega} \). For identification purposes, the displacement \( u^{obs} \) induced by excitation \( g \) is monitored over the measurement surface \( S_{obs} \subset S \). The inclusion is sought so as to minimize a misfit cost functional

\[
J(\hat{\Omega}, \hat{C}, \hat{\rho}) = \int_{S_{obs}} \varphi(u[\hat{\Omega}, \hat{C}, \hat{\rho}], w^{obs}) \, dS_{\xi},
\]

where function \( \varphi \), which quantifies the misfit between the predicted and observed displacements, is assumed to be differentiable with respect to its arguments. For example, the usual least-squares measure of misfit is defined through \( 2\varphi(u, u^{obs}) = |u - u^{obs}|^2 \).

\textit{Forward problem.} Let \( \mathcal{L} \) and \( \hat{\mathcal{L}} \) denote the Navier partial differential operator respectively associated with the reference solid and inclusion, i.e.

\[
\mathcal{L}u \equiv \nabla \cdot (C \nabla u) + \rho \omega^2 u, \quad \hat{\mathcal{L}}\hat{u} \equiv \nabla \cdot (\hat{C} \nabla \hat{u}) + \hat{\rho} \omega^2 \hat{u}.
\]

In (2) and thereafter, all quantities defined with reference to the inclusion or its constitutive parameters are indicated with a hat symbol. The trial displacement \( \hat{u} \), whose trace on \( S_{obs} \) is featured in cost functional (1), solves the forward problem defined by

\[
\mathcal{L}u = 0 \quad (\text{in } \Omega^-), \quad \hat{\mathcal{L}}\hat{u} = 0 \quad (\text{in } \hat{\Omega}), \quad (\text{elastodynamic field equations}), \\
u = \hat{u} \quad \text{(on } \Gamma), \quad (\text{perfect bonding conditions}), \\
t = g \quad (\text{on } S), \quad (\text{boundary condition}).
\]

Here \( t \equiv (C : \nabla u) \cdot n \) and \( \hat{t} \equiv (\hat{C} : \nabla \hat{u}) \cdot \hat{n} \) denote the boundary tractions acting respectively on the reference solid and the inclusion, where \( \hat{n} = -n \) and \( n \) is oriented toward the interior of \( \hat{\Omega} \).

If the reference domain \( \Omega \) extends to infinity, as is the case for the examples presented later in this article, \( u \) is in addition assumed to satisfy a radiation condition at infinity (an assumption which may be relaxed so as to include e.g. the scattering of plane waves by inclusions).

The forward problem (3)–(5) can be recast in terms of the following weak formulation:

\[
\text{Find } (u, \hat{u}) \in \mathcal{V}, \quad A((u, \hat{u}), (w, \hat{w})) - F((w, \hat{w})) = 0 \quad \forall (w, \hat{w}) \in \mathcal{V}
\]

with the function space \( \mathcal{V} \), the symmetric bilinear form \( A \), and the linear form \( F \) defined by

\[
\mathcal{V} = \{ (w, \hat{w}) \mid w \in [H^1_{\text{loc}}(\Omega^-)]^3, \quad \hat{w} \in [H^1(\hat{\Omega})]^3, \quad w = \hat{w} \text{ on } \Gamma \}, \\
A((u, \hat{u}), (w, \hat{w})) = \int_{\Omega^-} a(u, w) \, dV + \int_{\hat{\Omega}} \hat{a}(\hat{u}, \hat{w}) \, dV, \quad F((w, \hat{w})) = \int_{S} g \cdot w \, dS
\]

in terms of the bilinear energy densities \( a, \hat{a} \) for the reference medium and inclusion given by

\[
a(u, w) = \nabla u \cdot C : \nabla w - \rho \omega^2 u \cdot w, \quad \hat{a}(\hat{u}, \hat{w}) = \nabla \hat{u} \cdot \hat{C} : \nabla \hat{w} - \hat{\rho} \omega^2 \hat{u} \cdot \hat{w}.
\]
Boundary integral formulation for the forward problem. With reference to the Cartesian frame \( \{O, \xi_1, \xi_2, \xi_3\} \), let the host domain \( \Omega \) be semi-infinite \((\xi_3 \geq 0)\), bounded by the traction-free surface \( S = \{\xi \mid \xi_3 = 0\} \). Let \( U^\ell(\mathbf{x}, \xi; \omega) \), \( T^\ell(\mathbf{x}, \xi; \omega) \) denote the elastodynamic Green’s function, with \( T^\ell(\mathbf{x}, \xi; \omega) \) vanishing identically on \( S \), while \( U^\ell(\mathbf{x}, \xi; \omega) \), \( T^\ell(\mathbf{x}, \xi; \omega) \) denotes the (full-space) elastodynamic fundamental solution corresponding to the constitutive properties of the inclusion.

