# Reduced Order Modeling for First Order Hyperbolic Systems with Application to Multiparameter Acoustic Waveform Inversion\*

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Abstract. Waveform inversion seeks to estimate an inaccessible heterogeneous medium from data gathered by sensors that emit probing signals and measure the generated waves. It is an inverse problem for a second order wave equation or a first order hyperbolic system, with the sensor excitation modeled as a forcing term and the heterogeneous medium described by unknown, spatially variable coefficients. The traditional "full waveform inversion" (FWI) formulation estimates the unknown coefficients via minimization of the nonlinear, least squares data fitting objective function. For typical band-limited and high frequency data, this objective function has spurious local minima near and far from the true coefficients. Thus, FWI implemented with gradient based optimization algorithms may fail, even for good initial guesses. Recently, it was shown that it is possible to obtain a better behaved objective function for wave speed estimation, using data driven reduced order models (ROMs) that capture the propagation of pressure waves, governed by the classic second order wave equation. Here we introduce ROMs for vectorial waves, satisfying a general first order hyperbolic system. They are defined via Galerkin projection on the space spanned by the wave snapshots, evaluated on a uniform time grid with appropriately chosen time step. Our ROMs are data driven: They are computed in an efficient and noniterative manner, from the sensor measurements, without knowledge of the medium and the snapshots. The ROM computation applies to any linear waves in lossless and nondispersive media. For the inverse problem we focus attention on acoustic waves in a medium with unknown variable wave speed and density. We show that these can be determined via minimization of an objective function that uses a ROM based approximation of the vectorial wave field inside the inaccessible medium. We assess the performance of our inversion approach with numerical simulations and compare the results to those given by FWI.

Key words. hyperbolic systems, inverse wave scattering, data driven, reduced order modeling

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**1.** Introduction. Waveform inversion is an important technology in radar and sonar imaging [18, 16, 25, 7], seismology and geophysical exploration [36, 42], medical imaging with

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<sup>8</sup>Department of Mathematics, University of Houston, Houston, TX 77204-3008 USA (mamonov@math.uh.edu). <sup>¶</sup>Department of Information Technology, Division of Scientific Computing, Uppsala Universitet, 75105 Uppsala, Sweden (jorn.zimmerling@it.uu.se). ultrasound [38], and so on. It is an inverse problem concerned with the estimation of an inaccessible, heterogeneous medium, from time resolved measurements of the wave field, gathered with source and receiver sensors.

Mathematically, the heterogeneous medium is modeled by unknown variable coefficients in second order wave equations, or first order hyperbolic systems of equations. The forcing in these equations is localized at sources that emit probing signals, which are typically pulses. The unknown coefficients depend on the type of waves: They are the bulk modulus and mass density for acoustic waves, the dielectric permittivity and magnetic permeability for electromagnetic waves, and the Lamé parameters and density for elastic waves.

Much of the existing literature is concerned with scalar (acoustic pressure) waves, modeled by the second order wave equation with constant density and unknown variable bulk modulus, which in turn determines the variable wave speed. This is a simplification, but the problem remains difficult because the mapping between the unknown wave speed and the pressure field at the receivers is complicated and nonlinear. In fact, for application relevant high frequency probing pulses and back-scattering data acquisition geometries, where the sources and receivers lie on the same side of the medium, the nonlinear, least squares data fitting objective function has numerous spurious minima, far and near the true wave speed. This behavior is known as "cycle skipping." It is the main difficulty faced by the "full waveform inversion" (FWI) approach implemented with gradient based minimization of the least squares data misfit, even for reasonable initial guesses [42].

