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Kalman-based estimation of loading conditions from ultrasonic guided wave measurements

Andre Dalmora^{1,2,3}, Alexandre Imperiale¹ ✉, Sebastien Imperiale^{2,3},
Philippe Moireau^{2,3} 

¹CEA Saclay, LIST - DIN, Université Paris Saclay, 91191 Gif-sur-Yvette, France;

²Inria, Team-MEDISIM, Inria-Saclay Ile de France 91120 Palaiseau, France;

³LMS, Ecole Polytechnique, CNRS – Institut Polytechnique de Paris

✉ For
correspondence:
philippe.moireau@inria.fr

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Present address:
Team MEDISIM, Inria
Saclay, 1 Rue Honoré
d’Estienne d’Orves,
Palaiseau, 91128 France

Abstract

Ultrasonic guided wave-based Structural Health Monitoring (SHM) of structures can be perturbed by Environmental and Operations Conditions (EOCs) that alter wave propagation. In this work, we present an estimation procedure to reconstruct an EOC-free baseline of the structure suitable for SHM from the only available Ultrasonic guided wave measurements. Our approach is model-based, *i.e.* we use a precise modeling of the wave propagation altered by structure loading conditions. This model is coupled with the acquired data through a data assimilation procedure to estimate the deformation caused by the unknown loading conditions. From a methodological point of view, our approach is original since we have proposed an iterated Reduced-Order Unscented Kalman strategy, which we justify as an alternative to a Levenberg-Marquardt strategy for minimizing the non quadratic least-squares estimation criteria. Therefore, from a data assimilation perspective, we provide a quasi-sequential strategy that can valuably replace more classical variational approaches. Indeed, our resulting algorithm proves to be computationally very effective, allowing us to successfully apply our strategy to realistic 3D industrial SHM configurations.

1 Introduction

In various cutting-edge industrial fields, *e.g.* nuclear power generation, transportation, or aeronautics, the safe and reliable use of critical parts of structures is of paramount importance. To meet safety regulations in these areas, one must often be able to assess the integrity of the materials or equipment that make up these critical parts. To this end, numerous Non-Destructive Techniques (NDT) have been developed over the years. They are means of examining the material in question and obtaining quantitative information about its integrity without damaging it. Among them, Structural Health Monitoring (SHM) is an approach that – compared to other NDT techniques – generates a continuous stream of field data by incorporating actuators and sensors *in situ*. In other words, SHM systems monitor structures as it is used. One way to implement such systems is to rely on ultrasonic Guided Waves (GWs) [29, 41] because of their attractive properties, such as propagation over long distances to study a large volume of material, or sensitivity to local thickness variations due to

42 dispersion phenomena. Nevertheless, there are a number of challenges in the actual
43 implementation of GW-based SHM systems in realistic structures. To name just two of
44 them that drive the goals of our work, let us mention that the monitoring system should
45 be minimal to avoid overloading the structure of interest, and the Environmental and
46 Operations Conditions (EOCs) have a non-negligible impact on GW propagation [36].
47 Typical EOCs that can affect wave propagation include temperature variations and
48 the mechanical loading sustained by the structure during its use. We focus on the
49 latter because it is more general in terms of mathematical formulation and can indeed
50 lead to a change in wave velocities or even induce anisotropy. These effects are often
51 referred to by the term “acoustoelastic” propagation [21, 22]. These acoustoelastic
52 effects can alter the data registered by ultrasonic sensors, potentially affecting the
53 precision of GW-based monitoring systems. In this context, the main objective of our
54 work is the following: using the available data – the ultrasonic measurements – we aim
55 to remove the bias caused by the mechanical loading conditions in order to reconstruct
56 an EOC-free baseline. This objective solves the above two problems since the influence
57 of mechanical loading is captured without additional sensors. This EOC-free baseline
58 can then be used to find evidence of potential defects or damage within the structure
59 in the ultrasonic signals – assuming here that the contributions of the defects and the
60 EOCs are separable in the time or frequency domain.

61 In essence, our goal is to reconstruct a pre-deformation of the structure using only
62 the GW measurements. From the wave propagation point of view, this is an inverse
63 problem that we solve as a minimization problem of a fidelity-to-data functional under
64 the condition that wave propagation dynamics is satisfied. An important feature
65 arising from our EOC context is that the propagation model is in fact the one obtained
66 by linearizing the nonlinear elastodynamics model around the sought pre-deformation,
67 as presented in details in previous works [38] and recalled later in this article.

68 Solving such a non-linear optimization problem can be carried out through different
69 approaches. A first one is to resort to gradient descent iterations or quasi-Newton
70 processes [14, 7]. At each iteration, the gradient of the cost function can be obtained
71 by solving the so-called forward and backward adjoint problems. This approach is
72 arguably the most common one to address this type of problem, it is referred to as the
73 variational approach (4D-Var) [5, 16] in the data assimilation community with now
74 extension to mechanical systems [42], while in the geophysics community, it has been
75 labeled as Full Waveform Inversion (FWI) [32] with adaptation to tomography [30].
76 A strong advantage of FWI is its robustness *w.r.t.* the size of the parametric space,
77 *i.e.* the space in which lies the (discrete) solution of the minimization problem. In
78 fact, numerous successful applications of this method have led to the reconstruction of
79 wave velocity maps over large propagation domains. However, one significant difficulty
80 of this approach is managing the adjoint dynamics, which contains the tangent of
81 the propagation model around the forward trajectory. In the context of our work,
82 this tangent model is intricate. In particular, it entails the third derivative of the
83 hyperelastic potential ruling the constitutive behavior of the material. Also, storing
84 the forward trajectory to evaluate this tangent is prohibitive, since the state space
85 is very large in the context of high-frequency time-domain wave propagation. Note
86 that however, in the case of inviscid wave propagation, one can save storage space by
87 simply back-propagating the forward trajectory – a technique exploited in other wave
88 propagation inverse problems [18, 25]. However, this is done at the cost of yet another
89 call to the wave propagation solver.

90 A second approach is to resort to sequential methods and, in particular, to Kalman
91 filtering approaches that can be developed in a stochastic or a deterministic context
92 [1, 11]. The term sequential stems from the fact that the main building blocks of this

93 approach are (exclusively) forward problems, where the dynamics are modified by the
94 addition of a feedback loop. This feedback loop is proportional to the discrepancy
95 between the synthetic data generated from the model's current trajectory and the actual
96 measurements. The resulting modified dynamics is often referred to as a sequential
97 estimator (in the stochastic context) or an observer (in the deterministic context) of
98 the target trajectory. In Kalman-based filtering, the gain operator in the feedback
99 loop is computed from a covariance operator satisfying a Riccati equation [37]. For
100 Linear-Quadratic (LQ) problems, *i.e.* linear state dynamics with linear parameter-state
101 coupling and a quadratic misfit functional, the observer at the final time corresponds
102 exactly to the solution of the minimization problem [40]. Also, in the special case
103 where the uncertainty is limited exclusively to the parameter space, this method
104 leads to a specific application of the Reduced-Order Kalman Filter [15, 40]. This
105 method can be generalized to cases with non-linear parameter-state coupling, leading
106 to the so-called Reduced Order Extended Kalman Filter (EKF) or its gradient-free
107 version, the Reduced-Order Unscented Kalman Filter (UKF) [15, 19]. One of the main
108 advantages of these sequential estimators lies in their ability to provide a solution to
109 the minimization problem in one pass, consisting of embarrassingly parallel forward
110 problems. Moreover, thanks to their tangent-free alternative, *e.g.* UKF, they are
111 easy to interface with legacy code used in parallel as a black box propagating each
112 UKF *sigma-point*, also referred to as *particle*. Nevertheless, the usual computational
113 bottleneck of these sequential methods is to store and invert the (dense) covariance
114 matrix whose dimension corresponds to the size of the parameter space. This limits
115 the application of Kalman filters to relatively small parameter spaces compared to the
116 typical configurations handled by variational or FWI methods. Moreover, although
117 Kalman filters are exactly equivalent to the minimization problem LQ problems their
118 extension to nonlinear minimization problems is either prohibitively expensive [33, 40]
119 or approximate when relying on Extended or Unscented Kalman filters [15, 19, 40].

120 In our work, we develop a new estimation procedure that combines elements of the
121 two approaches. Namely, we first apply a Levenberg-Marquardt (LM) algorithm [8, 24]
122 to derive from the initial minimization problem a set of LQ subproblems satisfied by
123 parameter increments. Each of these LQ subproblems is then solved using a Kalman
124 filter approach, a sequential strategy already studied for wave or elasticity problems
125 [15, 28, 39]. We then revisit the UKF approach, to obtain a tangent-free algorithm
126 with increasing convergence at each iteration of the outer loop of LM descent. Thus,
127 we avoid the differentiation of the acoustoelastic wave propagation model and provide
128 an estimation algorithm that can be easily interoperated with blackbox industrial
129 codes. To be compatible with the dimensionality constraints of Kalman filtering, the
130 parameter space is built from a modal decomposition of the pre-deformation, which
131 in practice leads to the estimation of tens to hundreds of components on a modal
132 basis. Moreover, the number of LM iterations to achieve convergence is rather small,
133 leading overall to an almost sequential estimation approach. To illustrate the power of
134 our approach, both in computation efficiency and parameter estimation, we provide
135 extensive 3D results with synthetic noisy data in configurations associated with realistic
136 SHM applications.

137 The structure of this article is as follows. In *section 2*, we provide details on
138 the direct problem, *i.e.* the time-domain acoustoelasticity propagation model. This
139 leads us to the definition of the inverse problem we consider. In particular, we give a
140 precise definition of the observation operator that generates the GW measurements
141 and the modal basis that forms the parameter space. In *section 3*, we develop our
142 new method for identifying parameters using a combination of the LM algorithm
143 and Kalman-based filtering. In a first step, we provide meaningful insights into this

144 approach by considering continuous-time dynamics. In a second step, we give extensive
 145 details leading to the final fully discrete observer. Finally, in *section 4*, we give
 146 relevant numerical illustrations of the estimation of the 3D pre-deformation with our
 147 approach and noisy synthetic data in realistic industrial configurations.

148 2 Problem setting

149 We here consider a deformable system classically modeled in continuum mechanics in
 150 a Lagrangian referential defined from an initial stress-free configuration. Defining by
 151 Ω the reference domain with Lipschitz boundaries and the material position \mathbf{x} in the
 152 reference configuration, the dynamics principle reads

$$\begin{cases} \varrho_0 \partial_{tt}^2 \mathbf{u}_{\text{tot}}(\mathbf{x}, t) - \nabla \cdot \mathbf{T}(\mathbf{x}, t) = \varrho_0 \mathbf{f}_{\text{tot}}(\mathbf{x}, t) & (\mathbf{x}, t) \in \Omega \times (0, T), \\ \mathbf{u}_{\text{tot}}(\mathbf{x}, t) = 0 & (\mathbf{x}, t) \in \Gamma_D \times (0, T), \\ \mathbf{T} \cdot \mathbf{n}(\mathbf{x}, t) = 0 & (\mathbf{x}, t) \in \Gamma_N \times (0, T), \\ \mathbf{u}(\mathbf{x}, 0) = 0 & \mathbf{x} \in \Omega, \end{cases} \quad (1)$$

153 where, for the sake of simplicity, we consider homogeneous boundary conditions defined
 154 in the reference configuration. Moreover, we scale the volume loading with the volume
 155 mass for consistency. In (1) the first Piola-Kirchhoff stress tensor \mathbf{T} is here defined
 156 from the derivative of an hyperelastic potential \mathscr{W} , with respect to the deformation
 157 gradient $\mathbf{F}(\mathbf{x}, t) = \mathbf{Id} + \nabla \mathbf{u}_{\text{tot}}(\mathbf{x}, t)$, namely $\mathbf{T} = \mathbf{D}_{\mathbf{F}} \mathscr{W}(\mathbf{x}, \mathbf{F})$.

158 As an alternative to the strong form, the system is defined using the weak form of
 159 the dynamics principle, also known as the principle of virtual work, by defining a space
 160 of admissible displacements, typically $\mathcal{K} \subset \mathcal{V} = \{\mathbf{w} \in \mathbf{H}^1(\Omega)^3 \mid \mathbf{w}|_{\Gamma_D} = 0\}$ such that

$$\forall \mathbf{w} \in \mathcal{V}, \quad \int_{\Omega} \varrho_0 \partial_{tt}^2 \mathbf{u}_{\text{tot}} \cdot \mathbf{w} \, \mathrm{d}\mathbf{x} + \int_{\Omega} \mathbf{T} : \nabla \mathbf{w} \, \mathrm{d}\mathbf{x} = \int_{\Omega} \varrho_0 \mathbf{f}_{\text{tot}} \cdot \mathbf{w} \, \mathrm{d}\mathbf{x}. \quad (2)$$

161 In this general framework, we now consider that our system is inspected while being
 162 loaded by external unknown forces. These structural loading forces \mathbf{f}_0 are considered
 163 to be volume distributed, for the sake of simplicity, and quasi-static – namely not
 164 depending on time – albeit of possibly strong amplitude, as opposed to the ultrasonic
 165 excitation \mathbf{f} which is of high-frequency and low amplitude. In fact, the quasi-static
 166 assumption is considered with respect to the time scale of ultrasonic excitation so the
 167 total loading decomposes into

$$\mathbf{f}_{\text{tot}}(\mathbf{x}) = \mathbf{f}_0(\mathbf{x}) + \delta \mathbf{f}(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times (0, T), \quad (3)$$

168 where δ is a small parameter representing the fact that the amplitude of the ultrasonic
 169 excitation is small compared to the external loading. This allows us to separate scales
 170 and to consider that the resulting displacement is decomposed into

$$\mathbf{u}_{\text{tot}}(\mathbf{x}, t) = \mathbf{u}_0(\mathbf{x}) + \delta \mathbf{u}(\mathbf{x}, t) + O(\delta^2). \quad (4)$$

171 Injecting such ansatz into the principle of virtual work (2) and identifying the
 172 zero order terms *w.r.t.* δ , we formally showed in [38] that the displacement can be
 173 reconstructed from the solution $\mathbf{u}_0 \in \mathcal{K}$ of a large displacement static problem

$$\forall \mathbf{w} \in \mathcal{V}, \quad \int_{\Omega} \mathbf{T}(\mathbf{x}, \mathbf{F}_0) : \nabla \mathbf{w} \, \mathrm{d}\mathbf{x} = \int_{\Omega} \varrho_0 \mathbf{f}_0 \cdot \mathbf{w} \, \mathrm{d}\mathbf{x}, \quad (5)$$

174 where $\mathbf{F}_0 = \mathbf{Id} + \nabla \mathbf{u}_0$ is the deformation gradient associated with \mathbf{u}_0 . Then, identifying
 175 the first order term in δ , we find that $\mathbf{u} \in \mathbf{L}^2((0, T); \mathcal{V})$ should be a solution of the
 176 wave-propagation problem given by

$$\forall \mathbf{w} \in \mathcal{V}, \quad \int_{\Omega} \varrho_0 \partial_{tt}^2 \mathbf{u} \cdot \mathbf{w} \, \mathrm{d}\mathbf{x} + \int_{\Omega} \nabla \mathbf{u} : \mathbf{D}_{\mathbf{F}}^2 \mathscr{W}(\mathbf{x}, \mathbf{F}_0) : \nabla \mathbf{w} \, \mathrm{d}\mathbf{x} = \int_{\Omega} \varrho_0 \mathbf{f} \cdot \mathbf{w} \, \mathrm{d}\mathbf{x}. \quad (6)$$

177 From a mathematical viewpoint, the existence of a solution for the general problem
 178 formulation (1) is still an open problem. However, under suitable conditions, we can
 179 consider that problem (5) and (6) admits one and only one solution. For (5), this is
 180 typically the case when defining a hyperelastic law using a polyconvex potential [6],
 181 giving the existence of a displacement \mathbf{u}_0 in the space of admissible displacements
 182 $\mathcal{K} \subset \mathcal{V}$.

183 Then, moving to (6), this formulation can be recast into a general second-order
 184 in time weak formulation. Denoting by \mathcal{H} the space $L^2(\Omega)^3$ equipped with the scalar
 185 product

$$\forall(\mathbf{u}, \mathbf{w}) \in \mathcal{H}^2, \quad (\mathbf{u}, \mathbf{w})_{\mathcal{H}} = \int_{\Omega} \varrho_0 \mathbf{u} \cdot \mathbf{w} \, dx,$$

186 Moreover, we equip \mathcal{V} with the scalar product

$$\forall(\mathbf{u}, \mathbf{w}) \in \mathcal{V}^2, \quad (\mathbf{u}, \mathbf{w})_{\mathcal{V}} = \int_{\Omega} \nabla \mathbf{u} : D_{\mathbf{F}}^2 \mathscr{W}(\mathbf{x}, \mathbf{Id}) : \nabla \mathbf{w} \, dx + (\mathbf{u}, \mathbf{w})_{\mathcal{H}}.$$

187 Note that $D_{\mathbf{F}}^2 \mathscr{W}(\mathbf{x}, \mathbf{Id})$ actually corresponds to the standard Hooke's law in linear
 188 elasticity. We can identify \mathcal{H} with its dual so that we have the following Gelfand triple

$$\mathcal{V} \subset \mathcal{H} \equiv \mathcal{H}' \subset \mathcal{V}'.$$

189 Then, introducing the linear operator $A_0(\mathbf{u}_0) \in \mathcal{L}(\mathcal{V}, \mathcal{V}')$ such that

$$\forall(\mathbf{u}, \mathbf{w}) \in \mathcal{V}^2, \quad \langle A_0(\mathbf{u}_0) \mathbf{u}, \mathbf{w} \rangle_{\mathcal{V}', \mathcal{V}} = \int_{\Omega} \nabla \mathbf{u} : D_{\mathbf{F}}^2 \mathscr{W}(\mathbf{x}, \mathbf{F}_0) : \nabla \mathbf{w} \, dx,$$

190 the weak formulation (6) can be written in the following form

$$\forall \mathbf{w} \in \mathcal{V}, \quad \frac{d^2}{dt^2} (\mathbf{u}, \mathbf{w})_{\mathcal{H}} + \langle A_0(\mathbf{u}_0) \mathbf{u}, \mathbf{w} \rangle_{\mathcal{V}', \mathcal{V}} = (\mathbf{f}, \mathbf{w})_{\mathcal{H}}. \quad (7)$$

191 We now make the following assumption: there exists $\lambda \geq 0$ and $\alpha > 0$ such that

$$\forall \mathbf{w} \in \mathcal{V}, \quad \langle A_0(\mathbf{u}_0) \mathbf{w}, \mathbf{w} \rangle_{\mathcal{V}', \mathcal{V}} + \lambda \|\mathbf{w}\|_{\mathcal{H}}^2 \geq \alpha \|\mathbf{w}\|_{\mathcal{V}}^2. \quad (8)$$

192 Such assumption is satisfied for \mathbf{u}_0 small enough whereas for large displacement \mathbf{u}_0 , it
 193 may be violated. This is however very dependent on the potential \mathscr{W} that describes
 194 the elastic behavior of the medium. Some choices tend to make the assumption above
 195 more restrictive than others – see *e.g.* the examples in [38]. Thanks to this assumption
 196 – see for instance [2] – there exists one, and only one, *variational* solution of (7), namely
 197 $\mathbf{u} \in \mathcal{W}_T$ with

$$\mathcal{W}_T = \left\{ \mathbf{u} \in L^2((0, T); \mathcal{V}), \partial_t \mathbf{u} \in L^2((0, T); \mathcal{H}), \partial_{tt}^2 \mathbf{u} \in L^2((0, T); \mathcal{V}') \right\}.$$

198 Moreover, we can extend the operator $A_0(\mathbf{u}_0) \in \mathcal{L}(\mathcal{V}, \mathcal{V}')$ into an unbounded operator
 199 $(A_0(\mathbf{u}_0), \mathcal{D}(A_0))$ by defining

$$\mathcal{D}(A_0) = \left\{ \mathbf{u} \in \mathcal{V} \text{ such that } \exists \mathbf{r} \in \mathcal{H} : \forall \mathbf{w} \in \mathcal{V}, \quad \langle A_0(\mathbf{u}_0) \mathbf{u}, \mathbf{w} \rangle_{\mathcal{V}', \mathcal{V}} = (\mathbf{r}, \mathbf{w})_{\mathcal{H}} \right\}.$$

200 and

$$\forall \mathbf{u} \in \mathcal{D}(A_0), \quad \forall \mathbf{w} \in \mathcal{V}, \quad (A_0(\mathbf{u}_0) \mathbf{u}, \mathbf{w})_{\mathcal{H}} = \langle A_0(\mathbf{u}_0) \mathbf{u}, \mathbf{w} \rangle_{\mathcal{V}', \mathcal{V}}.$$

201 Then, for a given $\mathbf{u}_0 \in \mathcal{K}$, by introducing the operator

$$A(\mathbf{u}_0) = \begin{pmatrix} 0 & \text{Id} \\ -A_0(\mathbf{u}_0) & 0 \end{pmatrix} \text{ with } \mathcal{D}(A) = \mathcal{D}(A_0) \times \mathcal{V} \subset \mathcal{Z} := \mathcal{V} \times \mathcal{H},$$

202 we can rewrite the wave dynamics in the state-space form

$$\begin{cases} \frac{d}{dt}z = A(\mathbf{u}_0)z + r, & \text{in } (0, T) \\ z(0) = 0, \end{cases} \quad \text{with } z = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \text{ and } r = \begin{pmatrix} 0 \\ \mathbf{f} \end{pmatrix}, \quad (9)$$

203 and \mathbf{v} denotes the velocity unknown. In the sequel, we will denote $\dot{z} = \frac{d}{dt}z$. This
204 state-space form allows to define solutions using semi-group theory [12]. Namely for
205 $r \in L^2((0, T), \mathcal{Z})$ there exists one and only one mild solution of (9) in $C^0((0, T), \mathcal{Z})$
206 which is also a variational solution in \mathcal{W}_T of (7). We here underline that the variational
207 formalism is necessary to further justify finite element discretization of (7), whereas
208 the mild solution formulation in the sense of semi-group will simplify the presentation
209 of the estimation problem.