With the above definitions, the forward problem (3)–(5) for a semi-infinite solid can be reformulated in terms of a pair of boundary integral equations:

\[
\frac{1}{2} \mathbf{u}(\mathbf{x}) + \text{P.V.} \int_{\Gamma} \mathbf{u}(\xi) \cdot T^\ell(\mathbf{x}, \xi) \, dS_\xi - \int_{\Gamma} t(\xi) \cdot U^\ell(\mathbf{x}, \xi; \omega) \, dS_\xi = \mathbf{u}^\ell(\mathbf{x}) \quad (\mathbf{x} \in \Gamma) \tag{9}
\]

\[
\frac{1}{2} \mathbf{u}(\mathbf{x}) + \int_{\Gamma} \mathbf{u}(\xi) \cdot \bar{T}^\ell(\mathbf{x}, \xi) \, dS_\xi + \int_{\Gamma} t(\xi) \cdot \bar{U}^\ell(\mathbf{x}, \xi; \omega) \, dS_\xi = 0 \quad (\mathbf{x} \in \Gamma) \tag{10}
\]

written respectively for the “matrix” \( \Omega^- \) and inclusion \( \hat{\Omega} \), in terms of the traces \((\mathbf{u}, \mathbf{t})\) on \( \Gamma \) of the exterior field. The free field \( \mathbf{u}^\ell \) featured on the right-hand side of (9) is explicitly given by

\[
\mathbf{u}^\ell(\mathbf{x}) = \int_{S} g(\xi) \cdot U^\ell(\mathbf{x}, \xi; \omega) \, dS_\xi (\mathbf{x} \in \Omega) \tag{11}
\]

On solving (9) and (10) for \( \mathbf{u} \) and \( \mathbf{t} \) on \( \Gamma \), the displacement field in the (reference) solid surrounding the inclusion is computable from the integral representation formula

\[
\mathbf{u}(\mathbf{x}) = \mathbf{u}^\ell(\mathbf{x}) + \int_{\Gamma} \left\{ t(\xi) \cdot U^\ell(\mathbf{x}, \xi; \omega) - \mathbf{u}(\xi) \cdot T^\ell(\mathbf{x}, \xi; \omega) \right\} \, dS_\xi \quad (\mathbf{x} \in \Omega^-). \tag{12}
\]

3. Differentiation with respect to inclusion perturbations

To quantify the effect of the inclusion’s boundary and material-parameter perturbations on the cost function (1), the defect configuration \((\hat{\Omega}; \hat{\mathbf{C}}, \hat{\rho})\) is assumed to depend on a time-like evolution parameter \( \tau \) \cite{14}. The unperturbed, ‘initial’ configuration \((\hat{\Omega}; \hat{\mathbf{C}}, \hat{\rho})\) is conventionally associated with \( \tau = 0 \). In this study, only the first-order infinitesimal perturbations of \((\hat{\Omega}; \hat{\mathbf{C}}, \hat{\rho})\), i.e. the first-order “time” derivatives at \( \tau = 0 \), are considered. With such hypothesis, perturbations of the inclusion’s shape, elastic properties, and mass density can be expressed as

\[
\Omega_\tau = \Omega + \theta \tau, \quad \hat{\mathbf{C}}_\tau = \hat{\mathbf{C}} + \hat{\mathbf{C}}' \tau, \quad \hat{\rho}_\tau = \hat{\rho} + \hat{\rho}' \tau, \tag{13}
\]

where \( \theta(\mathbf{x}) \) is a given transformation velocity field, assumed to vanish outside of a neighbourhood of \( \hat{\Omega} \). A generic field variable \( g \) which depends on the inclusion configuration, e.g. the solution of the forward problem (3)–(5), can be represented in the form \( g(x; \Omega_\tau, \hat{\mathbf{C}}_\tau, \hat{\rho}_\tau) \). The total derivative \( \hat{g} \) is then a sum of contributions arising from geometric and material perturbations:

\[
\hat{g} = \hat{g} + \hat{g}', \quad \text{with} \quad \hat{g} = \lim_{\tau \to 0} \frac{1}{\tau} \left[ g(x; \Omega_{\tau}, \hat{\mathbf{C}}_{\tau}, \hat{\rho}_{\tau}) - g(x; \hat{\Omega}, \hat{\mathbf{C}}, \hat{\rho}) \right] \tag{14}
\]

\[
\hat{g}' = \lim_{\tau \to 0} \frac{1}{\tau} \left[ g(x; \hat{\Omega}, \hat{\mathbf{C}}_{\tau}, \hat{\rho}_{\tau}) - g(x; \hat{\Omega}, \hat{\mathbf{C}}, \hat{\rho}) \right] = \frac{\partial g}{\partial \hat{\mathbf{C}}} \cdot \hat{\mathbf{C}}' + \frac{\partial g}{\partial \hat{\rho}} \hat{\rho}'.
\]

The shape sensitivity thus corresponds to the Lagrangian time derivative of continuum kinematics with the physical time variable replaced with a pseudo-time. The total derivative of a generic domain integral \( I_\tau \) whose support \( D_\tau \) undergoes geometric perturbation (13a) is, upon noting that the shape sensitivity of a differential volume element \( dV \) is given by \( [\text{div} \theta] \, dV \), such that

\[
I_\tau = \int_{D_\tau} g(x; \hat{\Omega}_{\tau}, \hat{\mathbf{C}}_{\tau}, \hat{\rho}_{\tau}) \, dV \Rightarrow \hat{I} = \hat{I} + \hat{I}' = \int_{D} \{ \hat{g} + g \text{div} \theta \} \, dV + \int_{D} \hat{g}' \, dV. \tag{15}
\]

3.1. Shape sensitivity using an adjoint solution

Since \( S_{\text{obs}} \) is unaffected by geometric perturbation (13a), the shape sensitivity of (1) is given by

\[
\hat{J} = \text{Re} \left\{ \int_{S_{\text{obs}}} \frac{\partial \varphi}{\partial \mathbf{u}} (\mathbf{u}, \xi) \cdot \hat{\mathbf{u}} \, dS \right\}, \quad \text{with} \quad \frac{\partial \varphi}{\partial \mathbf{u}} \equiv \frac{\partial \varphi}{\partial \mathbf{u}_R} - i \frac{\partial \varphi}{\partial \mathbf{u}_I}, \quad (\mathbf{u} = \mathbf{u}_R + i \mathbf{u}_I). \tag{16}
\]
Displacement shape sensitivity – weak formulation. Since the weak formulation (6) of the forward problem (3)–(5) holds for all perturbed inclusion configurations, the governing weak formulation for the displacement shape sensitivity \((\hat{u}, \hat{u})\) can be obtained by exploiting

\[
\mathcal{A}((u, \hat{u}), (w, \hat{w})) = 0 \quad \forall (w, \hat{w}) \in \mathcal{V}.
\]

(17)

Application of the Lagrangian differentiation formula (15b) to (7) results in

\[
\mathcal{A}((u, \hat{u}), (w, \hat{w})) - \hat{\mathcal{F}}((w, \hat{w})) = \mathcal{A}((u, \hat{u}), (w, \hat{w})) - \mathcal{F}(\hat{w}, \hat{w}) + \mathcal{A}((u, \hat{u}), (w, \hat{w}))
\]

\[
+ \int_{\Omega} Lw \cdot (\nabla u \cdot \theta) \, dV + \int_{\Omega} \hat{L}w \cdot (\nabla \hat{u} \cdot \theta) \, dV + \int_{\Gamma} [n \cdot E(u, w) + \hat{n} \cdot E(\hat{u}, \hat{w})] \cdot \theta \, dS
\]

(18)

where the bilinear tensorial function \(E(u, w)\), related to the dynamic Eshelby energy-momentum, is defined by

\[
E(u, w) = a(u, w) I - (C \cdot \nabla w) \cdot \nabla u - (C \cdot \nabla u) \cdot \nabla w.
\]

(19)