The nonlinear least squares data fitting formulation of inversion has received a lot of attention since its introduction in geophysics in [29, 39]. It was named "full waveform inversion" in [33] to emphasize that it uses full seismogram information, not just arrival times. FWI is a computationally intensive, PDE constrained optimization that relies on application specific expertise in algorithms, parametrization, and regularization [32, 4]. Most studies consider the time domain formulation, but they may involve sequential frequency band filtering of the data, from low to high. Low frequencies help in estimating the kinematics (smooth part of the wave speed) which mitigates cycle skipping. There are also FWI methods that operate in the frequency domain, with low to high frequency sweeps and also with complex frequencies. The Ph.D. thesis [23] is a comprehensive study of such methods. The research in FWI continues and the methodology is used outside the geophysics community, for example, in brain imaging with low frequency ultrasound [17], ground penetrating radar [30], and nondestructive evaluation of corroded materials [34]. There remain challenges to overcome, especially for applications with high frequency waves, where the bandwidth is small with respect to the central frequency of the probing pulses.

There are other waveform inversion approaches, beyond FWI. For example, the source type integral equation (STIE) method introduced in [26] uses the observation that inhomogeneities in the medium introduce "scattering source currents" that are related to the measured wave field by linear integral operators. Unfortunately, these operators have a large null space. To deal with the nonuniqueness, the STIE method uses multiple excitations and frequencies and it estimates the scattering currents and subsequently the material properties via a nonlinear iterative procedure. The STIE methodology has been extended to medical imaging with MRI in [3].

Among other, more recent advances to waveform inversion, we mention the following three. One approach is to minimize the data misfit in the Wasserstein metric [21, 44]. The resulting objective function is improved; it is demonstrably convex for some simple models [22], although the result does not hold for general media [14, Figure 3.3]. Another approach is the "modeling operator extension" [28] or "extended FWI" [41, 43]. It introduces additional degrees of freedom in the optimization, e.g., an unknown source signal in addition to the wave speed, and then systematically drives the optimization toward a meaningful result. This approach has been analyzed for a transmission data acquisition geometry in a simple medium in [37], but guarantees for general media and back-scattering data are lacking. A third approach, introduced in [19] for one-dimensional media (see also the early study [40]) and then developed further in [20, 8, 9, 11, 13, 12, 14] for more general media, computes from the data a reduced order model (ROM). This is a matrix that captures essential features of wave propagation in the unknown medium, and therefore, it can be used to define objective functions that are amenable to gradient based minimization [13, 12, 14].

The advantage of FWI, extended FWI, and the Wasserstein metric approaches is that they work with arbitrary placement of the sources and receivers. So far, the ROM methodology has been limited to full knowledge of the "array response matrix" gathered by a collection (active array) of coinciding sources and receivers. Active arrays are used, for example, in radar and phased array ultrasonics, but are not feasible in all applications. Two other data acquisition setups, where the array response matrix can be obtained via some processing, are described in [14, section 4] and [12]. Nevertheless, general source and receiver placements have not been addressed so far. The advantage of the ROM approach, first documented in [12, 14], is that it can estimate strongly heterogeneous media for which the other approaches have failed.

In this paper we extend the ROM inversion methodology to first order hyperbolic systems that govern all types of linear waves in nondispersive and lossless media. The ROM derivation is general, but we focus attention on multiparametric inversion for acoustic waves, where the wave speed c and density  $\rho$  are to be estimated from measurements of the vectorial wave field, with components given by the acoustic pressure and velocity. Like in [20, 8, 9, 11, 13, 12, 14], the ROM is defined via Galerkin projection [5, 27, 15] on the space spanned by the wave snapshots, sampled on a uniform time grid, with step  $\Delta t$  chosen according to the Nyquist sampling criterion for the probing source signals. The snapshots are vector valued fields that are unknown at points inside the medium. We show that they satisfy an exact time stepping scheme driven by a "wave propagator" operator. The ROM is a matrix of size determined by the number of source excitations and time steps up to the duration of measurements. It is defined as the orthogonal projection of the wave propagator operator onto the unknown space of the snapshots. We derive the nonlinear mapping between the wave measurements at the sensors and the ROM and then obtain a data driven ROM construction via a noniterative procedure that uses efficient tools from numerical linear algebra.