210 In this modeling context, we consider that we have at our disposal some recorded
211 measurements on a subregion ω_i – of the boundary $\partial\Omega$ – from d sensors of the wave
212 propagation of a target wave solution $\check{\mathbf{u}}$. Typically we consider recordings $y = (y_i)_{1 \leq i \leq d}$
213 given by

$$[0, T] \ni t \mapsto \check{y}_i(t) = \frac{1}{|\omega_i|} \int_{\omega_i} \check{\mathbf{u}}(t, \mathbf{x}) \cdot \mathbf{d}_i \, d\mathbf{x} \in \mathbb{R}, \quad 1 \leq i \leq d,$$

214 up to certain measurement errors and where the fields \mathbf{d}_i represent the sensitivity
215 of the sensors to a displacement field. In fact, we do not have at our disposal
216 $[0, T] \ni t \mapsto \check{y}(t) \in \mathbb{R}$ but rather the perturbed measurement $y_\gamma \in L^2((0, T); \mathcal{Y})$ with
217 $\mathcal{Y} = \mathbb{R}^d$ such that for a given noise level $\gamma > 0$,

$$\int_0^T \|\check{y}_i - y_{\gamma,i}\|_{\mathcal{Y}}^2 \, dt \lesssim \gamma^2 T.$$

218 From a state-space point of view, this allows to define an observation operator $C \in$
219 $\mathcal{L}(\mathcal{Z}, \mathcal{Y})$ by

$$C : z = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \mapsto \left(\frac{1}{|\omega_i|} \int_{\omega_i} \mathbf{u}(\mathbf{x}) \cdot \mathbf{d}_i \, d\mathbf{x} \right)_{1 \leq i \leq d}. \quad (10)$$

220 **Remark 1.** *We would like to point out that in an alternative modeling approach,*
221 *we could have considered that the measurements are recorded from the deformed*
222 *configuration as the sensors are operating in this configuration. When rewriting the*
223 *integrals with respect to the reference configuration, this should lead to the definition of*
224 *an observation operator $C(\mathbf{u}_0)$ that depends on the deformation.*

225 We can now introduce the inverse problem that we want to solve. We assume
226 that \mathbf{u}_0 is unknown and we want to reconstruct it from the available measurements.
227 More precisely, we would like to specify the true $\check{\mathbf{u}}_0$ from an *a priori* displacement $\hat{\mathbf{u}}_0$
228 assuming that the true displacement is a regular perturbation with respect to the *a*
229 *priori*, typically there exists a constant M such that

$$\|\check{\mathbf{u}}_0 - \hat{\mathbf{u}}_0\|_{\mathcal{Y}}^2 \leq M^2.$$

230 Moreover in practice, we propose to decompose any $\mathbf{u}_0 \in \mathcal{H}$ on the basis made of the
231 eigenvectors $(\varphi_j)_{j \geq 0}$ of the compact operator $\Lambda_0 = A_0(\mathbf{0})^{-1} \in \mathcal{L}(\mathcal{V}', \mathcal{V})$. We recall that
232 there exists $(\mu_j)_{j \geq 0} \in (\mathbb{R}_+^*)^{\mathbb{N}}$ such that

$$A_0(\mathbf{0})\varphi_j = \mu_j\varphi_j \text{ with } \|\varphi_j\|_{\mathcal{H}}^2 = 1 \quad (11)$$

233 and $\lambda_j = \sqrt{\mu_j}^{-1}$ tends to 0 as j tends to infinity. Therefore, we can decompose

$$\mathbf{u}_0(\mathbf{x}) = \sum_{j \geq 0} \theta_j \varphi_j(\mathbf{x}) \quad (12)$$

234 and we can enforce

$$\mathbf{u}_0 \in \mathcal{V} \Leftrightarrow \sum_{j \geq 0} \frac{\theta_j^2}{\lambda_j^2} < +\infty.$$

235 In practice, we may even want to consider that \mathbf{u}_0 belongs to a more regular space \mathcal{V}^m
236 leading to increased convergence rate of the sequence $(\theta_j)_{k \geq 0}$ to 0, typically

$$\mathbf{u}_0 \in \mathcal{V}^m \Rightarrow \sum_{j \geq 0} \frac{\theta_j^2}{\lambda_j^{2m}} < +\infty. \quad (13)$$

237 However, as a first step, we remain with our choice of estimating $\mathbf{u}_0 \in \mathcal{V}^m$ which is
238 equivalent to estimating $\theta \in \mathcal{P} \subset \ell_2(\mathbb{R})$, equipped with a norm

$$\|\theta\|_{\mathcal{P}}^2 = (\theta, \Lambda_0^{-m} \theta)_{\ell_2}, \text{ with } (\Lambda_0)_{ij} = \lambda_j^{2m} \delta_{ij} \text{ and } \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (14)$$

239 Moreover, when we need to discretize \mathbf{u}_0 , we will consider a finite-dimensional space
240 corresponding to a finite number N_p of modes, hence $\theta \in \mathbb{R}^{N_p}$ and Λ_0 becomes typically
241 a diagonal matrix.

242 To conclude our problem setting, our objective is, therefore, to estimate $\check{\theta} \in \mathcal{P}$
243 from the available measurements, namely to invert the following operator

$$\Psi_T : \begin{cases} \mathcal{P} \rightarrow L^2((0, T); \mathcal{Y}) \\ \theta \mapsto \left[t \mapsto \int_0^t C e^{A(\theta)(t-s)} r(s) ds \right] \end{cases}$$

244 where we replace the \mathbf{u}_0 dependency by the θ dependency in the definition of the
245 operator A_0 . In the following, this inversion is based on a least-squares minimization
246 using Levenberg-Marquardt strategy.

247 3 Identification method

248 3.1 From Levenberg-Marquardt minimization scheme to an iterated 249 Extended Kalman strategy

Following [24], we approximate pseudo-inverse of Ψ_T with a Levenberg-Marquardt
minimization scheme [8] which consists of the following iterative procedure.

$$\begin{aligned} \theta^{k+1} &= \theta^k + \alpha^k \\ &= \theta^k + \left[D\Psi_T(\theta^k)^* D\Psi_T(\theta^k) + \varepsilon \frac{\gamma^2}{M^2} \Lambda_0^{-m} \right]^{-1} D\Psi_T(\theta^k)^* (y_\gamma - \Psi_T(\theta^k)), \end{aligned} \quad (15)$$

where the number of iterations of this scheme is finite, thus acting as a regularization,
and typically controlled by classical Morozov-like criteria, as advised in [24]. The
parameter $\frac{\gamma^2}{M^2}$ is a scaling parameter taking into account the prior over noise ratio,
while ε will give us an additional degree of freedom for weighting the regularization
in the LM algorithm, see below and in particular Remark 2. Then, we can see the
increment as

$$\alpha^k = \arg \min_{\alpha \in \mathcal{P}} \left\{ \frac{\varepsilon}{2M^2} \|\alpha\|_{\mathcal{P}}^2 + \frac{1}{2\gamma^2} \|y_\gamma - \Psi_T(\theta^k) - D\Psi_T(\theta^k)\alpha\|_{L^2((0, T); \mathcal{Y})}^2 \right\}, \quad (16)$$

250 **Remark 2.** Note again that by penalizing $\|\alpha\|_{\mathcal{P}}^2$ we penalize an incremental dis-
251 placement $\|\tilde{\mathbf{u}}_0(\alpha)\|_{\mathcal{V}^m}^2$. Therefore, we can force the first increments of the seeking

252 *displacement to belong to \mathcal{K} since a sufficiently smooth displacement with a sufficiently*
 253 *small amplitude will necessarily be admissible. However, this may come at the price*
 254 *of too much regularization, which can only be compensated by a higher number of*
 255 *iterations of the LM algorithm. This is illustrated in the numerical section.*

256 Let us now specify the tangent operator

$$\forall \theta \in \mathcal{P}, \quad D\Psi_T(\theta) : \begin{cases} \mathcal{H} \rightarrow L^2((0, T); \mathcal{Y}), \\ \alpha \mapsto y = C\zeta_{|\theta, \alpha} \end{cases}$$

257 and $\zeta_{|\theta, \alpha}$ is a mild solution of

$$\begin{cases} \dot{\zeta}_{|\theta, \alpha}(t) = A(\theta)\zeta_{|\theta, \alpha}(t) + B(\theta, z_{|\theta}(t))\alpha, & t \in [0, T] \\ \zeta_{|\theta, \alpha}(0) = 0, \end{cases}$$

258 where we have introduced the linear operator representing the tangent of $A(\theta)$ *w.r.t.*
 259 the parameter θ

$$\forall \theta \in \mathcal{P}, \quad \forall z \in \mathcal{D}(A), \quad \mathcal{L}(\mathcal{P}, \mathcal{Z}) \ni B(\theta, z) : \mathcal{P} \ni \alpha \mapsto (D_\theta A(\theta)\alpha)z \in \mathcal{Z}.$$

260 Therefore, we face a linear-quadratic optimal control problem, that can be mini-
 261 mized using the following Reduced-Order Kalman Filter (ROKF) sequential estimator
 262 reformulated from the initial design found in [15] – see also the more recent review
 263 [40]. To this end, let us first introduce the set of sensitivity operators $(L_{|\theta}(t))_{t \geq 0}$ in
 264 $\mathcal{L}(\mathcal{P}, \mathcal{Z})$ defined for all time $t \geq 0$ by

$$L_{|\theta}(t) : \alpha \mapsto \zeta(t) \text{ the mild solution of } \begin{cases} \dot{\zeta}(s) = A(\theta)\zeta(s) + B(\theta, z_{|\theta}(s))\alpha, & s \in [0, t] \\ \zeta(0) = 0. \end{cases} \quad (17)$$

265 We easily verify that $L_{|\theta} \in C^0([0, T]; \mathcal{L}(\mathcal{P}, \mathcal{Z}))$ the space of continuous mapping from
 266 $[0, T]$ to $\mathcal{L}(\mathcal{P}, \mathcal{Z})$ endowed with the uniform convergence topology [12].

267 Then, we introduce the time-dependent Riccati operator $(\Lambda_{|\theta})_{t \geq 0}$ – which can be
 268 interpreted as a parameter-covariance operator [12] – solution in $C^0([0, T]; \mathcal{S}_+^*(\mathcal{P}))$
 269 – with $\mathcal{S}_+^*(\mathcal{P})$ the space of symmetric positive definite bounded operators – of

$$\begin{cases} \dot{\Lambda}_{|\theta}(t) = -\frac{1}{\gamma^2} \Lambda_{|\theta}(t) L_{|\theta}(t)^* C^* C L_{|\theta}(t) \Lambda_{|\theta}(t), & t \in [0, T] \\ \Lambda_{|\theta}(0) = \frac{M^2}{\varepsilon} \Lambda_0^m \end{cases} \quad (18)$$

270 We would like to underline the fact that here the adjoint operator $L_{|\theta}(t)^*$ is here
 271 defined with respect to the ℓ^2 -norm as $\theta \in \mathcal{P} \subset \ell^2(\mathbb{R})$.

272 We then define the sequential estimator

$$\begin{cases} \hat{\zeta}^k(t) = A(\theta^k)\hat{\zeta}^k(t) + B(\theta^k, z_{|\theta^k}(t))\hat{\alpha}^k(t) + L_{|\theta^k}(t)\dot{\hat{\alpha}}^k(t), & t \in [0, T] \\ \dot{\hat{\alpha}}^k(t) = \frac{1}{\gamma^2} \Lambda_{|\theta^k}(t) L_{|\theta^k}(t)^* C^* (y_\gamma(t) - C z_{|\theta^k}(t) - C \hat{\zeta}^k(t)), & t \in [0, T] \\ \hat{\zeta}^k(0) = 0 \\ \hat{\alpha}^k(0) = 0 \end{cases} \quad (19)$$

273 which, ultimately, sequentially solve the minimization problem (16) as recall in the
 274 next theorem justified in [40].

275 **Theorem 1.** At every iteration k , the mild solution $\hat{\alpha}^k \in C^0([0, T]; \mathcal{P})$ and $\hat{\zeta}^k \in$
 276 $C^0([0, T]; \mathcal{Z})$ of (19) satisfies

$$\hat{\alpha}^k(T) = \alpha^k \text{ and } \hat{\zeta}^k(T) = \zeta_{|\theta^k, \alpha^k}(T). \quad (20)$$

277 In the previous theorem, we understand that we can sequentially compute $t \mapsto \hat{\alpha}^k$
 278 but also $t \mapsto \hat{\zeta}^k$ which is interpreted as a sequential estimator of the associated
 279 trajectory $t \mapsto \zeta_{|\theta^k, \alpha^k}$. Note that this estimator can be computed together with $\hat{\alpha}^k$ in
 280 only one coupled forward dynamics.

281 In fact, instead of a parameter increment, we are more interested in reconstructing
 282 the parameter itself, namely $t \mapsto \bar{\theta}^k(t) = \theta^k + \hat{\alpha}^k(t)$, and its associated trajectory
 283 $t \mapsto \bar{z}^k(t) = z_{|\bar{\theta}^k(t)}$. As $t \mapsto \hat{\alpha}^k(t)$ is a time-dependent trajectory, we have

$$\dot{\bar{z}}^k = \frac{d}{dt} [z_{|\bar{\theta}^k(\cdot)}] = \dot{z}_{|\bar{\theta}^k(\cdot)} + D_{\theta(\cdot)} z_{|\theta(\cdot)} \Big|_{\theta(\cdot) = \bar{\theta}^k(\cdot)} \hat{\alpha}^k,$$

284 and the sensitivity operator $L_{|\bar{\theta}^k(\cdot)} = D_{\theta(\cdot)} z_{|\theta(\cdot)} \Big|_{\theta(\cdot) = \bar{\theta}^k(\cdot)}$ is nothing else than, for all
 285 time $t \geq 0$,

$L_{|\bar{\theta}^k(\cdot)}(t) : \alpha \mapsto \zeta(t)$ is a mild solution of

$$\begin{cases} \dot{\zeta}(s) = A(\bar{\theta}^k(s))\zeta(s) + B(\bar{\theta}^k(s), z_{|\bar{\theta}^k(t)}(s))\alpha, & s \in [0, t] \\ \zeta(0) = 0 \end{cases} \quad (21)$$

286 Here note that in the previous dynamics, $s \mapsto \bar{\theta}^k(s)$ is a function of time, implying a
 287 time-dependent operator $s \mapsto A(\bar{\theta}^k(s))$. The existence of a solution for such dynamics
 288 is fundamentally based on the study of evolution equation operator in general [4,
 289 Chapter 5].

290 As $\hat{\alpha}^k = \dot{\bar{\theta}}^k$, and by approximating $z_{|\theta^k} + \hat{\zeta}^k \simeq z_{|\theta^k + \hat{\alpha}^k} = \bar{z}^k$ we could compute the
 291 sequential estimator

$$\begin{cases} \dot{\bar{z}}^k = A(\bar{\theta}^k)\bar{z}^k + r + L_{|\bar{\theta}^k}\dot{\bar{\theta}}^k, & t \in [0, T], \\ \dot{\bar{\theta}}^k = \frac{1}{\gamma^2}\Lambda_{|\theta^k}(t)L_{|\theta^k}(t)^*C^*(y_\gamma - C\bar{z}^k), & t \in [0, T], \\ \bar{z}^k(0) = 0 \\ \bar{\theta}^k(0) = \bar{\theta}^k, \end{cases} \quad (22)$$

292 such that at final time $\bar{\theta}^k(T) \simeq \bar{\theta}^{k+1}$.

293 One drawback in solving (22) is that it necessitates to propagate two sensitivity
 294 operators $L_{|\theta^k}$ and $L_{|\bar{\theta}^k}$. Moreover $L_{|\theta^k}$ necessitates to store the complete trajectory
 295 $z_{|\theta^k}$. To circumvent these drawbacks, one could imagine to instead solve

$$\begin{cases} \dot{\hat{z}}^k = A(\hat{\theta}^k)\hat{z}^k + r + L^k\hat{\theta}^k, & t \in [0, T], \\ \dot{\hat{\theta}}^k = \frac{1}{\gamma^2}\Lambda^k(t)L^k(t)^*C^*(y_\gamma - C\hat{z}^k), & t \in [0, T], \\ \hat{z}^k(0) = 0 \\ \hat{\theta}^k(0) = \hat{\theta}^{k-1}(T) \end{cases} \quad (23)$$

296 where, from now on, we simply use the notation $L^k = L_{|\hat{\theta}^k}$ and $\Lambda^k = \Lambda_{|\hat{\theta}^k}$ and we see
 297 that the sensitivity and the covariance operator are updated through time. Indeed, Λ^k
 298 is an operator that should be seen as a *mild* solution of the dynamics

$$\begin{cases} \dot{\Lambda}^k(t) = -\frac{1}{\gamma^2}\Lambda^k(t)L^k(t)^*C^*CL_{|\theta}(t)\Lambda^k(t), & t \in [0, T] \\ \Lambda^k(0) = \frac{M^2}{\varepsilon}\Lambda_0^m, \end{cases} \quad (24)$$

299 while L^k can be seen from (21) as a mild solution in $C^0([0, T], \mathcal{L}(\mathcal{P}, \mathcal{Z}))$ of

$$\begin{cases} \dot{L}^k(t) = A(\hat{\theta}^k)L^k(t) + B(\hat{\theta}^k(t), \hat{z}^k(t)) & t \in [0, T] \\ L^k(0) = 0. \end{cases} \quad (25)$$

300 We here recognize in (23) – combined with (24)-(25) – an iterated version of the
301 Reduced-Order-Extended-Kalman-Filter (ROEKF) estimator proposed in [15] for joint
302 state and parameter estimation for wave-like equations, here formally generalized to
303 infinite dimensional systems. One very strong advantage of such an estimator is that
304 it is fully sequential in the sense that it does not require storing any trajectory in
305 the iteration procedure. Note that the existence of a solution of (23) is much more
306 intricate and is based on justifying that L^k is well-defined even for time-dependent
307 parameter $\hat{\theta}^k$. This question is typically covered by the definition of stable families of
308 generators in evolution equation [4], see also [34] for similar questions when defining
309 the Extended Kalman Filter for infinite dimensional systems.

310 In this work, we call iROEKF the proposed iterated ROEKF. However, we must
311 warn the reader that in our case the iteration k is to be considered as an outer loop
312 of the LM descent. This iROEKF is therefore different from the classical iterated
313 Extended Kalman Filter presented in the literature [26].