(\(I\): second-order identity tensor). On invoking the equality obtained by setting \((w, \hat{w}) = (\hat{w}, \hat{w})\) in (6), the displacement shape sensitivity \((\hat{u}, \hat{u})\) is found to be governed by the weak formulation

\[
\text{Find } (\hat{u}, \hat{u}) \in \mathcal{V}, \quad \mathcal{A}((\hat{u}, \hat{u}), (w, \hat{w})) = - \int_{\Omega} Lw \cdot (\nabla u \cdot \theta) \, dV - \int_{\Omega} \hat{L}w \cdot (\nabla \hat{u} \cdot \theta) \, dV
\]

\[
- \int_{\Gamma} [n \cdot E(u, w) + \hat{n} \cdot E(\hat{u}, \hat{w})] \cdot \theta \, dS \quad \forall (w, \hat{w}) \in \mathcal{V}.
\]

(20)

Adjoint solution. The main motivation behind the adjoint state approach is to evaluate the shape sensitivity (16) in an indirect, and computationally faster, manner by circumventing the explicit computation of field sensitivities \(\hat{u}\). To this end, it is convenient to interpret the integral in (16) as a virtual work and treat the displacement sensitivity \(\hat{u}\) therein as a test function. Accordingly, let the adjoint state \((v, \hat{v})\) be defined as the solution of the adjoint transmission problem defined by the weak formulation

\[
\text{Find } (v, \hat{v}) \in \mathcal{V}, \quad \mathcal{A}((v, \hat{v}), (w, \hat{w})) = \int_{S_{\text{obs}}} \frac{\partial \varphi}{\partial u} (u, \xi) \cdot w \, dS \quad \forall (w, \hat{w}) \in \mathcal{V}
\]

(21)

The adjoint problem is then alternatively defined by strong formulation (3)–(5) or BIE formulation (9)–(11) with surface traction distribution \(g\) replaced with \(1_{\text{gobs}} \partial \varphi / \partial u\).

Shape sensitivity formula. Setting \((w, \hat{w}) = (\hat{u}, \hat{u})\) in (21), formula (16) for \(\hat{J}\) becomes

\[
\hat{J} = \mathcal{A}((v, \hat{v}), (\hat{u}, \hat{u})).
\]

Choosing \((w, \hat{w}) = (v, \hat{v})\) in (20) then readily yields, by virtue of field equations implied by (21) and the symmetry of \(\mathcal{A}(\cdot, \cdot)\), the following expression for \(\hat{J}\), where the displacement shape sensitivity no longer appears:

\[
\hat{J} = - \int_{\Gamma} [n \cdot E(u, v) + \hat{n} \cdot E(\hat{u}, \hat{v})] \cdot \theta \, dS.
\]

(22)

To make eq (22) tractable in a BIE/BEM framework, tensor function \(E(u, v)\) is rewritten in terms of the inferential tractions and tangential displacement gradients as

\[
n \cdot E(u, v) \cdot \theta = \left[ \nabla_s u \cdot C \cdot \nabla v + \Delta t \cdot D \cdot \Delta p - \rho \omega^2 u \cdot v \right] \theta_n - (t \cdot \nabla_s v + p \cdot \nabla_s u) \cdot \theta.
\]

in terms of the surface gradient operator \(\nabla_s\) defined through \(\nabla u = \nabla_s u + u \cdot n \otimes n\), having inverted the relationship \(t = (C \cdot \nabla u) \cdot n\) to express the normal derivative \(u_n\) in terms of \(\nabla_s u\) and \(t\) as

\[
u_n = D \cdot t.
\]

(23)

with the second-order tensor \(D\) and the combination \(\Delta t\) respectively defined by \(D = [n \cdot C \cdot n]^{-1}\).
(taking advantage of the minor symmetry of the elasticity tensor $C$), and $\Delta t = t - (C : \nabla u) \cdot n$. This in turn allows to express (22) in terms of quantities directly available from the boundary element solution, thus establishing, after some manipulations, the desired shape sensitivity as

$$
\dot{J} = \int_{\Gamma} \left[ \nabla_s u : (\dot{C} - C) : \nabla_s \dot{v} - \Delta \dot{t} \cdot \dot{D} \cdot \Delta \dot{p} + \Delta t \cdot D \cdot \Delta p - (\dot{\rho} - \rho) \omega^2 u \cdot \dot{v} \right] \theta_n \, dS.
$$