The results in [20, 8, 9, 11, 13, 12, 14] are specialized for the second order wave operator  $\partial_t^2 - c^2 \Delta$  and are based on the positive definiteness and self-adjointness of  $-c^2 \Delta$ , in the  $L_{c^{-2}}^2$  inner product, weighted by  $c^{-2}$ . For first order hyperbolic systems the wave operator is  $\partial_t + \mathcal{L}$ , with skew-adjoint, first order partial differential operator  $\mathcal{L}$ . This changes the technical aspects of the ROM construction, which is new and different from the previous studies. In the second order formulation [20, 8, 9, 11, 13, 12, 14], the wave field is scalar valued (acoustic pressure) and the propagator is a self-adjoint operator. Here, the wave field is vectorial and it can be expressed mathematically as a time-dependent flow, with unitary propagator operator  $e^{-\Delta t \mathcal{L}}$  defined in terms of the unitary semigroup generated by  $\mathcal{L}$ . The data driven

computation of the ROM is novel and the ROM propagator has a different algebraic structure. It was block tridiagonal and symmetric in [20, 8, 9, 11, 13, 12, 14], whereas here we obtain a block upper Hessenberg ROM propagator, that can be interpreted as a special, upwind finite difference scheme for the causal wave propagation. From the practical point of view, the first order formulation considered in this paper opens the door to addressing vector waves such as elastic and electromagnetic and to explore the use of different types of (polarized) sources and receivers.

We use the ROM to obtain an approximation of the vectorial wave field at the inaccessible points inside the medium, a.k.a. the "internal wave." This approximation is consistent with the measurements but the internal wave does not solve the hyperbolic system of equations unless the estimates of c and  $\rho$  are right. This motivates our multiparametric inversion approach which minimizes the discrepancy between the internal wave and the solution of the hyperbolic system, throughout the domain. This is different from the FWI approach, which minimizes the misfit of the wave at the sensor locations. As demonstrated by numerical simulations, our objective function is better suited for minimization with gradient based algorithms, like Gauss–Newton, than that of FWI.

As far as we know, no existing waveform inversion methodology comes with a mathematical guarantee of convergence to the true solution, i.e., the objective function is not convex. We cannot prove convexity either, but what we can show is that the ROM can resolve better the medium from the same data. There are many technical "tricks" that one can use to improve the performance of FWI [23, 32]. Our goal is to compare how the same optimization algorithm, with the same data, parametrization of the unknowns, and regularization strategy, performs on our objective function versus that of FWI. We point the reader to [12, 14] for an explicit comparison of the FWI and a ROM based objective function in a two-dimensional search domain for the velocity c. The performance of the ROM introduced in this paper is similar to that in [12, 14] for the case of a medium with constant density  $\rho$ . Thus, those results stand and demonstrate, at least in those simple cases, the advantage of the ROM based inversion. Here we are interested in the more difficult problem, where we search for both c and  $\rho$ .

The paper is organized as follows. We begin in section 2 with the derivation of the data driven ROM for a general first order hyperbolic system. In section 3 we specialize the result to acoustic waves in a medium with unknown wave speed c and density  $\rho$ . The multiparametric inversion is discussed in section 4. We also give there numerical simulation results. We end with a brief summary in section 5.

2. ROM for first order hyperbolic systems. Since we deal with a time domain formulation, where the measurements are recorded for a duration T, we use the hyperbolicity of the problem and the finite wave speed to truncate the domain of wave propagation, which is typically the whole space  $\mathbb{R}^d$ , to  $\Omega \subset \mathbb{R}^d$ , with  $d \in \{2,3\}$ . We let  $\Omega$  be a bounded and simply connected domain, with T dependent diameter, and with piecewise smooth boundary  $\partial\Omega$ , modeled with some appropriate homogeneous boundary conditions.<sup>1</sup> For example, for acoustic waves,  $\partial\Omega$  may be sound hard or sound soft. For electromagnetic waves, we may assume a perfectly conducting  $\partial\Omega$ .

<sup>&</sup>lt;sup>1</sup>Because  $\Omega$  is defined via truncation, the choice of boundary conditions does not affect the measurements up to time T.