314 **3.2 Space-time-discretized version of the iterated reduced-order Ex-** 315 **tended Kalman Filter**

316 Since we ultimately solve a discretized version of (23), we now present a discretiza-
317 tion strategy based on a stable discretization of the Levenberg-Marquardt increment
318 estimator (19). Our discretization strategy is based on the fundamental principle
319 *discretize-then-optimize*, which means that we first discretize the direct problem and
320 then reapply the equivalence of Levenberg-Marquardt and dynamic programming at
321 the discretized level, as recommended in [40]. For (7), we consider a finite-element
322 discretization based on the Spectral Finite Element Method (SFEM) [10] leading to
323 the formulation

$$\forall \mathbf{w}_h \in \mathcal{V}_h, \quad (\partial_{tt}^2 \mathbf{u}_h, \mathbf{w}_h)_{\mathcal{V}_h} + (A_{0h}(\mathbf{u}_{h0})\mathbf{u}_h, \mathbf{w}_h)_{\mathcal{V}_h} = (\mathbf{f}, \mathbf{w}_h)_{\mathcal{V}_h}. \quad (26)$$

324 To construct the finite dimensional space \mathcal{V}_h we assume given a partition \mathcal{T}_h of
325 quadrangles (in 2D) or hexahedra (in 3D) of the domain Ω , namely

$$\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K, \quad \forall (K, L) \in \mathcal{T}_h \times \mathcal{T}_h \quad \overset{\circ}{K} \cap \overset{\circ}{L} = \emptyset,$$

326 with maximum diameter given by h . Then $\mathcal{V}_h \subset \mathcal{V}$ is obtained using a \mathbb{Q}_k -Lagrangian
327 basis on a set of nodes $\{\xi_i\}_{i=1}^{N_h}$,

$$\mathcal{V}_h = (\text{span}\{\varphi_i\}_{i=1}^{N_h})^3, \quad \forall 1 \leq i, j \leq N_h, \quad \varphi_i(\xi_j) = \delta_{ij}, \quad \forall K \in \mathcal{T}_h, \quad \varphi_{i|K} \circ F_K \in \mathbb{Q}_k.$$

328 where the mapping from the reference element to any element $K \in \mathcal{T}_h$ is denoted F_K
329 – see [10] for more details. The nodes $\{\xi_i\}$ are obtained using Gauss-Lobatto integration
330 points on a reference square (in 2D) or cube (in 3D). One fundamental aspect of the
331 efficiency of the SFEM is that \mathcal{V}_h is equipped with a scalar product that – using a
332 quadrature formula on the nodes $\{\xi_i\}$ – leads at the algebraic level to a diagonal mass
333 matrix. This is called a mass-lumping strategy and preserves a near-optimal accuracy
334 [17]. The mentioned quadrature formula is also employed to compute the operator
335 $A_h(\mathbf{u}_{h0})$, thus given by

$$\forall (\mathbf{u}_h, \mathbf{w}_h) \in \mathcal{V}_h^2, \quad (A_{0h}(\mathbf{u}_{h0})\mathbf{u}_h, \mathbf{w}_h)_{\mathcal{V}_h} = \int_{\Omega} \nabla \mathbf{u}_h : \mathbb{D}_{\mathbf{F}}^2 \mathcal{W}(\mathbf{x}, \mathbf{F}_{0h}) : \nabla \mathbf{w}_h \, \text{d}\mathbf{x},$$

336 where \mathbb{f} stands for an integral computed from the quadrature formula, and $\mathbf{F}_{0h} =$
 337 $\mathbf{Id} + \nabla \mathbf{u}_{h0}$ with \mathbf{u}_{h0} an interpolation in \mathcal{V}_h of \mathbf{u}_0 . Note that the operator inherits some
 338 properties of the operator $A(\mathbf{u}_{h0})$, in particular it is self-adjoint. However it is not
 339 clear that it satisfies a positivity property of the form (8) for at least two reasons, the
 340 interpolation of \mathbf{u}_{0h} and the use of the quadrature formula. Therefore we are led to
 341 the following assumption that is sufficient to have a well-posed discrete problem,

$$\forall \mathbf{w}_h \in \mathcal{V}_h, \quad (A_{0h}(\mathbf{u}_{h0})\mathbf{w}_h, \mathbf{w}_h)_{\mathcal{V}_h} \geq 0.$$

342 The spatial discretization is then followed by an explicit time-discretization. Being
 343 given a time step Δt , the solution $\mathbf{u}_h(t)$ is approximated at time $t^n = n\Delta t$ by solving

$$\forall \mathbf{w}_h \in \mathcal{V}_h, \quad \left(\frac{\mathbf{u}_h^{n+1} - 2\mathbf{u}_h^n + \mathbf{u}_h^{n-1}}{\Delta t^2}, \mathbf{w}_h \right)_{\mathcal{V}_h} + (A_{0h}(\mathbf{u}_{h0})\mathbf{u}_h^n, \mathbf{w}_h)_{\mathcal{V}_h} = (\Pi_h \mathbf{f}(t^n), \mathbf{w}_h)_{\mathcal{V}_h}, \quad (27)$$

344 where $\Pi_h \mathbf{f}$ is a projection of \mathbf{f} in \mathcal{V}_h . Thanks to the mass-lumping strategy the
 345 computation of \mathbf{u}_h^{n+1} involves – at the algebraic level – only the inversion of a diagonal
 346 mass matrix. This discretization is stable for small enough time step Δt , namely the
 347 time step must satisfy the CFL condition

$$\Delta t \leq 2 \left(\sup_{\mathbf{w}_h \in \mathcal{V}_h} \frac{(A_{0h}(\mathbf{u}_{h0})\mathbf{w}_h, \mathbf{w}_h)_{\mathcal{V}_h}}{\|\mathbf{w}_h\|_{\mathcal{V}_h}^2} \right)^{-1/2}. \quad (28)$$

348 The CFL condition depends on the mesh size h (in particular Δt behaves like $O(h)$)
 349 and on the mesh quality but also on the gradient of the displacement field \mathbf{u}_{h0} . We
 350 can finally rewrite the time-discretization (27) as

$$\begin{cases} \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{\Delta t} = \mathbf{v}_h^{n+1} \\ \frac{\mathbf{v}_h^{n+1} - \mathbf{v}_h^n}{\Delta t} + A_{0h}(\theta_h)\mathbf{u}_h^n = \Pi_h \mathbf{f}(t^n) \end{cases} \quad (29)$$

351 where we replace the \mathbf{u}_{h0} dependency by the $\theta_h \in \mathcal{P}_h \simeq \mathbb{R}^{N_p}$ dependency such that

$$\mathbf{u}_{h0} = \sum_{j=1}^{N_p} \theta_{h,j} \boldsymbol{\varphi}_{h,j} \quad \text{with} \quad A_{0h}(0)\boldsymbol{\varphi}_{h,j} = \mu_{h,j} \boldsymbol{\varphi}_{h,j},$$

352 namely the $(\mu_{h,j}, \boldsymbol{\varphi}_{h,j})$ are the eigenelements of the discrete operators $A_{0h}(0)$ (ordered
 353 increasingly with respect to the eigenvalues). Then, by defining $z_h^n = (\mathbf{u}_h^n, \mathbf{v}_h^n)^\top$, we
 354 rewrite (29) in the following abstract state-space form

$$\begin{cases} z_h^{n+1} = \Phi_{h,\Delta t}(\theta_h) z_h^n + r_{h,\Delta t}^{n+1} \\ z_h^0 = 0 \end{cases} \quad (30)$$

355 where

$$\Phi_{h,\Delta t}(\theta_h) : z_h \mapsto \begin{pmatrix} \text{Id}_{\mathcal{V}_h} - \Delta t^2 A_{0h}(\theta_h) & \Delta t \text{Id}_{\mathcal{V}_h} \\ \Delta t A_{0h}(\theta_h) & \text{Id}_{\mathcal{V}_h} \end{pmatrix} z_h \quad \text{and} \quad r_{h,\Delta t}^{n+1} = \begin{pmatrix} \Delta t^2 \Pi_h \mathbf{f}(t^n) \\ \Delta t \Pi_h \mathbf{f}(t^n) \end{pmatrix}.$$

Using the time-discretized system (30), we propose to solve the Levenberg-Marquardt procedure

$$\begin{aligned} \theta_h^{k+1} &= \theta_h^k + \alpha_h^k \\ &= \theta_h^k + \left[\text{D}\Psi_{h,N}(\theta_h^k)^* \text{D}\Psi_{h,N}(\theta_h^k) + \varepsilon \frac{\gamma^2}{M^2} \Lambda_{0h}^{-m} \right]^{-1} \text{D}\Psi_{h,N}(\theta_h^k)^* (y_\gamma - \Psi_{h,N}(\theta_h^k)), \end{aligned}$$

356 where

$$\Psi_{h,N} : \begin{cases} \mathcal{P}_h \rightarrow \ell^2((1:N); \mathcal{Y}) \\ \theta_h \mapsto \left\{ \sum_{j=1}^n C_h \Phi_{h,\Delta t}^{n-j}(\theta_h) r_{h,\Delta t}^j \right\}_{n=1}^N \end{cases}$$

357 which can be equivalently rewritten in the following form

$$\alpha_h^k = \arg \min_{\alpha_h \in \mathcal{P}} \left\{ \frac{\varepsilon}{2M^2} \|\alpha_h\|_{\mathcal{P}}^2 + \frac{\Delta t}{2\gamma^2} \|y_\gamma - \Psi_{h,N}(\theta^k) - D\Psi_{h,N}(\theta^k)\alpha_h\|_{\ell^2((1:N); \mathcal{Y})}^2 \right\}. \quad (31)$$

358 Then, we define the fully discrete sensitivity operator, for all $n \in [0:N]$, as

$$L_{h|\theta_h}^{k,n} : \alpha_h \mapsto \zeta_h^n \text{ the solution of } \begin{cases} \zeta_h^{j+1} = \Phi_{h,\Delta t}(\theta_h) z_h^j + B_{h,\Delta t}(\theta_h, z_h^j) \alpha_h, & j \in [0:n-1] \\ \zeta_h^0 = 0 \end{cases}$$

359 with

$$B_{h,\Delta t}(\theta_h, z_h) \alpha_h = \begin{pmatrix} \Delta t^2 D_\theta A_{0h}(\theta_h) \alpha_h & 0 \\ -\Delta t D_\theta A_{0h}(\theta_h) \alpha_h & 0 \end{pmatrix} z_h.$$

360 Moreover, we define the fully discrete covariance operator $\Lambda_{h|\theta_h}^{k,n}$ satisfying the dynamics

$$\begin{cases} (\Lambda_{h|\theta_h}^{k,n+1})^{-1} = (\Lambda_{h|\theta_h}^{k,n})^{-1} + \frac{\Delta t}{\gamma^2} L_{h|\theta_h}^{k,n+1} C_h^* C_h L_{h|\theta_h}^{k,n+1}, & n \in [0:N] \\ \Lambda_{h|\theta_h}^{k,0} = \frac{M^2}{\varepsilon} \Lambda_{h0}^n. \end{cases}$$

361 If we now choose to solve from $\hat{\zeta}_h^{k,0} = 0$, and $\hat{\alpha}_h^{k,0} = 0$, for all $k \leq 0$ and $n \in [0:N-1]$

$$\begin{cases} \hat{\zeta}_h^{k,n+1-} = \Phi_{h,\Delta t}(\theta_h) \hat{\zeta}_h^{k,n} + B_{h,\Delta t}(\theta_h, z_{h|\theta_h}^n) \hat{\alpha}_h^{k,n} \\ \hat{\alpha}_h^{k,n+1} = \hat{\alpha}_h^{k,n} + \frac{\Delta t}{\gamma^2} \Lambda_{h|\theta_h}^{k,n+1} L_{h|\theta_h}^{k,n+1*} C_h^* (y_\gamma^{n+1} - C_h z_{h|\theta_h}^{n+1} - C_h \hat{\zeta}_h^{k,n+1-}) \\ \hat{\zeta}_h^{k,n+1} = \hat{\zeta}_h^{k,n+1-} + L_{h|\theta_h}^{k,n+1} (\hat{\alpha}_h^{k,n+1} - \hat{\alpha}_h^{k,n}) \end{cases} \quad (32)$$

362 where the “ $n-$ ” and “ n ” exponents correspond to the two steps of a splitting time-
363 scheme for $\hat{\zeta}_h^{k,n}$ – where the “ $n-$ ” step is often referred as the prediction (or forecast)
364 step and the “ n ” step is referred as the correction (or analysis) step – we have at the
365 discrete level the following equivalence proved in [40].

366 **Theorem 2.** *At every iteration k of the Levenberg-Marquardt minimization, we have*

$$\hat{\alpha}_h^{k,N} = \alpha_h^k \text{ and } \hat{\zeta}_h^{k,N} = \zeta_{h|\theta^k, \alpha^k}^N \quad (33)$$

367 The last theorem helps to understand that we keep at the discrete-time level the
368 same equivalence between the least square minimization of a discretized criterion and
369 the sequential approach. Therefore pursuing the same strategy than for the continuous-
370 time level leads us to defining the Discrete-Time iterated Reduced Order Extended
371 Kalman Filter (DT-iROEKF) as an approximation of the Levenberg-Marquardt min-
372 imization strategy for discrete-time dynamics. The resulting joint state-parameter
373 sequential estimator based on this DT-iROEKF is initialized from $\hat{z}_h^k = 0$, $\hat{\theta}_h^{k,0} = \hat{\theta}_h^{k-1,N}$
374 if $k > 1$ and $\hat{\theta}_h^{1,0} = \hat{\theta}_{0h}$, while $L^{k,0} = 0$, $\Lambda^{k,0} = \varepsilon^{-1} M^2 \Lambda_{h0}^n$. Then the recursive dynamics
375 reads for all $k \geq 1$ and for all $n \in [0:N-1]$

— Prediction / Forecast:

$$\begin{cases} \hat{z}_h^{k,n+1-} = \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})\hat{z}_h^{k,n} + r_{h,\Delta t}^{n+1}, \\ L_h^{k,n+1} = \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})L_h^{k,n} + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}). \end{cases}$$

— Correction / Analysis:

$$\begin{cases} (\Lambda_h^{k,n+1})^{-1} = (\Lambda_h^{k,n})^{-1} + \frac{\Delta t}{\gamma^2} L_h^{k,n+1} C_h^* C_h L_h^{k,n+1}, \\ \hat{\theta}_h^{k,n+1} = \hat{\theta}_h^{k,n} + \frac{\Delta t}{\gamma^2} \Lambda_h^{k,n+1} L_h^{k,n+1*} C_h^* (y_\gamma^{n+1} - C_h \hat{z}_h^{k,n+1-}), \\ \hat{z}_h^{k,n+1} = \hat{z}_h^{k,n+1-} + L_h^{k,n+1} (\hat{\theta}_h^{k,n+1} - \hat{\theta}_h^{k,n}). \end{cases}$$

376 Here again, the approximation relies on the fact that the sensitivity and the covariances
377 are computed sequentially from the current estimation $\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}$.

378 3.3 From a square root to a tangent-free formulation

379 We are now ready to formulate a practical implementation of our DT-iROEKF. In
380 this respect, we recast the DT-iROEKF formulation into a so-called square-root form
381 as commonly done in data assimilation for the robust implementation of the Kalman
382 approaches [11]. Then we show how we can replace, up to second-order terms, the
383 tangent computations by finite difference scheme over wave solution, hence leading to
384 an original tangent-free approach.

385 The SEEK algorithm for parameter identification.

In this section, we start by formulating a square-root approach of the reduced-order
Extended Kalman filter that we are going to apply to our state-parameter decomposi-
tion. This strategy is an adaption to parameter estimation of the square root algorithm
initially presented in [13]. Following their strategy, we choose to store not $L_h^{k,n}$ but
 $L_h^{k,n} D_h^{k,n}$ with $D_h^{k,n}$ a Cholesky factorization of $\Lambda_h^{k,n}$. More precisely, we define

$$D_h^{k,n} := \text{chol}(\Lambda_h^{k,n}) \text{ namely } \Lambda_h^{k,n} = D_h^{k,n} D_h^{k,n*} \quad (34)$$

$$S_h^{k,n} := L_h^{k,n} D_h^{k,n} \quad (35)$$

$$S_h^{k,n+1-} := L_h^{k,n+1} D_h^{k,n} \quad (36)$$

Note that $D_h^{k,n}$ can be equivalently represented as a collection of N_p members

$$\{D_{h,j}^{k,n}\}_{j=1}^{N_p} \in \mathcal{P}_h,$$

386 that can be seen as the ‘‘columns’’ of the matrix representations of the operator. Each
387 member is comparable to a parameter increment around the observer trajectory $\hat{\theta}_h^{k,n}$,
388 hence is associated with a reconstructed displacement

$$\mathbf{u}_{0h} = \sum_{1 \leq i \leq N_p} D_{h,ij}^{k,n} \boldsymbol{\varphi}_{h,i},$$

with $\boldsymbol{\varphi}_{h,i}$ the normalized eigenvectors of the operator A_{0h} . In the same manner $S_h^{k,n}$
and $S_h^{k,n+1-}$ can be equivalently represented as a collection of N_p members

$$\{S_{h,j}^{k,n}\}_{j=1}^{N_p} \in \mathcal{Z}_h.$$

389 Each member is comparable to the variation of a wave solution for the specific parameter
390 increment $D_{h,j}^{k,n}$. We are going to prove the following recursive dynamics, defining again
391 a splitting time-scheme with one prediction step followed by a correction step.

Theorem 3. For all $k \geq 1$ and for all $n \in [0:N-1]$, we define the Gramian operator $G^{k,n}$ by

$$G^{k,n} = \text{Id}_y + \frac{\Delta t}{\gamma^2} C_h S_h^{k,n-} S_h^{k,n-*} C_h^*,$$

392 and we denote by $Q^{k,n}$ the Cholesky decomposition of $(G^{k,n})^{-1} = Q^{k,n} Q^{k,n*}$. With
393 these notations, we obtain the following dynamics:

394 — Prediction / Forecast:

$$S_{h,j}^{k,n+1-} = \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n}) S_{h,j}^{k,n} + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}) D_{h,j}^{k,n}, \quad \forall j \in [1:N_p]. \quad (37)$$

395 — Correction / Analysis:

$$S_h^{k,n+1} = S_h^{k,n+1-} Q^{k,n+1}, \quad \text{and} \quad D_h^{k,n+1} = D_h^{k,n} Q^{k,n+1}. \quad (38)$$

Proof. We proceed by induction. This is true at $n = 0$ since $L_h^{k,0} = 0$. Let us now assume that (37) and (38) are valid at iteration n . For the prediction step, we have for all $j \in [1:N_p]$,

$$\begin{aligned} S_{h,j}^{k,n+1-} &= L_{h,j}^{k,n+1} D_{h,j}^{k,n} \\ &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n}) L_{h,j}^{k,n} D_{h,j}^{k,n} + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n+1-}) D_{h,j}^{k,n} \\ &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n}) S_{h,j}^{k,n} + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n+1-}) D_{h,j}^{k,n} \end{aligned}$$

so that (37) is satisfied at iteration n . From Woodbury inversion formula, we have that

$$\begin{aligned} (G^{k,n+1})^{-1} &= (\text{Id}_y + \frac{\Delta t}{\gamma^2} C_h S_h^{k,n+1-} S_h^{k,n+1-*} C_h^*)^{-1} \\ &= \text{Id}_{\mathcal{P}_h} - \Delta t S_h^{k,n+1-*} C_h^* [\gamma^2 \text{Id}_y + \Delta t C_h S_h^{k,n+1-} S_h^{k,n+1-*} C_h^*]^{-1} C_h S_h^{k,n+1-} \\ &= Q^{k,n+1} Q^{k,n+1*} \end{aligned}$$

Therefore if we now define $D_h^{k,n+1} = D_h^{k,n} Q^{k,n+1}$ then

$$\begin{aligned} D_h^{k,n+1} D_h^{k,n+1*} &= D_h^{k,n} Q^{k,n+1} Q^{k,n+1*} D_h^{k,n} \\ &= \Lambda_h^{k,n} \\ &\quad - \Delta t \Lambda_h^{k,n} L_h^{k,n+1*} C_h^* [\gamma^2 \text{Id}_y + \Delta t C_h L_h^{k,n+1} \Lambda_h^{k,n} L_h^{k,n+1*} C_h^*]^{-1} C_h L_h^{k,n+1} \end{aligned}$$

which, with a second use of Woodbury inversion formula gives $D_h^{k,n+1} D_h^{k,n+1*} = \Lambda_h^{k,n+1}$. Finally, we have that

$$S_h^{k,n+1} = L_h^{k,n+1} D_h^{k,n+1} = L_h^{k,n+1} D_h^{k,n} Q^{k,n+1} = S_h^{k,n+1-} Q^{k,n+1},$$

396 which concludes the proof. \square

Note that in practice, one can use the component-wise expression of the Gramian matrix, namely

$$G_{ij}^{k,n} = \delta_{ij} + \frac{\Delta t}{\gamma^2} (C_h S_{h,i}^{k,n-}, C_h S_{h,j}^{k,n-})_y, \quad \forall 1 \leq i, j \leq N_p.$$

In the same fashion, we have

$$S_{h,j}^{k,n+1} = \sum_{1 \leq i \leq N_p} Q_{ij}^{k,n+1} S_{h,i}^{k,n+1-}, \quad \text{and} \quad D_{h,i}^{k,n+1} = \sum_{1 \leq i \leq N_p} Q_{ij}^{k,n+1} D_{h,i}^{k,n}.$$

397 From the previous theorem, we then easily verify that the DT-iROEKF estimator can
398 be computed using only $S_h^{k,n-}$, $S_h^{k,n}$ and $D_h^{k,n}$ with

399 — Prediction / Forecast:

$$\hat{z}_h^{k,n+1-} = \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})\hat{z}_h^{k,n} + r_{h,\Delta t}^{n+1}, \quad (39)$$

— Correction / Analysis:

$$\begin{cases} \hat{\theta}_h^{k,n+1} = \hat{\theta}_h^{k,n} + \frac{\Delta t}{\gamma^2} D_h^{k,n+1} S_h^{k,n+1*} C_h^*(y_\gamma^{n+1} - C_h \hat{z}_h^{k,n+1-}), \\ \hat{z}_h^{k,n+1} = \hat{z}_h^{k,n+1-} + \frac{\Delta t}{\gamma^2} S_h^{k,n+1} S_h^{k,n+1*} C_h^*(y_\gamma^{n+1} - C_h \hat{z}_h^{k,n+1-}). \end{cases} \quad (40)$$

$$\hat{z}_h^{k,n+1} = \hat{z}_h^{k,n+1-} + \frac{\Delta t}{\gamma^2} S_h^{k,n+1} S_h^{k,n+1*} C_h^*(y_\gamma^{n+1} - C_h \hat{z}_h^{k,n+1-}). \quad (41)$$

And again in practice, solving (40) and (41) is performed by developing

$$\begin{cases} \hat{\theta}_h^{k,n+1} = \hat{\theta}_h^{k,n} + \frac{\Delta t}{\gamma^2} \sum_{1 \leq j \leq N_p} (C_h S_{h,j}^{k,n+1}, y_\gamma^{n+1} - C_h \hat{z}_h^{k,n+1-}) y D_{h,j}^{k,n+1}, \\ \hat{z}_h^{k,n+1} = \hat{z}_h^{k,n+1-} + \frac{\Delta t}{\gamma^2} \sum_{1 \leq j \leq N_p} (C_h S_{h,j}^{k,n+1}, y_\gamma^{n+1} - C_h \hat{z}_h^{k,n+1-}) y S_{h,j}^{k,n+1}. \end{cases}$$

400 **A tangent-free alternative.**

Ultimately, (37) can be seen as the tangent equation of

$$\begin{aligned} S_{h,j}^{k,n+1-} &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n}) S_{h,j}^{k,n} + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}) D_{h,j}^{k,n} \\ &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})(\hat{z}_h^{k,n} + S_{h,j}^{k,n}) + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}) D_{h,j}^{k,n} - \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n}) \hat{z}_h^{k,n} \\ &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n} + D_{h,j}^{k,n})(\hat{z}_h^{k,n} + S_{h,j}^{k,n}) - \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n}) \hat{z}_h^{k,n} + O(\|D_{h,j}^{k,n}\|^2) \\ &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n} + D_{h,j}^{k,n})(\hat{z}_h^{k,n} + S_{h,j}^{k,n}) + r_{h,\Delta t}^{n+1} - \hat{z}_h^{k,n+1-} + O(\|D_{h,j}^{k,n}\|^2). \end{aligned} \quad (42)$$

401 Therefore, by computing the forecast of each member $S_{h,j}^{k,n+1-}$ by a finite difference
402 between two wave equations, we do not need to compute the operator $B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n+1})$.
403 This means that the forecast step can be performed by simply forecasting $\hat{z}_h^{k,n}$ and
404 each member $S_{h,j}^{k,n}$.