(24)

where $p = (C : \nabla v) \cdot n$ and $\dot{p} = (\dot{C} : \nabla \dot{v}) \cdot \dot{n}$ are the traction vectors respectively associated with $v$ and $\dot{v}$. In the special case of isotropic elasticity (which is not a prerequisite for the derivation of (24)), and denoting by $I$ the symmetric fourth-order identity tensor, tensors $C$ and $D$ are given in terms of the shear modulus $\mu$ and Poisson’s ratio $\nu$ of the background solid as

$$
C = 2\mu \left[ \frac{\nu}{1 - 2\nu} I \otimes I + I \right], \quad D = \frac{1}{\mu} \left[ I - \frac{1}{2(1 - \nu)} n \otimes n \right].
$$

3.2. Material sensitivity

On the basis of (15c), the material sensitivity of the generic cost function (1) can be written as

$$
\mathcal{J}' = \text{Re} \left\{ \int_{S_{\text{obs}}} \frac{\partial \varphi}{\partial u} (u, \xi) \cdot u' \, dS \right\}.
$$

(25)

As an adjoint solution approach leads to material sensitivity formulae expressed as domain integrals, and hence not well-suited to the present BIE framework, the direct differentiation is used instead, with the material sensitivity $u'$ on $S_{\text{obs}}$ evaluated by differentiating the governing BIEs. On expressing the governing pair (9) and (10) in operator form as

$$
\begin{align*}
\mathcal{T}[u](\mathbf{x}) - \mathcal{U}[t](\mathbf{x}) &= u^s(\mathbf{x}) \quad (\mathbf{x} \in \Gamma), \\
\mathcal{T}'[u'](\mathbf{x}) - \mathcal{U}'[t'](\mathbf{x}) &= 0
\end{align*}
$$

(26)

and keeping in mind that the fundamental kernels $\hat{U}^t$ and $\hat{T}^t$ depend on the inclusion’s material parameters but $U^t$, $T^t$ and the free field $u^s$ do not, the sensitivity fields $t'$ and $u'$ on $\Gamma$ can be shown to solve the pair of integral equations

$$
\begin{align*}
\mathcal{T}'[u'](\mathbf{x}) - \mathcal{U}'[t'](\mathbf{x}) &= 0 \\
\mathcal{T}'[u'](\mathbf{x}) - \mathcal{U}'[t'](\mathbf{x}) &= \hat{u}'[t](\mathbf{x}) - \hat{T}'[u](\mathbf{x}) \\
\end{align*}
$$

(27)

where integral operators $\hat{U}'$, $\hat{T}'$ appearing in the right-hand side are defined in terms of the respective kernel derivatives ($\hat{U}' \cdot t'$ and $\hat{T}' \cdot t'$). Once equations (27) are solved for $u', t'$ on $\Gamma$, taking the material sensitivity of representation formula (12) yields the displacement material sensitivity $u'$ on $S_{\text{obs}}$. On substituting the resulting expression into (25), the material sensitivity of cost function (1) is finally given, using an operator notation similar to that in (26), by

$$
\mathcal{J}' = \text{Re} \left\{ \int_{S_{\text{obs}}} \frac{\partial \varphi}{\partial u} (u, \xi) \cdot \left( \hat{U}^{\text{obs}}[t'](\mathbf{x}) - \mathcal{T}^{\text{obs}}[u'](\mathbf{x}) \right) dS \right\}.
$$

(28)

4. Computational treatment

Defect parametrization. The geometry of the trial defect $\hat{\Omega}$ is, for the ensuing numerical experiments, described in terms of an ellipsoid whose principal axes are aligned with the reference Cartesian frame $\{O; \xi_1, \xi_2, \xi_3\}$; its evolution within the host domain $\Omega$ is restricted to i) translation and ii) stretch along the principal axes. For problems involving identification of a single isotropic defect, such description entails the use of a nine-dimensional parametric space

$$
a = (c_1/d, c_2/d, c_3/d, \alpha_1/d, \alpha_2/d, \alpha_3/d, \hat{\mu}/\mu, \hat{\nu}/\nu, \hat{\rho}/\rho),
$$