All linear waves in lossless and nondispersive media are governed by a first order hyperbolic system of the form

2.1) 
$$\partial_t \boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) + \mathcal{L} \boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = \boldsymbol{f}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}), \qquad t \in \mathbb{R}, \ \boldsymbol{x} \in \Omega.$$

The dimension m of the vectorial wave field  $\psi_{\epsilon} \in \mathbb{R}^{m}$  depends on d and the type of waves. For example, in d-dimensional acoustics, the components of  $\psi_{\epsilon}$  are the pressure and velocity, so m = d + 1. In three-dimensional electromagnetics (d = 3), the wave consists of the electric and magnetic fields, so m = 6. In two-dimensional electromagnetics (a three-dimensional case with medium invariant in one direction) the governing equations decouple into two polarizations with m = 3 each.

The variable t in (2.1) denotes time and  $\mathcal{L}$  is a first order, skew-adjoint partial differential operator with respect to  $\boldsymbol{x}$ , acting on m-dimensional vectorial functions in  $L^2(\Omega)$ , with homogeneous boundary conditions. The vector  $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2) \in \mathcal{E} \subset \mathbb{N}^2$  indexes the wave excitation, represented by the m-dimensional vector function  $\boldsymbol{f}_{\boldsymbol{\epsilon}}$  in  $L^2((-t_s, t_s) \times \Omega)$ , that models a source localized<sup>2</sup> at point  $\boldsymbol{x}_{\epsilon_1}$ , with polarization indexed by  $\epsilon_2$ . In some applications, the forcing  $\boldsymbol{f}_{\boldsymbol{\epsilon}}$ may be a separable function of t and  $\boldsymbol{x}$ . For generality, we allow the probing signals to change from one source to another. These signals are assumed to be pulses, supported in time in the interval  $(-t_s, t_s)$ , with modulation at central (carrier) frequency  $\nu$ . Prior to the excitation, there is no wave,

(2.2) 
$$\boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = \boldsymbol{0}, \quad t < -t_s, \, \boldsymbol{x} \in \Omega.$$

The unknown coefficients that model the heterogeneous medium are in  $\mathcal{L}$ . The waveform inversion problem is to determine them from the time-dependent array response matrix  $\boldsymbol{A}$  with entries

(2.3) 
$$\boldsymbol{A}_{\boldsymbol{\epsilon}',\boldsymbol{\epsilon}}(t) = \int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \left[ \boldsymbol{f}_{\boldsymbol{\epsilon}'}(-t',\boldsymbol{x}) \right]^T \boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}).$$

Here T denotes the transpose, while  $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2)$  and  $\boldsymbol{\epsilon}' = (\epsilon'_1, \epsilon'_2)$  are two-dimensional indexes in  $\mathcal{E} \subset \mathbb{N}^2$ . Since  $\boldsymbol{f}_{\epsilon'}$  is supported near the location  $\boldsymbol{x}_{\epsilon'_1}$  of one of the sensors, the measurements are approximated by  $\boldsymbol{\psi}_{\epsilon}$  evaluated there. That we consider this wave field along the force  $\boldsymbol{f}_{\epsilon'}$ is a requirement of our data driven ROM construction. We show in the next section that for acoustic waves, (2.3) models measurements of the velocity.

**2.1. Time stepping and the snapshots.** Denote by  $n_{\mathcal{E}}$  the cardinality of the set  $\mathcal{E} \subset \mathbb{N}^2$  of excitation indexes. To simplify notation, we gather the solutions of (2.1), for all the excitations, in the matrix valued wave field

(2.4) 
$$\boldsymbol{\psi}(t,\boldsymbol{x}) = \left(\boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x})\right)_{\boldsymbol{\epsilon}\in\mathcal{E}}$$

with m rows and  $n_{\mathcal{E}}$  columns. Similarly, we gather all the forces in

(2.5) 
$$\boldsymbol{f}(t,\boldsymbol{x}) = \left(\boldsymbol{f}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x})\right)_{\boldsymbol{\epsilon}\in\mathcal{E}} \in \mathbb{R}^{m \times n_{\mathcal{E}}},$$

<sup>&</sup>lt;sup>2</sup>Localized means that the support is contained in a ball centered at  $x_{\epsilon_1}$  with a radius that is small with respect to the wavelength.