405 3.4 The Reduced-Order UKF alternative

406 In the DT-iROEKF approach, we have seen that we can propagate the estimator
407 $\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}$ and the increment set $\{S_{h,j}^{k,n+1-}\}_{j=1}^{N_p}$ and $\{D_{h,j}^{k,n+1-}\}_{j=1}^{N_p}$. These increments
408 give the sensitivity direction around the estimator $\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}$. Revisiting [9, 19], the
409 Reduced-Order Unscented Kalman alternative (ROUKF) to ROEKF, we are going to
410 replace the computation of the increment sets by sets of so-called *sigma-points* around
411 $\hat{\theta}_h^{k,n}$ and $\hat{z}_h^{k,n}$ so that the estimator is computed by an averaging formula like in a
412 finite difference stencil. In essence, while EKF propagates a point-estimator and N_p
413 directions around this point-estimator, UKF computes a stencil of sigma-points such
414 that the point-estimator is a resulting average of this point. In practice we will need
415 at least $N_s = N_p + 1$ sigma-points when using a simplex stencil, but more complex
416 stencils with $N_s \geq N_p + 1$ can also be proposed with additional trajectories to be
417 computed. Note that our presentation clarifies the generalization of ROUKF to general
418 complex stencil initially proposed in [19, 20]. This may be of particular interest since
419 increasing the number of sigma points results in a potentially more precise sampling
420 and rendering of the sensitivity directions around the estimator.

421 **Empirical mean and empirical covariance.**

422 Let us introduce a set of strictly positive weights $\beta = \{\beta_j\}_{j=1}^{N_s} \in (\mathbb{R}_+^*)^{N_s}$ such that

$$\sum_{1 \leq j \leq N_s} \beta_j = 1.$$

423 From this set of weights, we introduce the following weight averaging operator defined,
424 for all sample set $\{s_j\}_{j=1}^{N_s} \in \mathcal{X}^{N_s}$ of elements of a Hilbert space \mathcal{X} (typically \mathcal{Z}_h , \mathcal{P}_h
425 or \mathcal{Y}), by

$$\mathbb{E}_\beta(\{s_j\}_{j=1}^{N_s}) = \sum_{1 \leq j \leq N_s} \beta_j s_j \in \mathcal{Z}.$$

426 This can be understood as an empirical mean of the $\{s_j\}_{j=1}^{N_s}$. In the same fashion, we
427 define the empirical covariance as the following linear operator

$$\mathbb{P}_\beta(\{s_j\}_{j=1}^{N_s}) : \mathcal{X} \ni s \mapsto \sum_{1 \leq j \leq N_s} \beta_j \left(s, s_j - \mathbb{E}_\beta(\{s_j\}_{j=1}^{N_s}) \right)_{\mathcal{X}} \left(s_j - \mathbb{E}_\beta(\{s_j\}_{j=1}^{N_s}) \right) \in \mathcal{X},$$

428 where $(\cdot, \cdot)_{\mathcal{X}}$ is the scalar product in \mathcal{X} . As soon as we are considering a finite-
429 dimensional Euclidian space $\mathcal{X} = \mathbb{R}^{N_x}$, then

$$\mathbb{P}_\beta(\{s_j\}_{j=1}^{N_s}) = \sum_{1 \leq j \leq N_s} \beta_j (s_j - \mathbb{E}_\beta(\{s_j\}_{j=1}^{N_s})) (s_j - \mathbb{E}_\beta(\{s_j\}_{j=1}^{N_s}))^\top.$$

430 **Sampling around the observer trajectory.**

431 Let us now introduce a scaling factor $\varrho \in \mathbb{R}_+^*$ and define a particular finite sequence of
432 sigma-points $\{e_j\}_{j=1}^{N_s}$ in the parameter space \mathcal{P}_h such that

$$\mathbb{E}_\beta(\{e_j\}_{j=1}^{N_s}) = 0 \text{ and } \mathbb{P}_\beta(\{e_j\}_{j=1}^{N_s}) = \frac{1}{\varrho^2} \text{Id}_{\mathcal{P}_h}.$$

433 Note that by choosing $\{e_j\}_{j=1}^{N_s}$ such that $\|e_j\|_{\mathcal{P}}^2 = O(1)$ then $\varrho = O(N_p^{-\frac{1}{2}})$. Again,
434 defining $D_h^{k,n}$ such as $\Lambda_h^{k,n} = D_h^{k,n} D_h^{k,n*}$ – namely $D_h^{k,n}$ can be the square root of $\Lambda_h^{k,n}$
435 or a Cholesky decomposition – and using $L_h^{k,n}$ at iteration n , we define the *sampling*
436 operation as constructing the following set of trajectories

$$\forall j \in [1 : N_s], \quad \begin{cases} \hat{z}_{h,j}^{k,n} = \hat{z}_h^{k,n} + \varrho L_h^{k,n} D_h^{k,n} e_j, \\ \hat{\theta}_{h,j}^{k,n} = \hat{\theta}_h^{k,n} + \varrho D_h^{k,n} e_j, \end{cases} \quad (43)$$

437 such that, by construction,

$$\mathbb{E}_\beta(\{\hat{z}_{h,j}^{k,n}\}_{j=1}^{N_s}) = \hat{z}_h^{k,n} \quad \text{and} \quad \mathbb{E}_\beta(\{\hat{\theta}_{h,j}^{k,n}\}_{j=1}^{N_s}) = \hat{\theta}_h^{k,n},$$

438 while

$$\mathbb{P}_\beta(\{\hat{z}_{h,j}^{k,n}\}_{j=1}^{N_s}) = L_h^{k,n} \Lambda_h^{k,n} L_h^{k,n*} \quad \text{and} \quad \mathbb{P}_\beta(\{\hat{\theta}_{h,j}^{k,n}\}_{j=1}^{N_s}) = \Lambda_h^{k,n}.$$

439 Different kinds of sigma-points can be used to perform this sampling operation – see for
440 instance [19]. In *Figure 1* we illustrate three different (albeit standard) sets of sigma-
441 points, and we compare it with the sampling strategy derived from the tangent-free
442 EKF approach presented in the previous section.

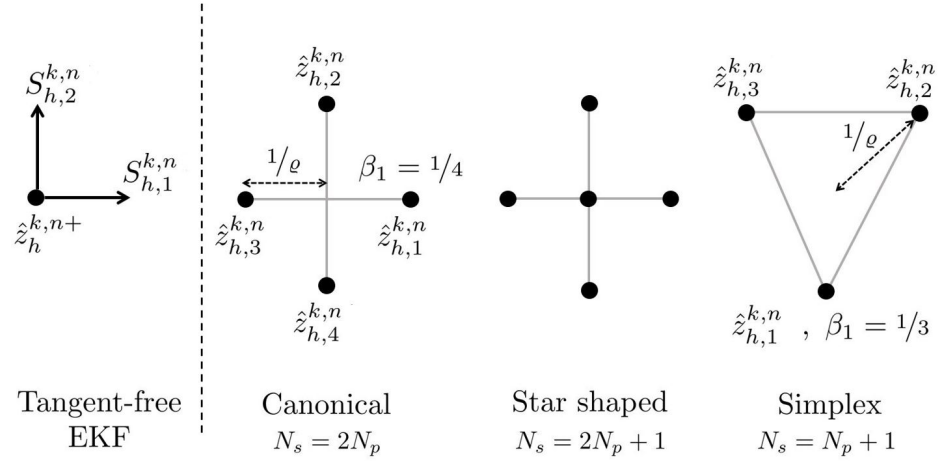


Figure 1. Definition of standard sigma-points for the simple case of $\mathcal{P} = \mathbb{R}^2$ and comparison with the state and sensitivity trajectories associated with the tangent-free EKF approach.

443 Prediction step of the reduced-order UKF.

The prediction step of the reduced-order UKF is simply obtained by propagating $\hat{z}_{h,j}^{k,n}$ using the discretized dynamics, namely

$$\hat{z}_{h,j}^{k,n+1-} = \Phi_{h,\Delta t}(\hat{\theta}_{h,j}^{k,n})\hat{z}_{h,j}^{k,n} + r_{h,\Delta t}^{n+1}.$$

444 Using the empirical average operator, we can derive the state and parameter sensitivity
445 around the estimator trajectory, namely we define the predictions

$$\forall j \in [1:N_s], \quad \begin{cases} \Sigma_{h,j}^{k,n+1-} &= \hat{z}_{h,j}^{k,n+1-} - \mathbb{E}_\beta(\{\hat{z}_{h,j}^{k,n+1-}\}_{j=1}^{N_s}), \\ \Delta_{h,j}^{k,n} &= \hat{\theta}_{h,j}^{k,n} - \mathbb{E}_\beta(\{\hat{\theta}_{h,j}^{k,n}\}_{j=1}^{N_s}). \end{cases} \quad (44)$$

446 From its definition, and using the definition of the sampling operation (43), one can
447 easily verify that the parameter sensitivity satisfies

$$\Delta_{h,j}^{k,n} = \varrho D_h^{k,n} e_j, \quad \forall j \in [1:N_s]. \quad (45)$$

448 The next lemma gives us a similar result for the state sensitivity.

449 **Lemma 4.** *The predicted state sensitivity defined in (44) satisfies*

$$\Sigma_{h,j}^{k,n+1-} = \varrho L_h^{k,n+1} D_h^{k,n} e_j + O(\varrho^2). \quad (46)$$

Proof. On the one hand, the state prediction of each sigma-point satisfies for any $j \in [1:N_s]$,

$$\begin{aligned} \hat{z}_{h,j}^{k,n+1-} &= \Phi_{h,\Delta t}(\hat{\theta}_{h,j}^{k,n})\hat{z}_{h,j}^{k,n} + r_{h,\Delta t}^{n+1} \\ &= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})\hat{z}_h^{k,n} + r_{h,\Delta t}^{n+1} + \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})(\hat{z}_{h,j}^{k,n} - \hat{z}_h^{k,n}) \\ &\quad + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n})(\hat{\theta}_{h,j}^{k,n} - \hat{\theta}_h^{k,n}) + O(\varrho^2). \end{aligned}$$

450 On the other hand, we can introduce

$$\hat{z}_h^{k,n+1-} = \mathbb{E}_\beta(\hat{z}_{h,j}^{k,n+1-}) = \mathbb{E}_\beta(\{\Phi_{h,\Delta t}(\hat{\theta}_{h,j}^{k,n})\hat{z}_{h,j}^{k,n} + r_{h,\Delta t}^{n+1}\}_{j=1}^{N_s}),$$

451 and a Taylor expansion gives

$$\hat{z}_h^{k,n+1-} = \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})\hat{z}_h^{k,n} + r_{h,\Delta t}^{n+1} + O(\varrho^2).$$

Using the sampling operations defined in (43) we obtain

$$\begin{aligned}
\Sigma_{h,j}^{k,n+1-} &= \hat{z}_{h,j}^{k,n+1-} - \hat{z}_h^{k,n+1-} \\
&= \Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})(\hat{z}_{h,j}^{k,n} - \hat{z}_h^{k,n}) + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n})(\hat{\theta}_{h,j}^{k,n} - \hat{\theta}_h^{k,n}) + O(\varrho^2) \\
&= \varrho(\Phi_{h,\Delta t}(\hat{\theta}_h^{k,n})L_h^{k,n} + B_{h,\Delta t}(\hat{\theta}_h^{k,n}, \hat{z}_h^{k,n}))D_h^{k,n}e_j + O(\varrho^2) \\
&= \varrho L_h^{k,n+1}D_h^{k,n}e_j + O(\varrho^2).
\end{aligned}$$

452

□

453 Correction step of the reduced-order UKF.

454 From the relations (45) and (46) we see that – up to second order terms – storing
455 $\Sigma_{h,j}^{k,n+1-}$ and $\Delta_{h,j}^{k,n}$ is equivalent to the storing $S_h^{k,n+1-}$ and $D_h^{k,n}$ except that $N_s > N_p$.
456 Then, following the definition of the correction (or analysis) step of the SEEK algorithm,
457 namely (38), we propagate the state and parameter sensitivity through

$$\Sigma_{h,j}^{k,n+1} = \sum_{1 \leq i \leq N_s} Q_{ij}^{k,n+1} \Sigma_{h,i}^{k,n+1-} \quad \text{and} \quad \Delta_{h,j}^{k,n+1} = \sum_{1 \leq i \leq N_s} Q_{ij}^{k,n+1} \Delta_{h,i}^{k,n},$$

where for all n , $Q^{k,n} \in \mathbb{M}_{N_s}(\mathbb{R})$ is given by the Cholesky decomposition of $(G^{k,n})^{-1} = Q^{k,n}Q^{k,n*}$ a Gramian matrix defined by

$$G_{ij}^{k,n} = \delta_{ij} + \frac{\Delta t}{\gamma^2} (C_h \Sigma_{h,i}^{k,n-}, C_h \Sigma_{h,j}^{k,n-})_{\mathcal{Y}}, \quad \forall i, j \in [1:N_s].$$

Using the same analogy, the corrected estimator can be rewritten in the form

$$\begin{cases}
\hat{\theta}_h^{k,n+1} = \hat{\theta}_h^{k,n} + \frac{\Delta t}{\gamma^2} \sum_{1 \leq j \leq N_s} (C \Sigma_{h,j}^{k,n+1}, y_{\gamma}^{n+1} - C \hat{z}_h^{k,n+1-})_{\mathcal{Y}} \Delta_{h,j}^{k,n+1}, \\
\hat{z}_h^{k,n+1} = \hat{z}_h^{k,n+1-} + \frac{\Delta t}{\gamma^2} \sum_{1 \leq j \leq N_s} (C \Sigma_{h,j}^{k,n+1}, y_{\gamma}^{n+1} - C \hat{z}_h^{k,n+1-})_{\mathcal{Y}} \Sigma_{h,j}^{k,n+1}.
\end{cases}$$

458 Furthermore, with a proof very similar to the proof of *Theorem 3* (introducing in finite
459 dimension the matrix $E = [e_1 | \dots | e_{N_s}]$ and concatenating in columns the sigma-points
460 $\{e_j\}_{j=1}^{N_s}$), one can verify that for all $j \in [1:N_s]$,

$$\Sigma_{h,j}^{k,n+1} = \varrho L_h^{k,n+1} D_h^{k,n+1} e_j + O(\varrho^2) \quad \text{and} \quad \Delta_{h,j}^{k,n+1} = \varrho D_h^{k,n+1} e_j + O(\varrho^2). \quad (47)$$

Hence, $\Sigma_{h,j}^{k,n+1}$ and $\Delta_{h,j}^{k,n+1}$ are equivalent to $S_h^{k,n+1}$ and $D_h^{k,n+1}$, up to second order terms, as for the prediction step. Once again, the only – but fundamental – difference compared to the EKF version is the fact that the Gramian is defined in $\mathbb{M}_{N_s}(\mathbb{R})$ instead of $\mathbb{M}_{N_p}(\mathbb{R})$. Note that, one important aspect of the relations (47) is that it enables us to rewrite the sampling operation (43) exclusively in terms of the computed state and parameter sensitivities. Namely, we recreate the sample at $n + 1$ by discarding second-order terms in the following relations

$$\hat{z}_{h,j}^{k,n+1} = \hat{z}_h^{k,n+1} + \Sigma_{h,j}^{k,n+1} + O(\varrho^2), \quad \text{and} \quad \hat{\theta}_{h,j}^{k,n+1} = \hat{\theta}_h^{k,n} + \Delta_{h,j}^{k,n+1} + O(\varrho^2).$$

461 We provide in *Figure 2* an illustration of its main steps, in order to fully apprehend
462 the various unknowns appearing in the algorithm.

463 Final algorithm.

464 We can now summarize the complete algorithm used in this work.

The Discrete-Time iterated Reduced-Order Unscented Kalman Filter (DT-iROUKF)

- ▶ Choice of the UKF sigma-points $\{e_j\}_{j=1}^{N_s}$ and the associated weights $\{\beta_j\}_{j=1}^{N_s}$.
- ▶ Initialization of the parameter prior from the modal decomposition

$$\hat{\mathbf{u}}_0(\mathbf{x}) = \sum_{1 \leq j \leq N_p} \hat{\theta}_{0h,j} \boldsymbol{\varphi}_j(\mathbf{x}).$$

- ▶ For all $k \geq 1$ until convergence:

- Initialization at $n = 0$:
- ↪ Parameter initialization:

$$\hat{\theta}_h^{k,0} = \hat{\theta}_h^{k-1,N} \quad \text{if } k > 1, \quad \hat{\theta}_h^{1,0} = \hat{\theta}_{0h} \quad \text{otherwise.}$$

- ↪ Parameter and state particles initialization:

$$\forall j \in [1:N_s], \quad \begin{cases} \hat{\theta}_{h,j}^{k,0} = \hat{\theta}_h^{k,0} + \varrho D^{k,0} e_j, & \text{with } D^{k,0} = \text{chol}(\Lambda_0^m), \\ \hat{z}_{h,j}^{k,0} = 0. \end{cases}$$

- For $0 \leq n \leq N$:
- ↪ Prediction step:

$$\forall j \in [1:N_s], \quad \begin{cases} \hat{z}_{h,j}^{k,n+1-} = \Phi_{h,\Delta t}(\hat{\theta}_{h,j}^{k,n}) z_{h,j}^{k,n} + r_{h,\Delta t}^{n+1}, \\ \Sigma_{h,j}^{k,n+1-} = \hat{z}_{h,j}^{k,n+1-} - \mathbb{E}_\beta(\{z_{h,j}^{k,n+1-}\}_{j=1}^{N_s}), \\ \Delta_{h,j}^{k,n} = \hat{\theta}_{h,j}^{k,n} - \mathbb{E}_\beta(\{\hat{\theta}_{h,j}^{k,n}\}_{j=1}^{N_s}). \end{cases}$$

- ↪ Correction step:

- Compute Gramian matrix and Cholesky decomposition of its inverse:

$$\begin{cases} G^{k,n+1} = (\delta_{ij} + \frac{\Delta t}{\gamma^2} (C_h \Sigma_{h,i}^{k,n+1-}, C_h \Sigma_{h,j}^{k,n+1-})_{1 \leq i,j \leq N_s}), \\ Q^{k,n+1} = \text{chol}((G^{k,n+1})^{-1}). \end{cases}$$

- Compute corrected sensitivity matrices:

$$\forall j \in [1:N_s], \quad \begin{cases} \Sigma_{h,j}^{k,n+1} = \sum_{1 \leq i \leq N_p} Q_{ij}^{k,n+1} \Sigma_{h,i}^{k,n+1-}, \\ \Delta_{h,j}^{k,n+1} = \sum_{1 \leq i \leq N_p} Q_{ij}^{k,n+1} \Delta_{h,i}^{k,n}. \end{cases}$$