(29)

which incorporates the defect’s centroid $(c_1, c_2, c_3)$, principal axes $(\alpha_1, \alpha_2, \alpha_3)$, and material characteristics $(\mu, \nu, \rho)$. Definitions (29) are made dimensionless using material characteristics $(\mu, \rho)$ of the reference solid and an arbitrary length scale $d$. With such definitions, analytical dependence of the nodal coordinates, $\xi^T = \xi^T(a)$, of the surface mesh on the evolving defect boundary $\Gamma$ is introduced as an affine deformation of the boundary element mesh for a reference
unit sphere $S$ (described by Lagrange coordinates $(X_1, X_2, X_3)$) so that $\xi_i^b = c_i + \alpha_i X_i^b$ ($X_i^b \in S$, $i = 1, 2, 3$). Introducing an auxiliary notation $J_a(a) \equiv J(\bar{\Omega}(a_1, \ldots, a_6), \bar{C}(\hat{\mu}, \hat{\nu}, \hat{\rho}))$ to reflect the featured defect parametrization and making reference to (14), the necessary sensitivities $\partial J_a/\partial a_d$ required for the minimization of $J_a(a)$ are accordingly computable as

$$\frac{\partial J_a}{\partial a_d} = \mathcal{J}|_{r=a_d}, \quad d = 1, 2, \ldots, 6 \quad \text{Material:} \quad \frac{\partial J_a}{\partial a_d} = \mathcal{J}|_{r=a_d}, \quad d = 7, 8, 9 \quad (30)$$

**Evaluation of shape sensitivities.** The computation of $\mathcal{J}$ and $\mathcal{J}'$ entails the solution of three boundary value problems, associated respectively with the primary field $u$, the adjoint field $\nu$, and the material-sensitivity field $u'$. With reference to (11), (26), (27), and after a standard BEM discretization process, the discrete algebraic systems for these fields can be written as

$$\begin{align*}
\text{Primary} & : \quad \mathbf{H} \mathbf{u} - \mathbf{G} \mathbf{T} = \mathbf{U}^f, \\
\text{Adjoint} & : \quad \mathbf{H} \mathbf{v} - \mathbf{G} \mathbf{P} = \mathbf{V}^f, \\
\text{Material-sensitivity} & : \quad \mathbf{H} \mathbf{u'} - \mathbf{G} \mathbf{T'} = \mathbf{G}' \mathbf{T} - \mathbf{H}' \mathbf{U}
\end{align*} \quad (31)$$

where vectors $\mathbf{U}$ and $\mathbf{T}$ contain the nodal approximations of the primary field $u$ and $t$; coefficient matrices $\mathbf{H}$, $\mathbf{G}$, $\mathbf{H}$ and $\mathbf{G}$ approximate the respective integral operators $\mathcal{T}, \mathcal{U}, \mathcal{T}$ and $\mathcal{U}$ in (26); $\mathbf{U}^f$ and $\mathbf{V}^f$ collect the nodal values of the forward and adjoint free fields; $\mathbf{V}$ and $\mathbf{P}$ are identified with the adjoint field $u$ and $t$; vectors $\mathbf{U}'$ and $\mathbf{T}'$ refer respectively to $u'$ and $t'$, while $\mathbf{H}'$ and $\mathbf{G}'$ are the matrix discretizations of $\mathcal{T}'$ and $\mathcal{U}'$ in (27). One may note that the coefficient matrices are the same for all three discretized systems, which allows for a computationally-effective evaluation of the adjoint and material-sensitivity fields once the primary problem has been solved.

**Parallel computation.** Owing to the high computational cost that is commonly associated with 3D void scattering, regularized boundary integral treatment [12] of the primary, adjoint, and material-sensitivity problems in (31a–c) is implemented, together with formulas (24) and (28), in a data parallel code using the message-passing interface (MPI) [11].

**Minimization.** Preliminary identification studies on sample inclusion configurations demonstrated that the unconstrained (quasi-Newton) minimization algorithm, successfully used in previous studies [7] for 3D void reconstruction, is ill-equipped to deal with the geometric-material identification problem at hand. This prompted the development of a more robust algorithm based on the augmented-Lagrangian cost functional [10], as a means to deal with physical inequality constraints that have to be enforced on some of the arguments of $J_a$, most notably the material characteristics of the trial defect, to maintain the physical relevance of the solution. In the present context, one must have $\hat{\mu} > 0$ and $-1 < \hat{\nu} < 0.5$ besides $\hat{\rho} > 0$. To aid the strict enforcement of these constraints, the defect parametrization (29) is restated using the transformed variables $b = (b_1, b_2, \ldots, b_9) = (a_1, \ldots, a_6, \log a_7, \log(0.5 - a_8), \log a_9) \in \mathbb{R}^9$, which ensure that $\mu > 0$, $\nu < 0.5$, and $\rho > 0$. The featured cost function is then expressed through $J_b(b) = J_a(a)$, and the required sensitivities of $J_b$ can be computed as