The solution of (2.1) can be written as

(2.6) 
$$\boldsymbol{\psi}(t,\boldsymbol{x}) = \int_{-t_s}^{t} dt' \, e^{-(t-t')\mathcal{L}} \boldsymbol{f}(t',\boldsymbol{x}),$$

where  $e^{-t\mathcal{L}}$  is the unitary semigroup generated by  $\mathcal{L}$ . This operator is understood to act columnwise on  $\mathbf{f}$ . Let us shift the time axis by a finite time<sup>3</sup>  $\tau \geq t_s$  and define the new, *m*-dimensional field

(2.7) 
$$\boldsymbol{\varphi}(t, \boldsymbol{x}) = \boldsymbol{\psi}(t + \tau, \boldsymbol{x})$$

with initial state

(2.8) 
$$\boldsymbol{\varphi}(0,\boldsymbol{x}) = \boldsymbol{\varphi}_0(\boldsymbol{x}) = \int_{-t_s}^{t_s} dt' \, e^{-(\tau-t')\mathcal{L}} \boldsymbol{f}(t',\boldsymbol{x}).$$

Here we used that f is supported in  $(-t_s, t_s)$ . Equation (2.6) implies that  $\varphi$  satisfies the homogeneous equation

(2.9) 
$$\partial_t \boldsymbol{\varphi}(t, \boldsymbol{x}) + \mathcal{L} \boldsymbol{\varphi}(t, \boldsymbol{x}) = \boldsymbol{0}, \quad t > 0, \, \boldsymbol{x} \in \Omega,$$

and it takes the form of the time-dependent flow

(2.10) 
$$\boldsymbol{\varphi}(t, \boldsymbol{x}) = e^{-t\mathcal{L}} \boldsymbol{\varphi}_0(\boldsymbol{x}).$$

The time stepping equation follows easily from (2.10): Let  $t_j = j\Delta t$  be a uniform time grid, with  $j \in \mathbb{N}$  and  $\Delta t \leq 1/(2\nu)$ , so that the Nyquist sampling criterion for the signal s is satisfied. Define the wave snapshots on this grid by

(2.11) 
$$\boldsymbol{\varphi}_{j}(\boldsymbol{x}) = \boldsymbol{\varphi}(t_{j}, \boldsymbol{x}), \qquad j \geq 0.$$

These satisfy the time stepping iteration

(2.12) 
$$\boldsymbol{\varphi}_{j+1}(\boldsymbol{x}) = \mathcal{P}\boldsymbol{\varphi}_j(\boldsymbol{x}), \qquad j \ge 0, \ \boldsymbol{x} \in \Omega,$$

driven by the wave propagator operator

(2.13) 
$$\mathcal{P} = e^{-\Delta t \mathcal{L}}.$$

This unitary operator contains all the information about the medium and the ROM approximates it by the matrix  $\mathcal{P}^{\text{ROM}}$ , called the "ROM propagator."

<sup>&</sup>lt;sup>3</sup>We show later that, since  $e^{-t\mathcal{L}}$  is unitary, the ROM construction is invariant with respect to  $\tau$ .

**2.2. Galerkin approximation of the snapshots.** We are interested in the Galerkin projection of the time stepping equation (2.12) on the space  $\mathcal{S}^{GAL}$  spanned by the first  $n_t$  snapshots, gathered in the matrix valued field

(2.14) 
$$\Phi(\boldsymbol{x}) = (\boldsymbol{\varphi}_0(\boldsymbol{x}), \dots, \boldsymbol{\varphi}_{n_t-1}(\boldsymbol{x})),$$

with m rows and  $n_t n_{\mathcal{E}}$  columns. The ROM is defined using the following assumption.

Assumption 1. The columns of  $\Phi(x)$  are linearly independent vector fields.