- Compute corrected state and parameter:

$$\begin{cases} \hat{\theta}_h^{k,n+1} = \hat{\theta}_h^{k,n} + \frac{\Delta t}{\gamma^2} \sum_{1 \leq j \leq N_s} (C \Sigma_{h,j}^{k,n+1}, y_\gamma^{n+1} - C \hat{z}_h^{k,n+1-})_{1 \leq j \leq N_s} \Delta_{h,j}^{k,n+1} \\ \hat{z}_h^{k,n+1} = \hat{z}_h^{k,n+1-} + \frac{\Delta t}{\gamma^2} \sum_{1 \leq j \leq N_s} (C \Sigma_{h,j}^{k,n+1}, y_\gamma^{n+1} - C \hat{z}_h^{k,n+1-})_{1 \leq j \leq N_s} \Sigma_{h,j}^{k,n+1} \end{cases}$$

- ↪ Sampling step:

$$\forall j \in [1:N_s], \quad \begin{cases} \hat{\theta}_{h,j}^{k,n+1} = \hat{\theta}_h^{k,n+1} + \Delta_{h,j}^{k,n+1}, \\ \hat{z}_{h,j}^{k,n+1} = \hat{z}_h^{k,n+1} + \Sigma_{h,j}^{k,n+1}. \end{cases}$$

Additionally, for output purposes, we can re-define up to second-order terms the

parameter covariance operator from the stored $\{\Delta_{h,j}^{k,n}\}_{j=1}^{N_s}$ and $\{\hat{z}_h^{k,n+1-}\}_{j=1}^{N_s}$:

$$\Lambda_h^{k,n} : \mathcal{P}_h \ni \theta \mapsto \sum_{1 \leq j \leq N_s} \beta_j(\Delta_{h,j}^{k,n}, \theta) \mathcal{P}_{\Delta_{h,j}^{k,n}} \in \mathcal{P}_h.$$

In the same fashion, the parameter sensitivity operator reads

$$L_h^{k,n+1} : \mathcal{P}_h \ni \theta \mapsto \sum_{1 \leq j \leq N_s} \beta_j((\Lambda_h^{k,n})^{-1} \theta, \Delta_{h,j}^{k,n}) \mathcal{P}(\hat{z}_h^{k,n+1-} - \hat{z}_h^{k,n+1-}) \in \mathcal{Z}_h.$$

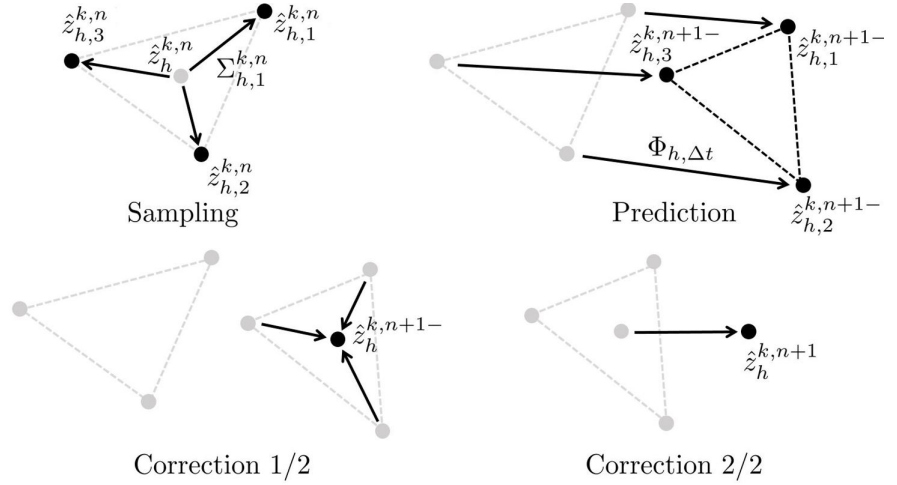


Figure 2. Illustration of the main steps of the reduced-order UKF algorithm in the specific case of $\mathcal{P} = \mathbb{R}^2$ and focusing specifically on the state estimation part.

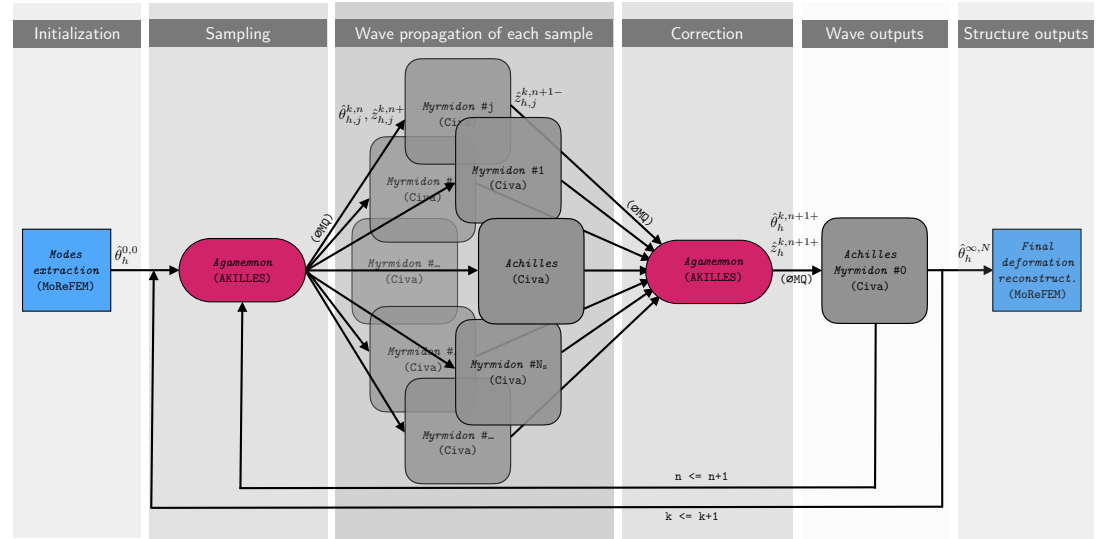


Figure 3. Parallel implementation of the DT-iROUKF in AKILLES.

465 Finally let us give some implementation details, see also Figure ???. We implemented
466 the DT-iROUKF algorithm in a specific Python library called AKILLES¹ based on
467 the message passing library $\mathcal{O}MQ^2$. The objective of this library is to couple the
468 estimator library with any model, written in any language that can receive and send

¹<https://gitlab.inria.fr/AKILLES/AKILLES>

²<https://zeromq.org>

469 vector quantities through $\otimes\text{MQ}$. In **AKILLES**, the Gramian, Cholesky decomposition,
 470 corrected states and parameters are computed by the main process of **AKILLES** called
 471 *Agamemnon* who communicates through $\otimes\text{MQ}$ with *Achilles'* army of *Myrmidons* –
 472 here they represent wave solvers built upon the SFEM kernel of the commercial
 473 software **CIVA**³. The physical outputs are finally processed after the correction step by
 474 the process *Achilles*, a specific *Myrmidon* wave solver in **CIVA** in charge of extra output
 475 computations. Note that the non-linear mechanical deformation and the corresponding
 476 modal decomposition are initially computed using the Finite Element Library **MoReFEM**⁴
 477 for solving large deformation mechanical problems.

478 4 Numerical results

479 In this section, we illustrate the use of the presented algorithm for estimating the
 480 deformation caused by the mechanical loading in structures using GW measurements.
 481 Three different cases are presented in increasing order of complexity. The first case is
 482 a small-scale problem with the objective of testing the robustness and analyzing the
 483 estimation results of the proposed strategies. The second case is an aluminum plate
 484 under traction forces based on an experiment [23] done in the context of acoustoelasticity
 485 to retrieve the material third-order elastic constants. The third case is a pipe subjected
 486 to a 4-point bending test based on an experiment [31] related to the detection of
 487 welding defects under operational conditions employing ultrasound. All the illustrated
 488 cases are presented with the structure described below.

489 Noisy synthetic data generation.

First, let us describe the numerical experimental setup for generating noisy synthetic
 data, and comprising mechanical loading, ultrasonic excitation and signal acquisition. A
 quasi-static structural problem is defined to compute the structural deformation caused
 by mechanical loading. For all the cases, the constitutive behavior of the material is
 modeled by the Compressible Neo Hookean (CNH) hyperelastic law. With λ and μ
 being the Lamé parameters, its hyperelastic potential reads

$$\mathscr{W}^{\text{CNH}} = \frac{\lambda}{2}(\sqrt{I_3} - 1)^2 + \frac{\mu}{2}(I_1 - 3 - \log(I_3)),$$

490 with $I_1 = \text{tr } \mathbf{C}$ and $I_3 = \det \mathbf{C}$ being invariants of the right Cauchy-Green deformation
 491 tensor $\mathbf{C} = \mathbf{F}^\top \mathbf{F}$. The mesh, type of forces and boundary conditions configuring the
 492 quasi-static problem are given for every configurations considered in the following.
 493 After defining the configuration for the structural deformation problem, we define the
 494 configuration for the excitation, propagation and measurement of ultrasonic waves. A
 495 force acting upon the outer surface generates a wavefield radially with respect to the
 496 structure surface. It represents a force \mathbf{f} defined in a sufficiently thin layer on the outer
 497 surface. Its ring geometry has an inner radius of 10mm and an outer radius of 20mm.
 498 The excitation signal is a 5-cycle cosine Hanning windowed at a specific frequency for
 499 each case. We consider zero initial conditions for the wavefield. The observation data
 500 are generated by using the operator in (10) with the domain ω_i defined upon the outer
 501 surface as a sufficiently thin layer in which the wavefield does not vary in the thickness
 502 direction. This amounts to modeling a point or surface probe with specific sensitivity.
 503 One may note that during the estimation procedure, as the estimated deformation
 504 changes while the wave propagation problem is running, the CFL condition (28) also
 505 changes. However, the time step is computed once at the initialization and this changes

³<https://www.extende.com>

⁴<https://gitlab.inria.fr/MoReFEM>

506 may cause numerical instability. To avoid such an issue, the time step is computed to
 507 satisfy the CFL condition for the expected deformation extrema.

To emulate signals obtained from an acquisition system in real scenarios, we generate synthetic observation data using the target deformation and the wave propagation solver. Gaussian noise is added to the simulated data to represent potential electronic and environmental noise. The Gaussian noise is added to the simulated measurements as

$$y_{\gamma,i}^n = \check{y}_i^n + \frac{\gamma}{\sqrt{\Delta t}} \|\check{y}_i\|_{\ell_2} \chi_i^n,$$

508 where χ_i^n is a realization of a random variable with distribution $\mathcal{N}(0,1)$. The noise
 509 level is set by adjusting γ .

510 Reducing the parametric space using mode decomposition.

To represent the parametric space on a reduced basis, we use the eigenmodes of the quasi-static problem as defined in (11). First, we compute a finite set of eigenmodes \mathcal{I} ordered in ascending eigenvalue order, *i.e.* from the lower to highest spatial frequency. A reduced parametric space for reconstructing the deformation is selected as a subset $\mathcal{I}^* \subset \mathcal{I}$. This selection is made by having a guess \mathbf{u}_0^* of the deformation decomposed in the eigenbasis of \mathcal{I} and selecting the smallest subset \mathcal{I}^* that satisfy a representation error criterion. More precisely, by decomposing \mathbf{u}_0^* in the eigenmodes of \mathcal{I} we select a set of modes associated with the components θ_i^* that have a minimum relative ℓ_2 -error τ^* defined as

$$\tau^* = \frac{\|\mathbf{u}_0^* - \sum_{j \in \mathcal{I}^*} \theta_j^* \boldsymbol{\varphi}_j\|}{\|\mathbf{u}_0^*\|}.$$

To better visualize the relevance of the selected modes we plot the representation error for the first m modes in \mathcal{I} , namely $1 - \tau_m$, where

$$\tau_m = \frac{\|\mathbf{u}_0^* - \sum_{j \in \mathcal{I}_m} \theta_j^* \boldsymbol{\varphi}_j\|}{\|\mathbf{u}_0^*\|}$$

511 and \mathcal{I}_m being the set of the m lowest frequency modes in \mathcal{I} .

512 Initializing the estimator.

To initialize the estimator, we must give an *a priori* parameter and its covariance. Even though one could use θ^* as an *a priori* parameter value, we set $\hat{\theta}_h^{1,0}$ to zero in order to test the robustness of our estimator with respect to the initial guess. Regarding the initial covariance, we consider that $\max_{i \in \mathcal{I}^*} \theta_i^*$ is a relevant estimation of the standard deviation of the lowest frequencies, assuming that the lowest frequency is the most relevant for reconstruction. Then, the initial covariance Λ_0 is computed as, based on (14),

$$(\Lambda_0)_{ij} = \frac{\lambda_i^2}{\lambda_{\min}^2} (\max_{i \in \mathcal{I}^*} \theta_i^*)^2 \delta_{ij}, \quad \forall i, j \in \mathcal{I}^*,$$

where the subscript min is associated with the lowest-frequency component in \mathcal{I}^* . The constant M used to normalize the regularization term is computed as

$$M = \sum_{i \in \mathcal{I}^*} \frac{\lambda_{\min}^2}{\lambda_i^2}.$$

513 Finally, the constant ε , which weights the regularization and misfit terms, is adjusted
 514 for each case. The parameter m appearing in the parametric space norm is set as
 515 $m = 1$.

516 **Presentation of the estimation results.**

517 At each outer iteration k of our estimator, the last estimated parameter $\hat{\theta}_h^{k-1,N}$ is used
 518 as an initial parameter for the next one $\hat{\theta}_h^{k,0}$ while the initial covariance restarts at
 519 Λ_0 . We plot for each case the evolution in $n \in [1 : N]$ of the estimated parameters
 520 $\hat{\theta}_h^{k,n}$ and a region representing an estimation of the associated standard deviation
 521 $\sqrt{(\Lambda^{k,n+1})_{ii}}$. Regarding the later, the initial covariance is propagated through the
 522 estimation process while retrieving information from the observations. It provides
 523 qualitative information about how the uncertainty evolves, although a quantitative
 524 interpretation of this uncertainty must be considered carefully.

525 **Sensitivity analysis.**

Instead of using the subset \mathcal{I}^* , the estimation could be done using a larger set of
 eigenmodes, \mathcal{I} for instance, eliminating the need for \mathbf{u}_0^* . However, the ill-posedness
 of the problem combined with the potential instability of the forward model, as the
 estimated pre-deformation varies in time, makes it unviable. To circumvent this
 difficulty, we assume to know a set \mathcal{I}^* of eigenmodes that best represents the target
 deformation. Nonetheless, one may like to gather \mathcal{I}^* directly from the measurements,
 instead of using \mathbf{u}_0^* . As an attempt to do so, we perform a sensitivity analysis using
 one Levenberg-Marquardt iteration of the proposed estimator and the set \mathcal{I} . As we
 run the estimator in the whole set \mathcal{I} , we must avoid instability by constraining the
 trajectory $\hat{\theta}_h^{1,n}$. This can be done by setting the covariance as

$$(\Lambda_0)_{ii} = \gamma^2 = 10^{-8}$$

with a parameter $\varepsilon = 1$, initially. Although at the end of the iteration the estimated
 $\hat{\theta}_h^{1,N}$ have no quantitative significance, it still retains qualitative information relating
 the parametric space to the observations. To visualize and assess this relation, we plot
 the normalized estimated parameters at the end of the estimation,

$$\frac{\hat{\theta}_{h,i}^{1,N}}{\max_{i \in \mathcal{I}} \hat{\theta}_{h,i}^{1,N}}, \quad \forall i \in \mathcal{I},$$

as well as the estimated parameters $\hat{\theta}_{h,i}^{1,n}$ over time. Additionally to the estimated
 values, the covariance matrix is also an output of the estimation process and can be
 used for this purpose. We plot its normalized inverse,

$$(\Lambda_0^{-\frac{1}{2}}) \left((\Lambda^{0,N})^{-1} - \Lambda_0^{-1} \right) (\Lambda_0^{-\frac{1}{2}}),$$

526 representing the normalized Gramian matrix, related to the system's observability [3].

527 **4.1 Results and discussion**

528 **4.1.1 A test case on robustness to noise**

529 To illustrate and test the estimator robustness to noise, we model an aluminum cube
 530 of dimensions $60 \times 60 \times 60 \text{ mm}^3$. The configuration for the quasi-static problem is
 531 shown in *Figure 4a*. The target deformation shown in *Figure 4b* is computed by
 532 solving the quasi-static problem for a body force of $50\text{N}/\text{mm}^3$ in the Y direction.

533 From zero initial conditions, the wave field is excited at one of its faces at 100kHz
 534 in a ring region as described previously. The configuration for the wave propagation
 535 model is depicted in *Figure 5a*, where the characteristic Gauss-Lobatto points of the
 536 SFEM discretization are represented. Examples of extracted signals are plotted in
 537 *Figure 5b*. In this case, the observations are point measurements at ten positions,

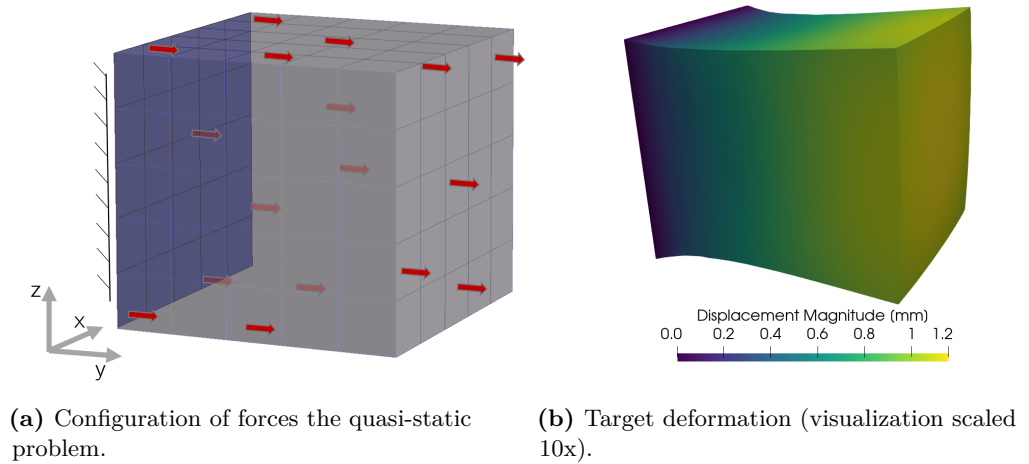
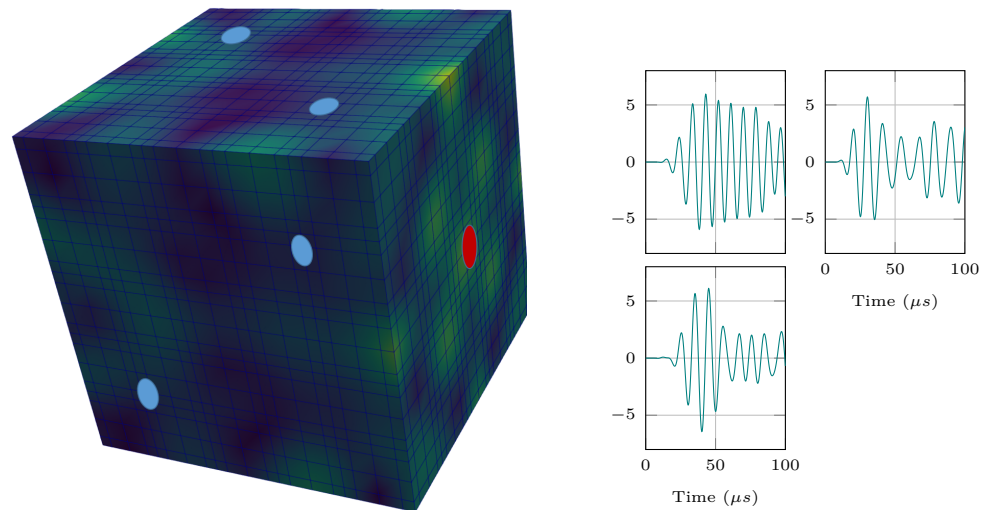


Figure 4. Quasi-static problem configuration for the illustration on the cube.

538 where the three components of the displacement field are obtained. Considering the
 539 definition of the observation operator (10), ω_i is a sufficiently small volume for which
 540 the displacement field is considered constant. The three components are taken as
 541 sensitivity \mathbf{d}_i , resulting in $d = 30$, the number of measured signals. Each face, except
 542 the excited one, has two measurement points on the surface at a distance of 15 mm
 543 from the edges. We run the wave propagation solver up to $100\mu\text{s}$ to generate the
 544 synthetic observation data. In *Figure 5b* we show the extracted field components for
 the point located at $(15,15,0)$.



(a) Configuration of the wave propagation problem. An example of the wave field is illustrated.

(b) Example of measured signals (three components) at $(15,15,0)$.

Figure 5. Configuration and examples of measured signals for the wave propagation problem. The measurement regions are represented in blue and the excited region in red.

545 To test the effect of noise in the estimation, different sets of observed data are
 546 constructed with different levels of noise $\gamma = [10^{-4}, 0.01, 0.1, 0.2]$. Examples of the
 547 different levels of added noise are shown in *Figure 6*.