$$\begin{align*}
\frac{\partial J_b}{\partial b_d} = \frac{\partial J_a}{\partial a_d}, & \quad d \leq 6, \\
\frac{\partial J_b}{\partial b_d} = \frac{\partial J_a}{\partial a_d} a_d, & \quad d = 7, 9 \\
\frac{\partial J_b}{\partial b_8} = \frac{\partial J_a}{\partial a_8} (a_8 - 0.5)
\end{align*}$$

with $\partial J_a/\partial a_i$ given by (24), (28) and (30). With the above parametrization, the optimization problem is posed in terms of the minimization of an augmented Lagrangian functional

$$\min_b \mathcal{L}_\lambda(b, \lambda, \gamma) = J_b(b) + \sum_{i \in I} \psi(C_i(b), \lambda_i; \gamma), \quad \psi(C, \lambda, \gamma) = \begin{cases} C^2/(2\gamma) - \lambda C & (C \leq \gamma \lambda), \\ -\gamma \lambda^2/2 & (C > \gamma \lambda) \end{cases} \quad (32)$$

(where the “soft” inequality constraints $C_i$ ($I$ being a set of integers) reflect any additional restrictions on $b$), whose gradient is computable as

$$\nabla_b \mathcal{L}_\lambda(b, \lambda^m; \gamma_m) = \nabla J_b(b) - \sum_{i \in I \bar{C}_i(b) \leq \gamma_m \lambda^m i} \left(\lambda^m_i - \frac{C_i(b)}{\gamma_m i}\right) \nabla C_i(b). \quad (33)$$
Given the initial penalty parameter \( \gamma_0 > 0 \), tolerance \( \tau_0 > 0 \), starting point \( b^0 \), and starting vector of Lagrange multipliers \( \lambda^0 \), the augmented Lagrangian method introduces a sequence \( (m = 1, 2, \ldots) \) of unconstrained minimization problems with explicit Lagrange multiplier estimates \( \lambda^m \) and decreasing penalties \( \gamma_m \) that produce a good estimate of the local Karush-Kuhn-Tucker minimizer \( b^* \) even when the penalty parameter \( \gamma \) is not particularly close to zero [10]. This latter feature is highly desirable as it reduces the possibility of ill-conditioning that commonly occurs for vanishing values of \( \gamma \). For any given iterate \( m \), the nonlinear minimization of \( \mathcal{L}_A(b, \lambda^m, \gamma_m) \) is effected (with \( \lambda^m \) and \( \gamma_m \) fixed) using the BFGS quasi-Newton method [10].

5. Results

The effectiveness of the proposed shape-material sensitivity approach as a tool for reconstructing buried penetrable objects is now demonstrated on numerical results. The buried obstacle is “illuminated” using \( 4 \times 4 = 16 \) point forces, sequentially applied in the \( \xi_3 \)-direction over the square testing grid \( (\xi_1, \xi_2) \in [-3d, 3d] \times [-3d, 3d] \) in the \( \xi_3 = 0 \) plane; for each source, the response of the solid is monitored using \( 5 \times 5 = 25 \) triaxial receivers arranged (in the same plane) as shown in Fig. 1. The reference solid is characterized by \( \nu = 0.35 \). The frequency of illumination is \( \omega = 3(\rho/\mu d^2)^{1/2} \), corresponding to a shear wavelength \( \lambda_S = 2\pi d/3 \).

Sensitivity evaluation. To verify the numerical implementation, geometric and material sensitivities \( \partial J_a/\partial a_d \) stemming from (24) and (28) are compared with their central difference approximations computed using the boundary integral approach and a surface mesh with 650 elements. The comparison is performed at \( a = (1, 1, 3; 5, 5, 5; 2, 35, 9) \) for a “true” ellipsoid given by \( a_{\text{true}} = (0, 0, 3; 5, 5, 5; 5, 25, 1) \), assuming an infinite reference domain \( \Omega = \mathbb{R}^3 \). From Table 1, the relative discrepancy between the sensitivity formulas and their central difference approximations (computed using \( \pm 4\% \) perturbation on each parameter) does not exceed 0.4%.