Remark 2.1. Assumption 1 holds in general, i.e., its converse is unlikely to occur. Indeed, suppose that the columns of  $\mathbf{\Phi}$  were linearly dependent. Then, there exists a linear combination  $\mathbf{\Phi}\gamma$  of these columns that is vanishing in  $\Omega$ , where the coefficients are stored in the column vector  $\boldsymbol{\gamma} = (\gamma_{j,\epsilon})_{j=0,\ldots,n_t-1,\epsilon\in\mathcal{E}}$  of size  $n_t n_{\mathcal{E}}$ . Equivalently, it is possible to build the source

$$\boldsymbol{f}^{(\boldsymbol{\gamma})}(t,\boldsymbol{x}) = \sum_{j=1}^{n_t} \sum_{\boldsymbol{\epsilon} \in \mathcal{E}} \gamma_{j,\boldsymbol{\epsilon}} \boldsymbol{f}_{\boldsymbol{\epsilon}}(t-t_j-\tau,\boldsymbol{x}),$$

supported in space on the sensor locations and in time in  $(-(n_t - 1)\Delta t - \tau - t_s, 0)$  such that the resulting wave vector field vanishes in  $\Omega$  at time 0, and hence at any positive time. It is very unlikely that a null controllability problem can be solved by "chance" that way.

We will see later that the Gramian matrix of the snapshots stored in  $\Phi$  plays a key role in the data driven computation of the ROM. Assumption 1 implies that the Gramian is nonsingular. This is sufficient for the theory in this section. However, to get a stable ROM computation, the Gramian must also be well-conditioned. In our experience, this occurs for arrays with sensor separation of about half the wavelength, calculated at frequency  $\nu$ , in the reference medium near the sensors, and with time sampling step  $\Delta t \leq 1/(2\nu)$ . If the Gramian is ill-conditioned or even singular (i.e., Assumption 1 does not hold), then the ROM construction requires regularization. We discuss this in section 4.

The Galerkin approximation of the snapshots is

(2.15) 
$$\boldsymbol{\varphi}_{j}^{\text{GAL}}(\boldsymbol{x}) = \boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{g}_{j} \in \mathcal{S}^{\text{GAL}}, \qquad j \ge 0, \ \boldsymbol{x} \in \Omega,$$

where  $\boldsymbol{g}_j \in \mathbb{R}^{n_t n_{\mathcal{E}} \times n_{\mathcal{E}}}$  are the matrices of Galerkin coefficients, calculated so that, when substituting (2.15) into (2.12), we get a residual that is orthogonal to the approximation space. We write this orthogonality relation using a particular orthonormal basis of  $\mathcal{S}^{\text{GAL}}$ , given by the Gram–Schmidt orthogonalization procedure, summarized in the equation

(2.16) 
$$\Phi(\boldsymbol{x}) = \boldsymbol{V}(\boldsymbol{x})\boldsymbol{R}, \qquad \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{V}^{T}(\boldsymbol{x})\boldsymbol{V}(\boldsymbol{x}) = \boldsymbol{I}_{n_{t}n_{\mathcal{E}}},$$

where  $I_q$  denotes the  $q \times q$  identity matrix, for any  $q \in \mathbb{N}$ . The Gram–Schmidt procedure is good for our context, because it gives a causal basis. That is to say, if we write V, similar to (2.14),

(2.17) 
$$V(x) = (v_0(x), \dots, v_{n_t-1}(x)),$$

we have

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2.18) 
$$\boldsymbol{v}_j(\boldsymbol{x}) \in \text{span} \{ \boldsymbol{\varphi}_l(\boldsymbol{x}), 0 \leq l \leq j \}, \quad j = 0, \dots, n_t - 1,$$

with

(2.19) 
$$\int_{\Omega} d\boldsymbol{x} \, \boldsymbol{v}_j^T(\boldsymbol{x}) \boldsymbol{v}_l(\boldsymbol{x}) = \delta_{j,l} \boldsymbol{I}_{n_{\mathcal{E}}}.$$

The causality (2.18) is reflected in (2.16) by the block upper triangular algebraic structure of the matrix  $\mathbf{R} \in \mathbb{R}^{n_t n_{\mathcal{E}} \times n_t n_{\mathcal{E}}}$  with  $n_{\mathcal{E}} \times n_{\mathcal{E}}$  blocks.