549 The eigenmodes associated with the hundred lowest eigenvalues are computed,
 550 embodying \mathcal{I} . We decompose a guess of the deformation generated by an axial body

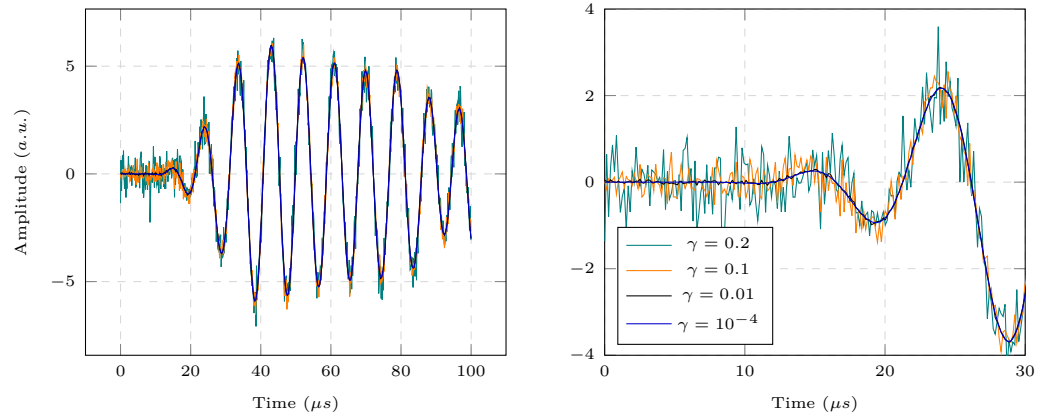
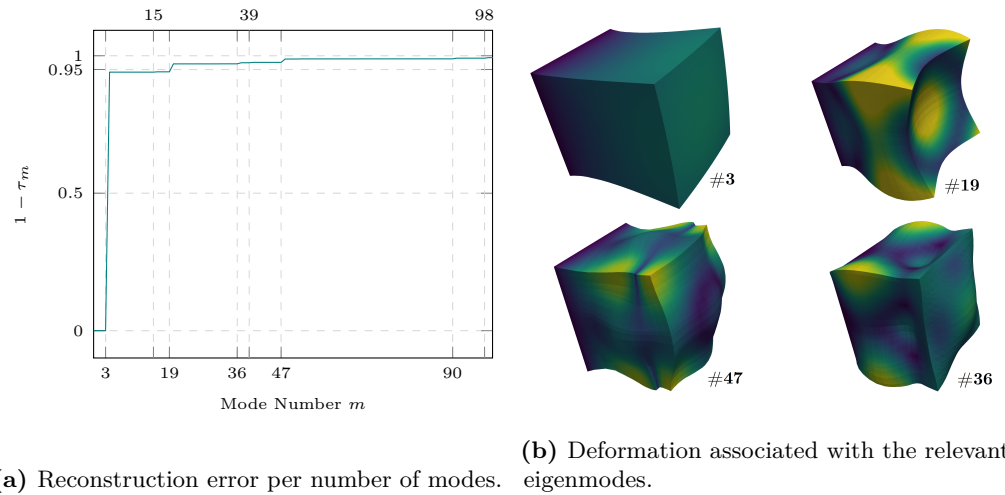


Figure 6. Example of different noise levels added to the synthetic data for the cube case.

551 force with low amplitude, \mathbf{u}_0^* , in the basis associated with \mathcal{I} . Using this decomposition
 552 we plot $1 - \tau_m$ and the associated relevant modes in **Figure 7**. Then, the most relevant
 553 modes can be selected and are therefore highlighted, making, for $\tau^* = 0.01$, $\mathcal{I}^* =$
 554 $\{3, 15, 19, 36, 39, 47, 90, 98\}$, meaning that with 8 selected modes we can reconstruct
 555 99% of its deformation.



(a) Reconstruction error per number of modes. (b) Deformation associated with the relevant eigenmodes.

Figure 7. Reconstruction of \mathbf{u}^* using the lowest frequency modes from which the selection of the most relevant modes is done.

556 We run the estimation algorithm for the different noise levels γ . We first use $\varepsilon = 1$
 557 as the regularization and misfit terms in function (16) are normalized. The iterative
 558 process is shown in **Figure 8** with the time evolution of the estimated parameters $\hat{\theta}_h^k$.
 559 To illustrate the evolution of the estimated deformation, we reconstruct it at given
 560 iterations and time and compare it with the target deformation in **Figure 9**, for the
 561 case with $\gamma = 0.2$.

562 Discussion.

563 At relatively low noise levels ($\gamma \leq 0.01$), the estimate converges in one iteration, and at
 564 each subsequent iteration, the estimate deviates slightly from the converged value and
 565 converges again. At higher noise levels ($\gamma \geq 0.1$), a few iterations may be required to
 566 converge with significant errors *w.r.t.* the target, although it presents a good estimation
 567 of the reconstructed deformation, as shown in **Figure 9**. In addition, the estimator
 568 updates the estimated parameter at a lower rate as γ increases, as we can see in the

569 case of $\gamma = 0.2$. This is due to the fact that γ weights the mismatch term, as can be
570 seen in (16), and gives less credibility to the observed data when noise increases. In
571 such a case, the parameter ε can be adjusted to increase the rate at which the estimator
572 updates the parameter based on the observed data. For example, we set $\varepsilon = 0.025$ and
573 show the corresponding estimate in *Figure 10*. We can see that when the update rate
574 is increased, the noise causes larger instabilities in the estimated parameter during an
575 iteration. The variable ε can be adjusted on a case-by-case basis. As discussed earlier,
576 the tangent stiffness operator in (6) can be ill-posed, *i.e.* the coercivity assumption
577 (8) for the forward problem is not guaranteed. Therefore, ε must be adjusted taking
578 into account the direct-problem stability issues due to strong oscillations during the
579 estimation.

580 As mentioned earlier, we can restrict the estimation to a reduced parametric space
581 without resorting to an initial deformation prior, but by retrieving information from
582 the observations. For this case, we evaluate the possibility of doing this through a
583 sensitivity analysis using a low noise level, $\gamma = 10^{-4}$, and $\varepsilon = 1$. The normalized
584 estimated parameters are shown in *Figure 11a* and the quantity \mathcal{I}^* is highlighted.
585 Based on these results, the most important modes cannot be completely distinguished,
586 but one could empirically set a threshold to select them. At the risk of overlooking some
587 important modes, an iterative selection process can be proposed but it is not discussed
588 here. The evolution of these parameters during estimation is shown in *Figure 11b*,
589 with the \mathcal{I}^* set highlighted. The main modes do not appear to exhibit any particular
590 dynamic behavior that could be used to distinguish them. Finally, *Figure 11c* plots
591 the Gramian for the 50 first modes in \mathcal{I} . The Gramian quantifies how observable and
592 distinguishable the different modes are from each other and information about the
593 overall observability of the inverse problem can be retrieved. High observability can
594 lead to overestimation, as in the case of the higher frequency modes, for example,
595 mode 47. Inversely, low observability can lead to underestimation, as in the case of
596 mode 3. The diagonal values quantifies the observability of the associated modes while
597 off-diagonal terms quantifies how indistinguishable the associated modes are from each
598 other.

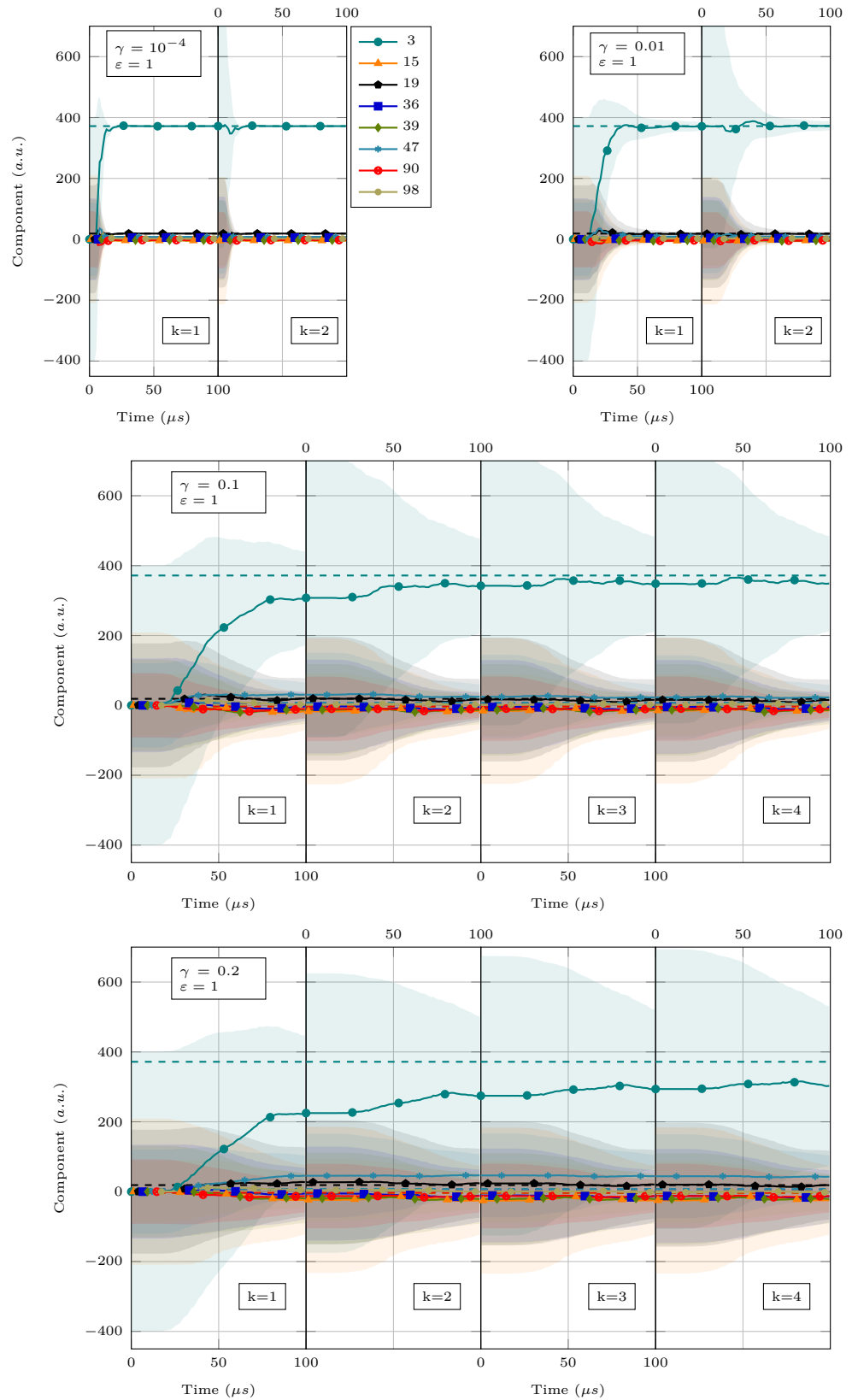


Figure 8. Evolution in time for the estimation $\hat{\theta}_h^k$ for the cube case. The estimated modes components are plotted with a highlighted region corresponding to the standard deviation. The target values are represented as dashed lines. Different γ noise levels are tested with a regularization $\varepsilon = 1$.

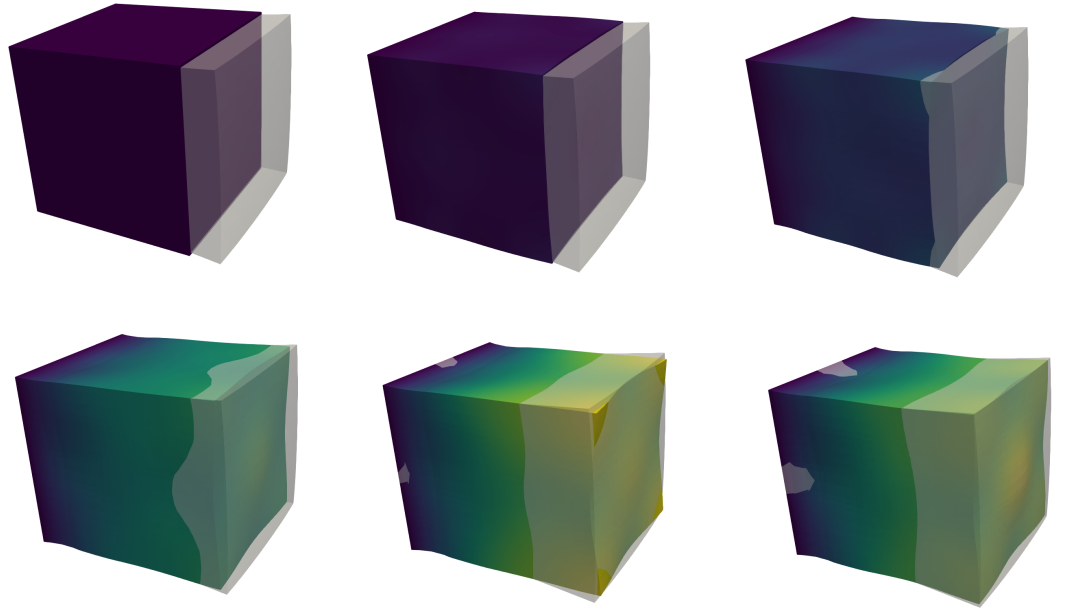


Figure 9. Snapshots at given iterations k and time t of the estimated deformation compared with the target deformation (transparent) for a high level of noise, $\gamma = 0.2$. From left to right, top to bottom we have $(k=0, t=0\mu s)$ $(k=0, t=25\mu s)$ $(k=0, t=35\mu s)$ $(k=1, t=25\mu s)$ $(k=2, t=75\mu s)$ and $(k=3, t=100\mu s)$.

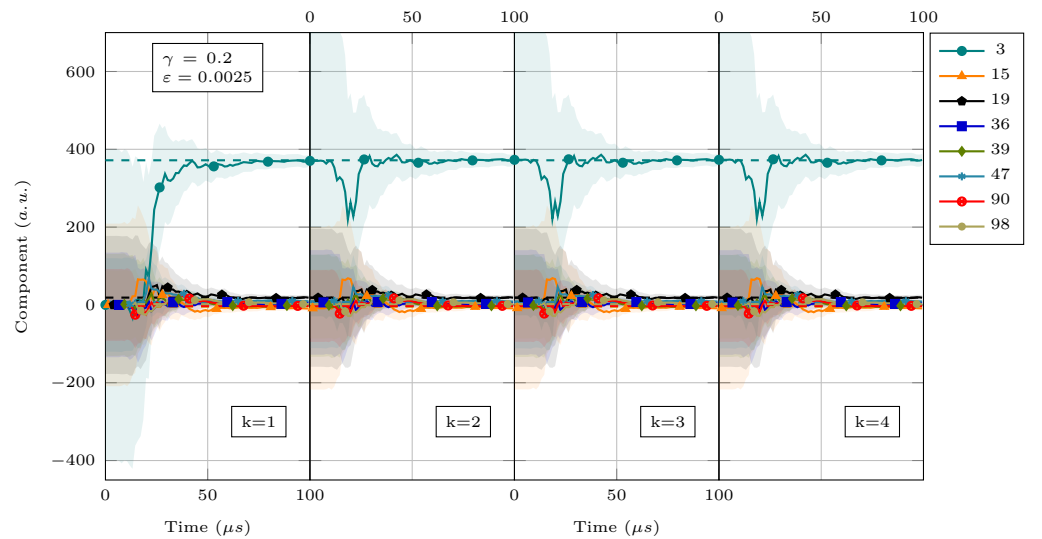
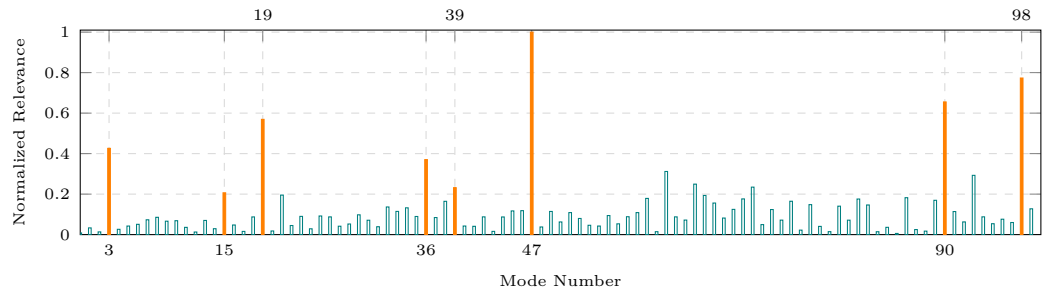
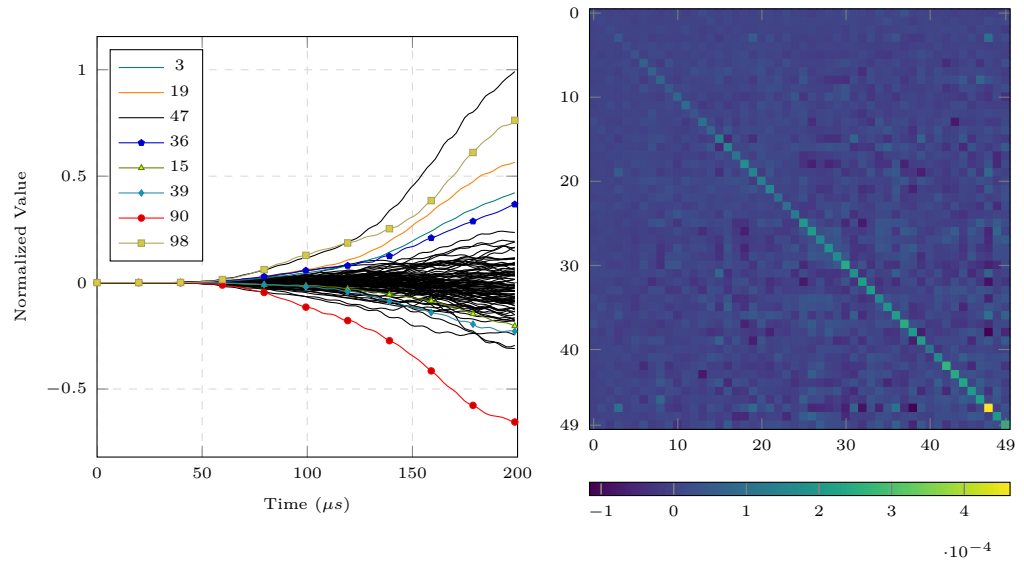


Figure 10. Evolution in time for the estimation $\hat{\theta}_h^k$ for the cube case. The estimated modes components are plotted with a highlighted region corresponding to the standard deviation. The target values are represented as dashed lines. A weak regularization, $\varepsilon = 0.0025$, and noise $\gamma = 0.2$ is used.



(a) Normalized estimated value for each parameter at the end of the sensitivity analysis.

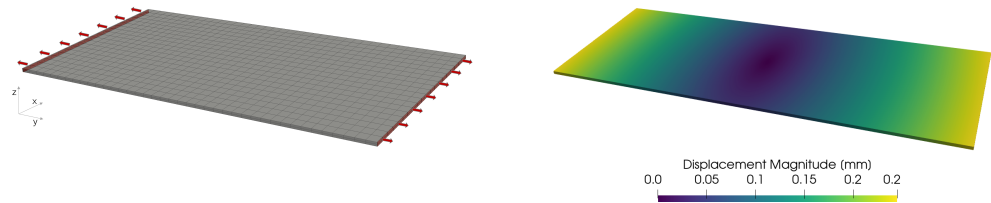


(b) Evolution of $\hat{\theta}_h$ for every parameter in \mathcal{I} . (c) Normalized Gramian at the end of the analysis.

Figure 11. The estimation is done for the larger set \mathcal{I} to perform a sensitivity analysis in the cube illustration. Different outputs of the estimation procedure are plotted and the set \mathcal{I}^* is highlighted.

599 4.1.2 Aluminum plate under traction

600 We present here a case based on the experiment done in [23] to model guided wave
 601 propagation in axially loaded structures. The specimen is an aluminum plate of
 602 dimensions $610 \times 305 \times 6.35 \text{ mm}^3$ under traction forces. The configuration for the
 603 quasi-static problem is shown in *Figure 12a*. We compute the target deformation with
 604 an axial stress of 57.5 MPa, resulting in the deformation illustrated in *Figure 12b*.

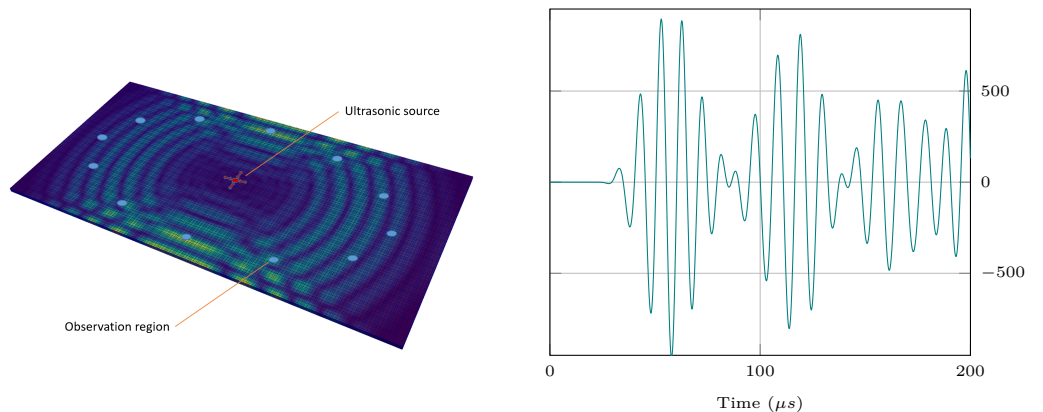


(a) Configuration.