Reconstruction of a hard obstacle. For this example the testing grid, placed on the surface of the half-space \( (\xi_3 = 0) \), and the true defect (indicated as “Hard”) are shown in Fig. 1. The true defect, centered at \( (a_1, a_2, a_3)_{\text{true}} = (1, 5, 3) \), is described as an ellipsoid with semi-axes \( (a_4, a_5, a_6)_{\text{true}} = (0.4, 6, .5) \) and material properties \( (\mu, \nu, \rho)_{\text{true}} = (4\mu, 0.25, 1.1\rho) \); the initial iterate is placed at \( a^0 = (-4, -2, 2.5; 5, 5, 5; 1.8, 3, 1) \), see Fig. 1.

![Figure 1: Reconstruction of a hard defect (\( \omega = 3, \hat{\mu}^{\text{true}} = 4\mu \)).](image-url)
Synthetic observations $\mathbf{u}^{\text{obs}}$ are generated using a “dense” boundary element mesh (1,460 elements), whereas the minimization is effected using a “coarse” mesh (650 elements). Fig. 1 illustrates the iterative reconstruction process for the featured problem. The solution converges to the global minimum of $\mathcal{J}$ after approximately 70 iterations. Not surprisingly, the centroidal coordinates exhibit the fastest convergence, followed by that in terms of the semi-axes and material properties. To examine the effect of measurement uncertainties, synthetic observations in terms of the total field $\mathbf{u}^{\text{obs}}$ are next corrupted as $\mathbf{u}^{\text{obs}} = (1 + \varrho \chi) \mathbf{u}^{\text{obs}}$, where $\varrho$ is the noise amplitude and $\chi \in [-1, 1]$ is a uniform random variable. The induced perturbation in terms of the scattered field $\mathbf{u}^{\text{s}} - \mathbf{u}^{F}$, which is the sole carrier of information about the defect, exceeds 50% for selected source-receiver pairs when $\varrho = 1\%$. Table 2, which lists the reconstructed defect parameters for $\varrho = 0, 1, 2\%$, shows that the solution is fairly sensitive to measurement noise. In practical situations, this problem may be mitigated using a combination of multi-tonal illumination and Bayesian (e.g. maximum likelihood) data analysis [17].

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| Parameter | $c_1$ | $c_2$ | $c_3$ | $\alpha_1$ | $\alpha_2$ | $\alpha_3$ | $\mu$ | $\nu$ | $\hat{\rho}$ |
|-----------|------|------|------|----------|----------|----------|------|------|--------|
| Formulae  | 0.3884 | 0.3884 | 3.669 | -8.384    | -8.384    | -9.803    | -3.286 | 7.205E-02 | -2.857 |
| Finite diff. | 0.3873 | 0.3873 | 3.666 | -8.384    | -8.384    | -9.802    | -3.289 | 7.231E-02 | -2.856 |

Table 1: Sensitivities $\partial \mathcal{J} / \partial a_i$: comparison with central differences

| Parameter | $c_1$ | $c_2$ | $c_3$ | $\alpha_1$ | $\alpha_2$ | $\alpha_3$ | $\hat{\mu}$ | $\hat{\nu}$ | $\hat{\rho}$ |
|-----------|------|------|------|----------|----------|----------|---------|---------|--------|
| True      | 1.0  | 0.50 | 3.0  | 0.40     | 0.60     | 0.50     | 5.0     | 0.25    | 1.1    |
| Identified, $\varrho = 0\%$ | 1.0  | 0.50 | 3.0  | 0.40     | 0.60     | 0.50     | 5.0     | 0.25    | 1.1    |
| Identified, $\varrho = 1\%$ | 0.996 | 0.496 | 3.0  | 0.408    | 0.607    | 0.508    | 3.76    | 0.297   | 1.1    |
| Identified, $\varrho = 2\%$ | 0.992 | 0.492 | 2.99 | 0.367    | 0.583    | 0.481    | 5.19    | 0.016   | 1.06   |

Table 2: Sensitivity of the solution to experimental noise (hard defect)