The equation for the Galerkin coefficients is

(2.20) 
$$\int_{\Omega} d\boldsymbol{x} \boldsymbol{V}^{T}(\boldsymbol{x}) [\boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{g}_{j+1} - \mathcal{P}\boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{g}_{j}] = \boldsymbol{0}, \qquad j \ge 0,$$

or, equivalently,

(2.21) 
$$\boldsymbol{R}^{-T} \mathbb{M} \boldsymbol{g}_{j+1} = \boldsymbol{R}^{-T} \mathbb{S} \boldsymbol{g}_j, \qquad j \ge 0,$$

with  $\mathbf{R}^{-T}$  the transpose of the inverse of  $\mathbf{R}$ . Here we solved for  $\mathbf{V}$  in (2.16) and introduced the Gramian, a.k.a. the "mass" matrix

(2.22) 
$$\mathbb{M} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\Phi}^{T}(\boldsymbol{x}) \boldsymbol{\Phi}(\boldsymbol{x}) \in \mathbb{R}^{n_{t} n_{\mathcal{E}} \times n_{t} n_{\mathcal{E}}},$$

and the "stiffness" matrix

(2.23) 
$$\mathbb{S} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\Phi}^{T}(\boldsymbol{x}) \mathcal{P} \boldsymbol{\Phi}(\boldsymbol{x}) \in \mathbb{R}^{n_{t} n_{\mathcal{E}} \times n_{t} n_{\mathcal{E}}}$$

There are a few important observations for the Galerkin version (2.21) of the time stepping equation:

1. The matrices  $\mathbf{R}$  and  $\mathbb{M}$  are invertible due to Assumption 1, so all the Galerkin coefficients  $\mathbf{g}_j$  are uniquely defined by (2.21), in terms of  $\mathbf{g}_0$ . We choose

(2.24) 
$$g_0 = i_0$$

where  $\{i_j\}_{j=0}^{n_t-1}$  denote the  $n_t n_{\mathcal{E}} \times n_{\mathcal{E}}$  "column blocks" of the identity matrix  $I_{n_t n_{\mathcal{E}}} = (i_0, \ldots, i_{n_t-1})$ . The choice (2.24) ensures that the Galerkin approximation (2.15) satisfies exactly the initial condition.

2. The first  $n_t$  matrices of Galerkin coefficients are trivial, meaning that

$$(2.25) \boldsymbol{g}_{j} = \boldsymbol{i}_{j}, 0 \leq j \leq n_{t} - 1,$$

and therefore,

(2.26) 
$$\boldsymbol{I}_{n_t n_{\mathcal{E}}} = (\boldsymbol{g}_0, \dots, \boldsymbol{g}_{n_t-1}) = (\boldsymbol{i}_0, \dots, \boldsymbol{i}_{n_t-1}).$$

3. The block upper triangular matrix  $\mathbf{R}$  in the Gram–Schmidt orthogonalization is the block Cholesky square root of the mass matrix

$$(2.27) M = \mathbf{R}^T \mathbf{R}$$

Note that (2.25) is equivalent to saying that the Galerkin approximation (2.15) is exact not only at  $t = t_0$ , but also at  $t = t_j$ , for  $j = 1, ..., n_t - 1$ . This follows from the definition of the approximation space  $\mathcal{S}^{GAL}$  and the fact that (2.12) implies

(2.28) 
$$\boldsymbol{\varphi}_{j+1}(\boldsymbol{x}) - \mathcal{P}\boldsymbol{\varphi}_j(\boldsymbol{x}) = \boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{i}_{j+1} - \mathcal{P}\boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{i}_j = \boldsymbol{0}, \qquad 0 \le j \le n_t - 2$$

Equation (2.27) is derived from the definition (2.22) of the mass matrix and the Gram–Schmidt equation (2.16),