(b) Deformation for an axial stress of 57.5MPa.

Figure 12. Quasi static problem configuration and target deformation for the plate illustration.

605 The ultrasonic excitation is done as previously described at the center of the
 606 plate (upper surface) at 100kHz. The observation data are obtained by defining the
 607 observation operator in twelve surface regions ω_i distributed in an ellipse as depicted
 608 in *Figure 13a*. The mesh used in the wave propagation problem is also depicted. The
 609 synthetic observed data are generated by running the simulation up to $200\mu\text{s}$. An
 610 example of the obtained signal is shown in *Figure 13b*.

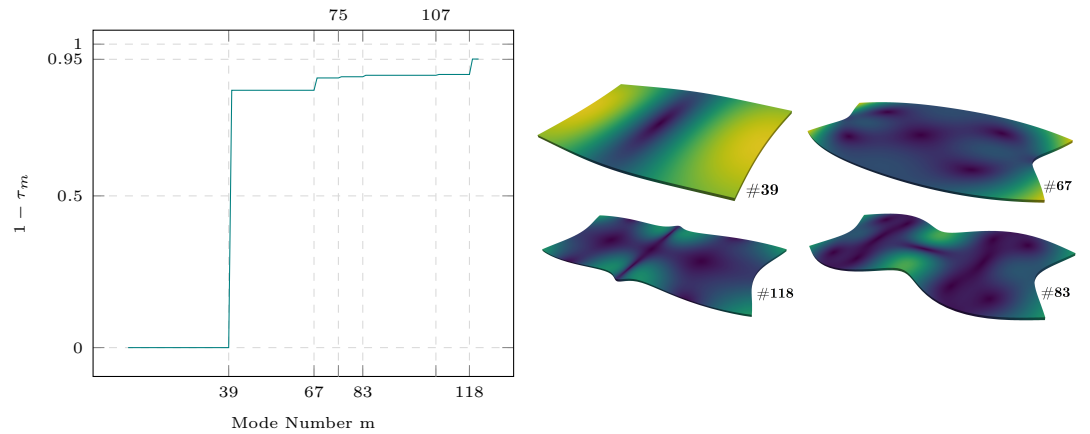


(a) Wave propagation problem configuration, mesh, excitation and measurement regions.

(b) Example of measure signals.

Figure 13. Configuration and examples of measured signals for the wave propagation problem. The measurement regions are represented in blue and the excited region in red.

611 For the larger set of eigenmodes \mathcal{I} we compute those associated with the 120
 612 lowest eigenvalues. As the experiment has no essential boundary conditions, rigid body
 613 movements are penalized and the first 6 eigenmodes, associated to them, are removed.
 614 From a guess of the deformation \mathbf{u}_0^* generated by the traction surface forces with lower
 615 amplitude, we can select a smaller set of eigenmodes by analyzing its decomposition
 616 on a parametric basis. In *Figure 14* we plot $1 - \tau_m$ from which the most relevant
 617 modes can be selected. For $\tau^* = 0.05$, we have $\mathcal{I}^* = \{39, 67, 75, 83, 107, 118\}$.



(a) Reconstruction error per number of modes. (b) Deformation associated with the relevant eigenmodes.

Figure 14. Reconstruction of \mathbf{u}^* using the lowest frequency modes from which the selection of the most relevant modes is done.

618 After acquiring the observed data from the simulated measurements on the target
619 deformation, we add different levels of noise, $\gamma = [0.01, 0.1]$, as plotted in *Figure 15*.

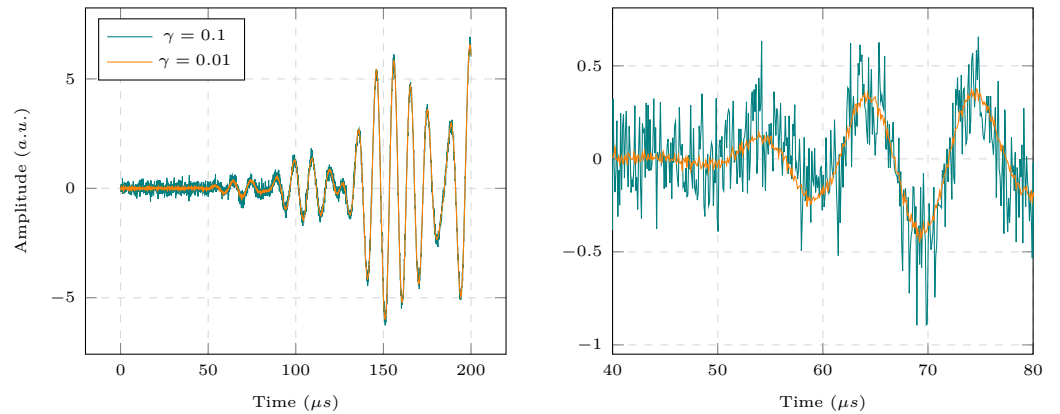


Figure 15. Example of different noise levels for the aluminum plate illustration.

620 Discussion.

621 As in the previous case of the cube, a few specific modes are important to the
622 reconstruction of the deformation although the first relevant mode is of relatively high
623 frequency. This must be taken into account when computing \mathcal{I} as we risk not including
624 the relevant modes. The estimation shown in *Figure 16* required more iterations
625 to achieve apparent convergence, even with the lowest noise. As noise increases, the
626 differentiation between modes becomes more difficult although the most important
627 mode, 39, remains pronounced. For visualization purposes, the estimated deformation
628 is reconstructed at different times of the estimation and depicted in *Figure 17*. As
629 previously done, by adjusting ε we can achieve a faster response of the estimate by
630 reducing the number of iterations needed until apparent convergence, as shown in the
631 estimation for this adjusted case, *Figure 18*.

632 Regarding performance, the model for the quasi-static problem has 7750 degrees
633 of freedom (DoFs) and the computation of the first 120 eigenmodes takes 9 minutes.
634 Finite elements of order one is used for the quasi-static problem as numerical locking
635 is negligible in pure extensional deformation. The wave propagation problem has

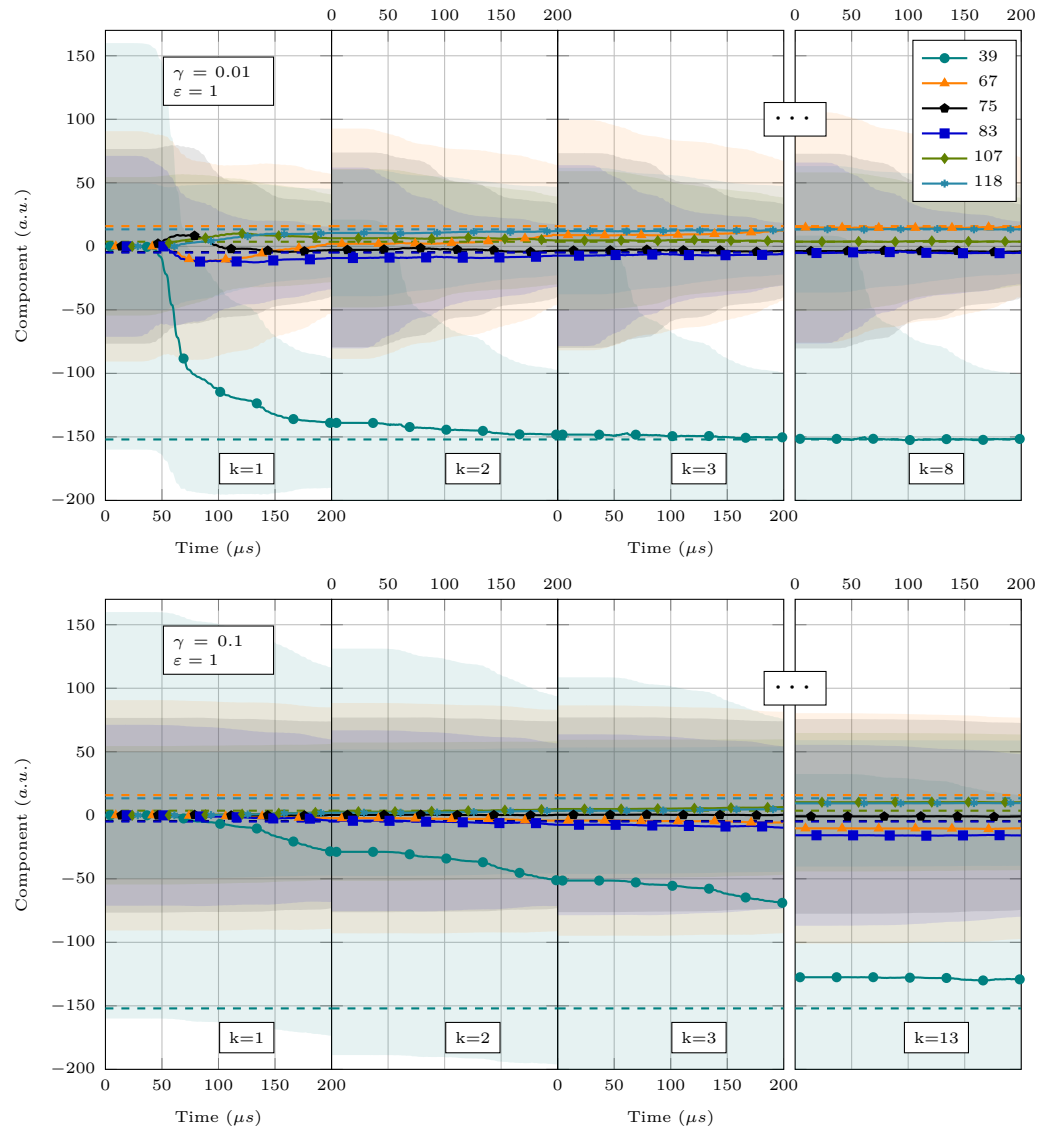


Figure 16. Evolution in time for the estimation $\hat{\theta}_h^k$ for the plate case. The estimated modes components are plotted with a highlighted region corresponding to the standard deviation. The target values are represented as dashed lines. Different γ noise levels are tested with a neutral regularization $\varepsilon = 1$.

636 420k DoFs and a total of 2223 time steps. One run of the wave propagation problem
 637 to generate the observations takes less than a minute and requires 180MB of RAM.
 638 During an estimation of 6 mode components, 7 wave propagation problems are run
 639 in parallel and each iteration of the estimation procedure takes 12 minutes. The
 640 computational cost of solving a wave propagation problem is higher during estimation
 641 due to parameter change at each time step, requiring extra computations related to
 642 the update of the tangent stiffness operator. We use a laptop computer equipped with
 643 a *Intel i9-9880H* CPU and 32GB of RAM for computing the presented results.

644 Finally, the sensitivity analysis is done for a negligible noise $\gamma = 10^{-4}$ and $\varepsilon = 1$.
 645 The final estimated values for the sensitivity analysis are plotted in *Figure 19a*.
 646 In this case, the relevant modes are well distinguishable. The observability can be
 647 analyzed in the Gramian matrix, *Figure 19c*. Due to its sparsity, we conclude that
 648 there are only a few observable modes and the fact that the diagonal is not pronounced
 649 means that the modes are less indistinguishable from each other. This can be seen in

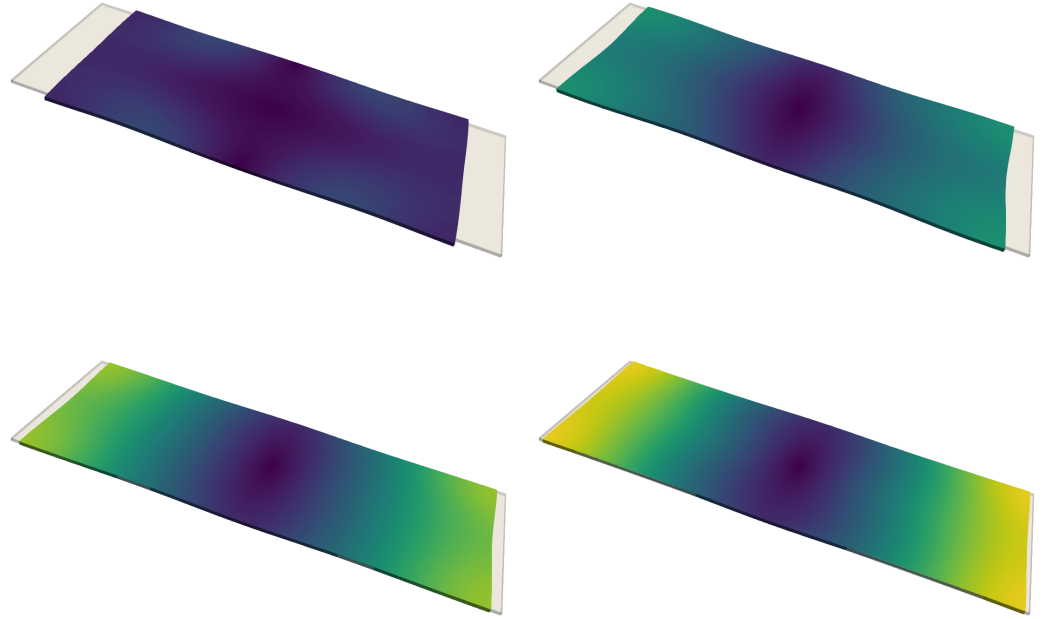


Figure 17. Snapshots at given iterations k and time t of the estimated deformation compared with the target deformation (transparent). Estimation for $\gamma = 0.1$. From left to right, top to bottom we have $(k=0, t=60\mu s)$ $(k=0, t=130\mu s)$ $(k=0, t=180\mu s)$ and $(k=1, t=200\mu s)$. Visualization is scaled 300x.

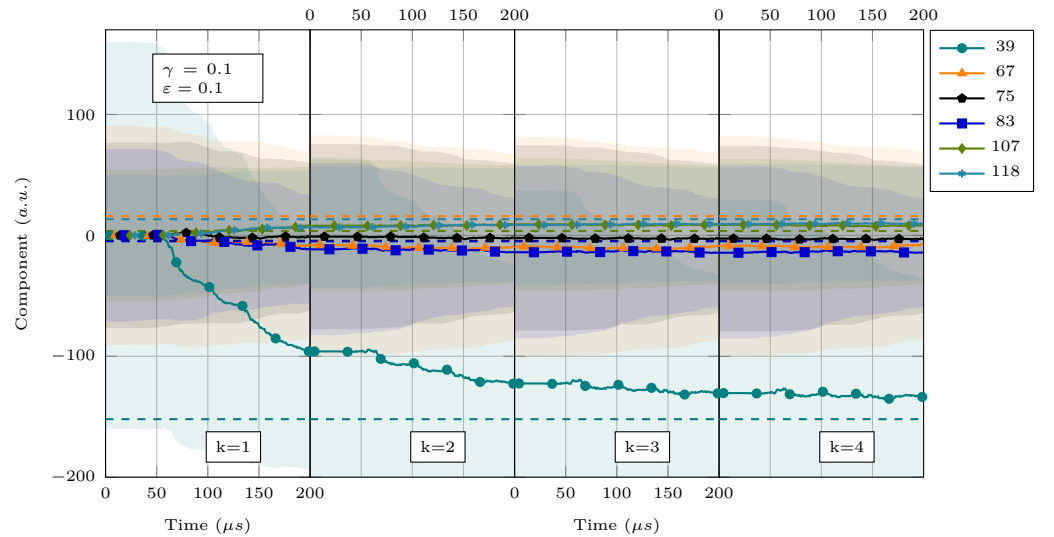
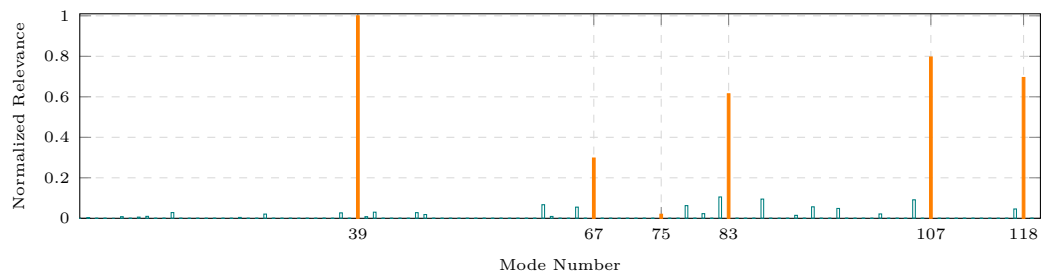


Figure 18. Evolution in time for the estimation $\hat{\theta}_h^k$ for the plate case. The estimated modes components are plotted with a highlighted region corresponding to the standard deviation. The target values are represented as dashed lines. A weaker regularization, $\varepsilon = 0.1$, is used.

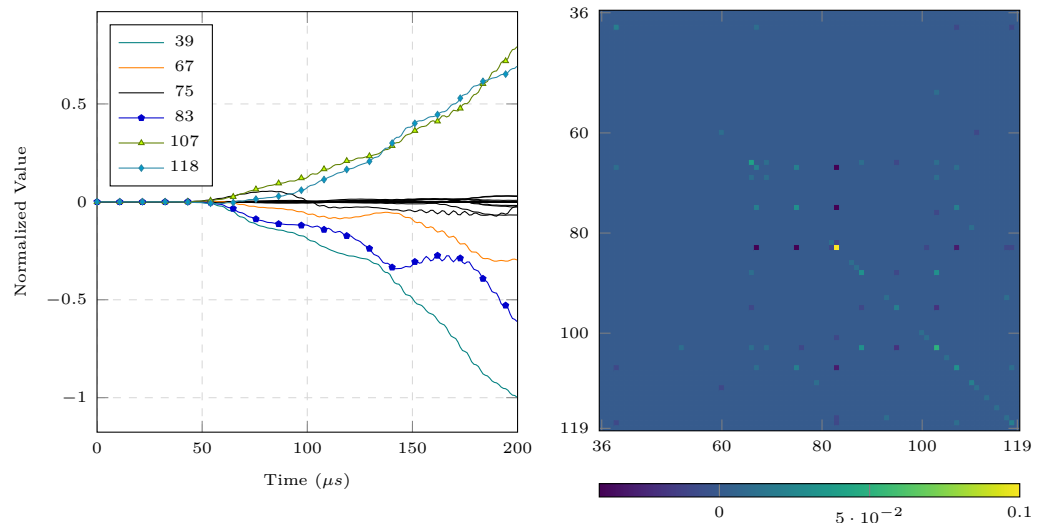
650 the results with the reduced set of eigenmodes, where the estimation of less relevant
 651 modes are highly affected by noise. The high observability shown in *Figure 19a* is due
 652 to the fact that the deformation of the structure is of relatively high frequency, hence
 653 more observable according to the Gramian. Also, the relevant modes are not clustered
 654 around a certain frequency, which helps their spatial differentiation. The evolution of

655 the parameters shown in *Figure 19b* can be analyzed and provide some insights into
 656 the process of estimation. Modes 67 and 87 present non-monotonic behavior since the
 657 deformation related to these modes is concentrated farther from the center where the
 658 waves were excited (see *Figure 14*), hence the wave takes longer to travel through
 659 these regions and its carried information to be considered.

660 Regarding performance of the sensitivity analysis, 115 wave propagation problems
 661 had to be run in parallel, taking 5 hours to complete and requiring 271GB of RAM,
 662 in total. The memory usage for each problem was significantly higher than when
 663 estimating only 6 modes as each problem had to store the deformation gradient of all
 664 114 modes. Other strategies for accessing such gradients can be proposed, leaving room
 665 for improvement. A desktop workstation equipped with 2**Intel Xeon Platinum 8276*
 666 CPU and 512GB of RAM was used to run these problems. Note that, although we
 667 use only one workstation, our implementation with $\text{\textcircled{O}MQ}$ allows parallelization through
 668 workstations and clusters.



(a) Normalized estimated value for each parameter at the end of the sensitivity analysis.



(b) Evolution of $\hat{\theta}_h$ for every parameter in \mathcal{I} .

(c) Normalized Gramian at the end of the analysis.

Figure 19. The estimation is done for the larger set \mathcal{I} to perform a sensitivity analysis in the plate illustration. Different outputs of the estimation procedure are plotted and the set \mathcal{I}^* is highlighted..

669 4.1.3 Experiment-based 4-point bending on a steel pipe

670 To increase complexity, we consider the experiment done in [31], where the authors use
 671 ultrasonic guided waves to detect weld damage in a steel pipe while it was subjected to
 672 a 4-point bending test. They assess the performance of traditional imaging techniques
 673 to detect the damage while the specimen is subjected to mechanical load. To overcome

674 the bias introduced by the mechanical load to the ultrasonic signal, they perform signal
 675 acquisitions in pristine conditions for different loads and use them as baselines to,
 676 through comparison, detect changes in the signal due to potential damage. The baseline
 677 should be acquired for every expected load condition, which requires experimental
 678 manipulation and reduces the robustness of a detection system. An alternative to
 679 acquiring several baselines is to estimate the deformation of the structure using the
 680 already available signals. For that purpose, we illustrate the use of our method in this
 681 more complex and application-related configuration. The modeled pipe has a length
 682 of 2.94 meters, a diameter of 0.1973m and is 8mm thick. The quasi-static problem is
 683 depicted in *Figure 20a*. For a total applied force of 220kN, the target deformation is
 684 depicted in *Figure 20b*.

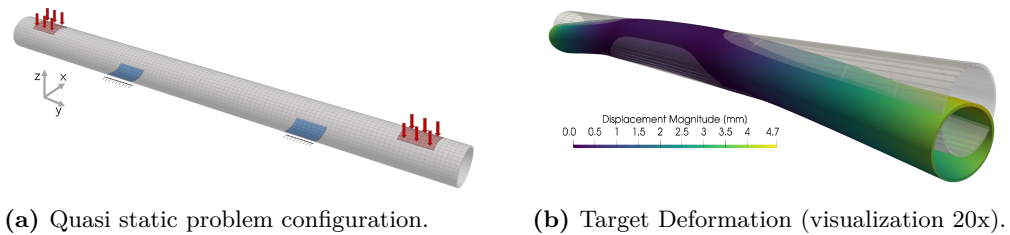


Figure 20. Quasi static problem configuration and target deformation for the pipe illustration.

685 The excitation is done at the top outer-upper surface of the steel pipe at 30kHz,
 686 the observations are obtained from applying the observation operator, as previously
 687 described, with radial sensitivity in 48 regions distributed in 4 circular evenly distributed
 688 sections as depicted in *Figure 21a*. Each section of transducers is rotated 15 degrees
 689 with respect to each other. The synthetic observed data are obtained from simulating
 690 the wave propagation problem up to $1000\mu s$. An example of the obtained signal
 691 is shown in *Figure 21b*.

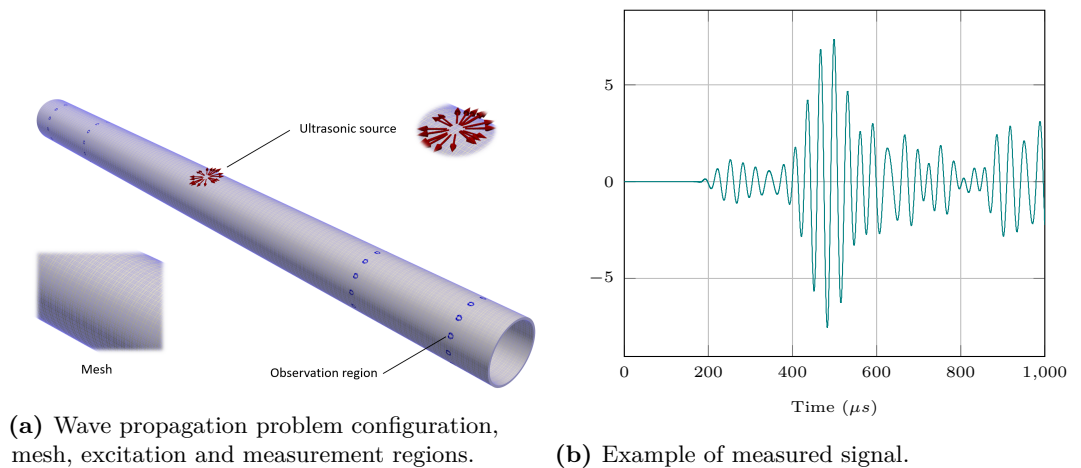


Figure 21. Configuration and examples of measured signals for the wave propagation problem. The measurement regions are represented in blue and the excited region in red.

692 The set \mathcal{I} is embodied by the eigenmodes associated with the 60 lowest eigenvalues.
 693 From a guess of the deformation \mathbf{u}_0^* generated by the bending surface forces, we can
 694 analyze its decomposition in the eigenbasis. In *Figure 22* we plot $1 - \tau_m$ from which
 695 the most relevant modes can be selected and are therefore highlighted, making, for

696 $\tau^* = 0.05$, $\mathcal{I}^* = \{0, 1, 2, 4, 6, 7, 8, 9\}$. Differently from the previous cases, the relevant
 697 modes are concentrated in the lowest frequencies and are poorly distributed.

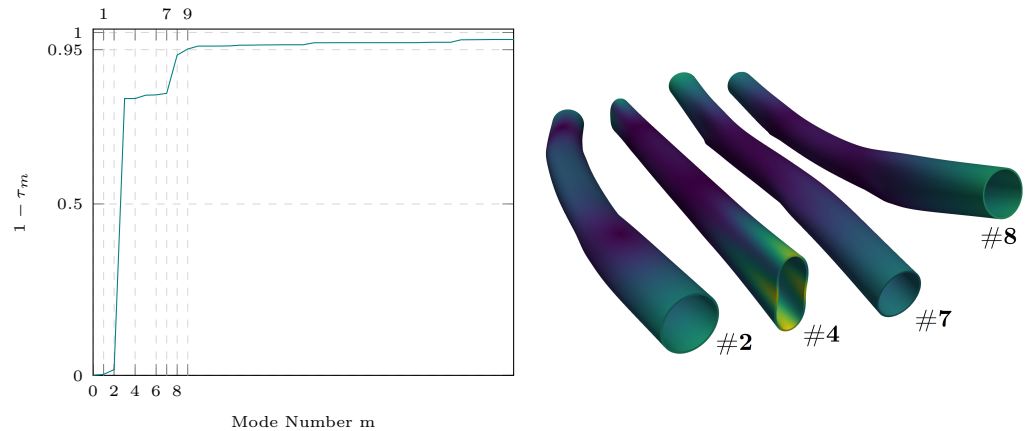


Figure 22. Reconstruction error of \mathbf{u}^* using the lowest frequency modes from which the selection of the most relevant modes is done.

698 Due to the stability issues associated with the potential non-coercivity of the
 699 wave propagation problem, the estimation has to be adjusted with $\varepsilon = 10^4$, setting
 700 a relatively low update rate for the estimation, hence avoiding instabilities during
 701 estimation. The evolution of the parameter can be seen in *Figure 23* for two different
 702 levels of noise, $\gamma = 10^{-4}$ and $\gamma = 0.1$. For both levels of noise, the estimation succeeds
 703 in differentiating the modes. The estimated deformation are reconstructed at different
 704 steps of the estimation procedure and is depicted in *Figure 24*.

705 Discussion.

706 Using high regularization and a large amount of observed data, the estimate is stable
 707 and shows good convergence to the target in a few iterations, even when noise increases.
 708 By comparison with the plate case, we believe that this is because sensors are well
 709 positioned and the acquisition time is long enough so that this case benefits from
 710 rather strong observability, allowing it to well distinguish the deformation modes. This
 711 illustrates the importance of a robust and well-designed acquisition configuration for a
 712 correct estimation.

713 Regarding performance of the estimation, The model for the quasi-static problem
 714 had 148k DoFs and the computation of the first 60 eigenmodes takes 8 hours to
 715 complete using a *Intel(R) Xeon(R) W-3245* CPU. Finite elements of order two is
 716 used for the quasi-static problem. The wave propagation problem has $2M$ DoFs and a
 717 total of 4662 time steps. One run of the wave propagation problem to generate the
 718 observations takes 5 minutes and requires 1GB of RAM. During an estimation of 8
 719 mode components, 9 wave propagation problems are computed in parallel and each
 720 iteration of the estimation procedure takes 2 hours. A workstation equipped with a
 721 *Intel i9-9880H* CPU and 32GB of RAM is used for the estimation.

722 Note, however, that while we obtain satisfactory results when the estimation is
 723 performed in a reduced set of modes, the sensitivity analysis performs poorly when it
 724 comes to selecting the relevant modes from a larger set, as can be seen in *Figure 25a*.
 725 The high-frequency modes are overestimated because they are more observable, as seen
 726 in the Gramian (*Figure 25c*). This overestimation of the less relevant modes due to
 727 observability is a cause of instability when trying to estimate the deformation using the
 728 larger set of modes. The evolution of the sensitivity analysis in *Figure 25b* shows that
 729 some irrelevant modes compensate for each other when trying to minimize the misfit

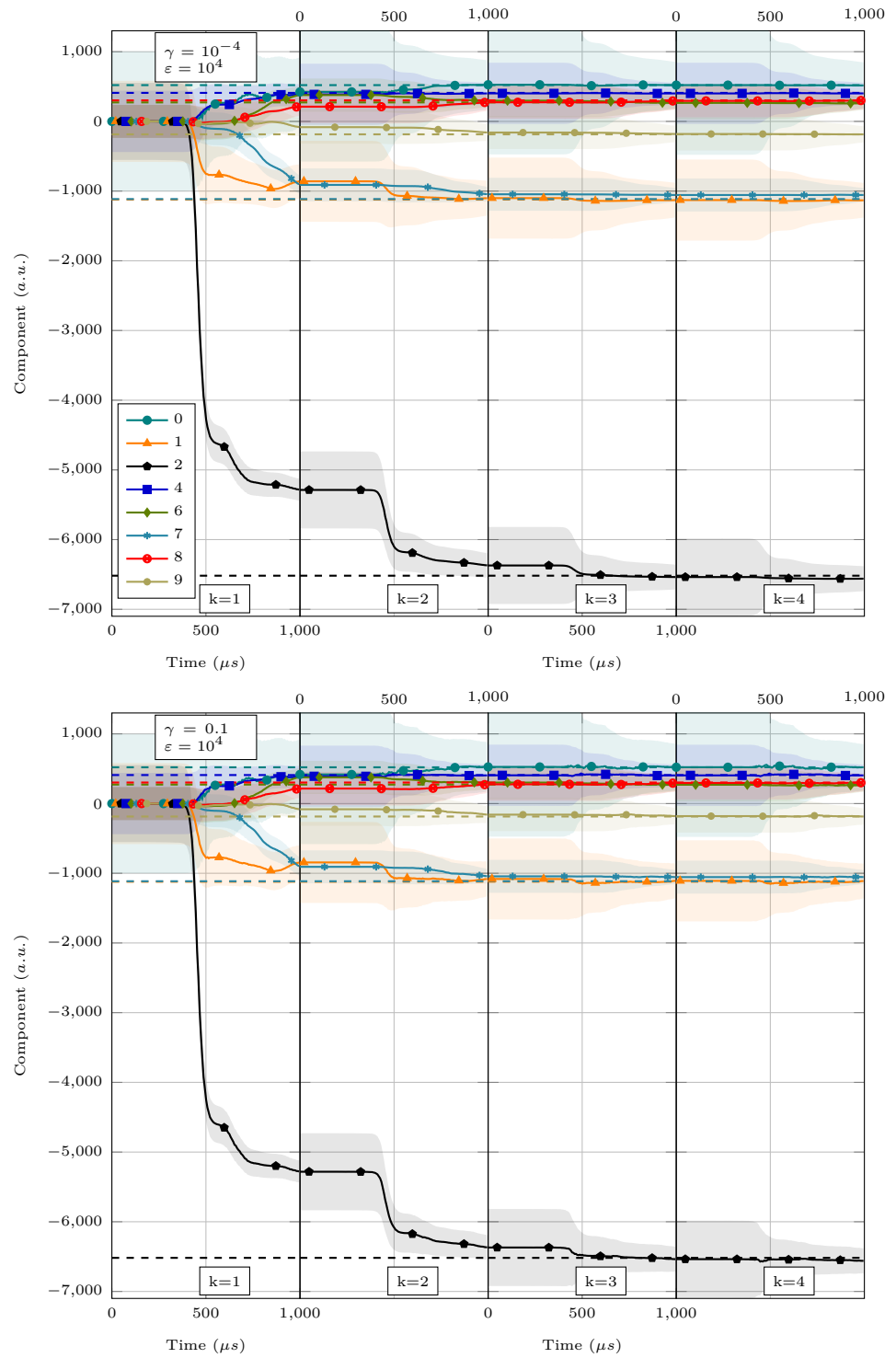


Figure 23. Evolution in time for the estimation $\hat{\theta}_h^k$ for the pipe case. The estimated modes components are plotted with a highlighted region corresponding to the standard deviation. The target values are represented as dashed lines. Different γ noise levels are tested with a strong regularization $\varepsilon = 10^4$.

730 because they are less distinguishable. Without the potential instability issue of the
 731 wave propagation problem, the Gramian diagonal indicates that the modes are readily
 732 observable. The Gramian diagonal can also be used to group the modes that conflict
 733 with each other in minimizing the mismatch, allowing selection of distinguishable modes

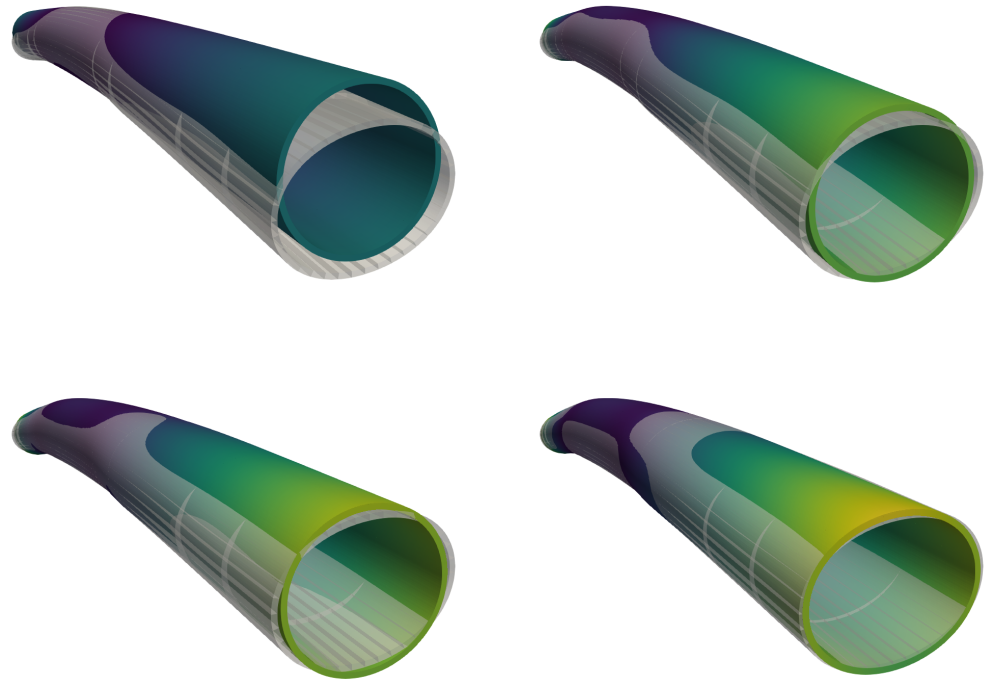


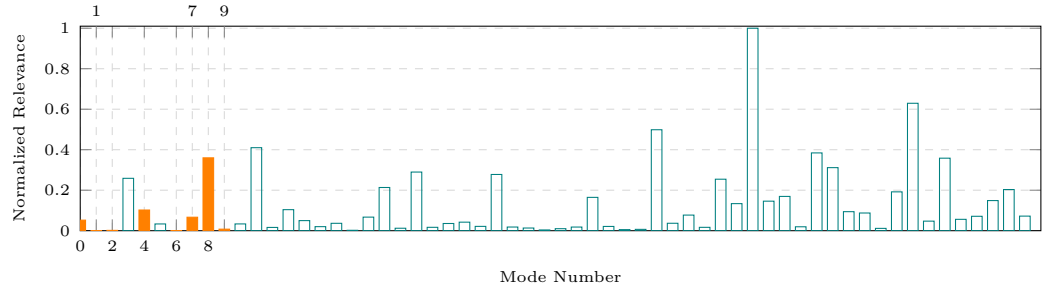
Figure 24. Snapshots at given iterations k and time t of the estimated deformation compared with the target deformation (transparent). Estimation for $\gamma = 0.01$. From left to right, top to bottom we have $(k=0, t=60\mu s)$ $(k=0, t=130\mu s)$ $(k=0, t=180\mu s)$ and $(k=1, t=200\mu s)$. Visualization is scaled 20x.

734 and adaptive estimation. This is typical of ill-posed inverse problems, where estimation
 735 is efficient once we accept a regularization that here comes from a reconstruction in a
 736 parameter space with a small dimension.

737 Regarding performance of the sensitivity analysis, 61 wave propagation problems
 738 are computed in parallel, taking 5 hours to complete and using 400GB of RAM, in
 739 total. A desktop workstation equipped with $2 \times$ Intel Xeon Platinum 8276 and 512GB
 740 of RAM was used. The same remarks done for the plate case regarding performance
 741 are valid here.

742 5 Conclusion and perspectives

743 In this paper, we show how to reconstruct in nondestructive tests a baseline free of
 744 environmental loading conditions using available SHM measurements. Our model-
 745 based approach is inspired by Full-Wave Inversion (FWI) strategies, but here we take
 746 advantage of dynamic programming principles to avoid multiple iterations of adjoint
 747 minimization. In fact, we still rely on an iterative strategy, the Levenberg-Marquardt
 748 algorithm, to transform the initial nonlinear inverse problem into successive linear-
 749 quadratic estimation problems. Each of these linear-quadratic estimation problems is
 750 then solved using a Kalman-based approach. By relying on the Unscented-Kalman
 751 filter, we also avoid the computation of the tangent operator required by the Levenberg-
 752 Marquardt algorithm. The final algorithm converges in a limited number of iterations
 753 compared to standard FWI and is therefore mostly sequential and inherently parallel
 754 with respect to the sigma-points covering the reconstruction space. As a result, our
 755 algorithm efficiency remains comparable to solving the direct guided wave propagation



(a) Normalized estimated value for each parameter at the end of the sensitivity analysis.

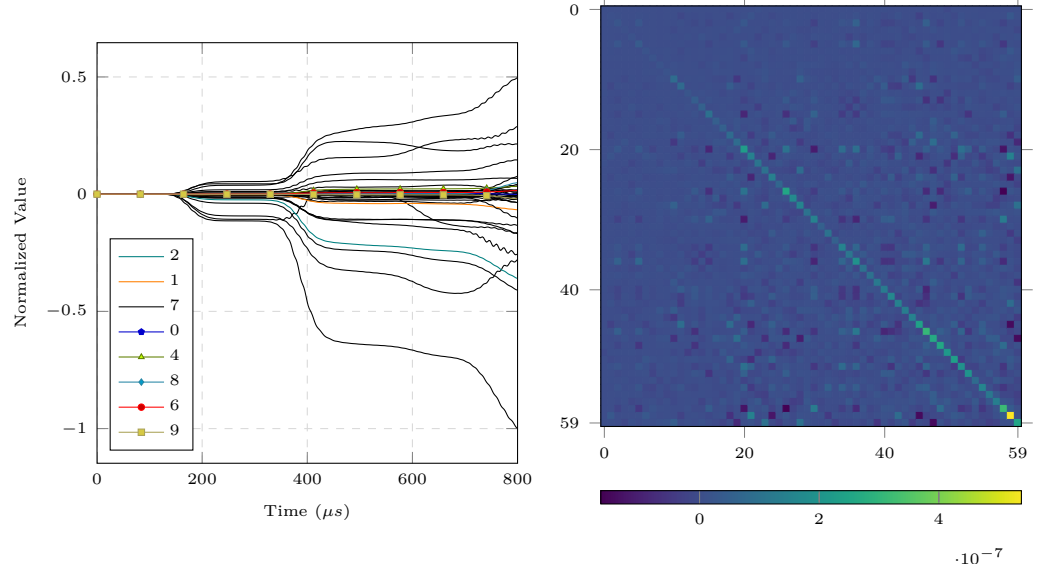
(b) Evolution of $\hat{\theta}_h$ for every parameter in \mathcal{I} . (c) Normalized Gramian at the end of the analysis.

Figure 25. The estimation is done for the larger set \mathcal{I} to perform a sensitivity analysis in the pipe illustration. Different outputs of the estimation procedure are plotted and the set \mathcal{I}^* is highlighted.

756 problem. The main limitation of our approach is that, due to followed dynamic
 757 programming point of view, we are limited to a low-dimensional representation of the
 758 estimated deformation, i.e., only about a hundred modes can be estimated. Moreover,
 759 and this will be the goal of future developments, our approach first considers the
 760 reconstruction of the displacement field, while from the identification perspective,
 761 it might be better suited to reconstruct a strain tensor, for instance, the Cauchy-
 762 Green strain or its invariants. In particular, we believe that this research direction
 763 will help us to better control some deformation constraints related to a potentially
 764 ill-posed wave propagation problem that limits the trust region neighborhood of our
 765 current method. Moreover, our method now needs to be extended to more general
 766 observational operators, some of which may depend on the estimated deformation,
 767 making the presented approach more complex. Moreover, our approach suffers from the
 768 same limitation as the classical FWI method in terms of the choice of the discrepancy
 769 measure between the model and the data. Recently, [27, 35] has been shown that the
 770 use of Wasserstein-based distances can overcome cycle-skipping effects in wave field
 771 inversions.

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