(2.29) 
$$\mathbb{M} = \int_{\Omega} d\boldsymbol{x} \left[ \boldsymbol{V}(\boldsymbol{x}) \boldsymbol{R} \right]^T \boldsymbol{V}(\boldsymbol{x}) \boldsymbol{R} = \boldsymbol{R}^T \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{V}^T(\boldsymbol{x}) \boldsymbol{V}(\boldsymbol{x}) \, \boldsymbol{R} = \boldsymbol{R}^T \boldsymbol{R}$$

**2.3. Galerkin projection ROM.** Equation (2.21) is the algebraic, a.k.a. ROM, equivalent of (2.12). The ROM snapshots are the  $n_t n_{\mathcal{E}} \times n_{\mathcal{E}}$  matrices defined by

(2.30) 
$$\boldsymbol{\varphi}_{j}^{\text{ROM}} = \boldsymbol{R}\boldsymbol{g}_{j}, \qquad j \ge 0,$$

and due to the block Cholesky factorization (2.27), they satisfy the time stepping equation

(2.31) 
$$\boldsymbol{\varphi}_{j+1}^{\text{ROM}} = \boldsymbol{\mathcal{P}}^{\text{ROM}} \boldsymbol{\varphi}_{j}^{\text{ROM}}, \qquad j \ge 0,$$

driven by the ROM propagator matrix

$$(2.32) \qquad \qquad \mathcal{P}^{\text{ROM}} = \mathbf{R}^{-T} \mathbb{S} \mathbf{R}^{-1}.$$

This is a projection ROM: According to (2.15)-(2.16), the ROM snapshots are the projection of the Galerkin approximation of the snapshots of the wave field,

(2.33) 
$$\boldsymbol{\varphi}_{j}^{\text{ROM}} = \boldsymbol{R}\boldsymbol{g}_{j} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{V}^{T}(\boldsymbol{x}) \boldsymbol{\Phi}(\boldsymbol{x}) \boldsymbol{g}_{j} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{V}^{T}(\boldsymbol{x}) \boldsymbol{\varphi}_{j}^{\text{GAL}}(\boldsymbol{x}), \qquad j \ge 0,$$

and from (2.23) we get

(2.34) 
$$\boldsymbol{\mathcal{P}}^{\text{ROM}} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{R}^{-T} [\boldsymbol{V}(\boldsymbol{x})\boldsymbol{R}]^{T} \boldsymbol{\mathcal{P}} [\boldsymbol{V}(\boldsymbol{x})\boldsymbol{R}] \boldsymbol{R}^{-1} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{V}^{T}(\boldsymbol{x}) \boldsymbol{\mathcal{P}} \boldsymbol{V}(\boldsymbol{x}).$$

**2.4.** Data driven ROM. From the ROM definition above, it appears that its computation requires the matrix  $\Phi$  of snapshots. The next theorem states that the ROM is data driven.

Theorem 2.2. The ROM can be computed directly from the array response matrix (2.3) that defines the "data matrices"

(2.35) 
$$\boldsymbol{D}_j = \boldsymbol{A}(t_j) + \boldsymbol{A}^T(-t_j), \qquad j \ge 0.$$

The data matrices satisfy

(2.36) 
$$\boldsymbol{D}_{j} = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_{0}^{T}(\boldsymbol{x}) \boldsymbol{\varphi}_{j}(\boldsymbol{x})$$

(2.37) 
$$= (\boldsymbol{\varphi}_0^{\text{ROM}})^T \boldsymbol{\varphi}_j^{\text{ROM}}, \qquad j = 0, \dots, n_t - 1,$$

where the second equality means that the ROM interpolates the measurements on the uniform time grid. The ROM is computed from  $\{D_j\}_{j=0}^{n_t}$  and its propagator matrix (2.32) has an unreduced, upper Hessenberg block structure.

*Proof.* The proof of (2.36) follows, basically, from energy conservation. Recall definition (2.7) of  $\varphi$  and define the matrix

(2.38) 
$$\boldsymbol{Q}(t;t_j) = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\psi}^T(t+\tau,\boldsymbol{x}) \boldsymbol{\psi}(t+t_j+\tau,\boldsymbol{x}).$$

The trace of  $Q(\cdot; t_0 = 0)$  is the total energy of the system at time  $t + \tau$  for all excitations. According to (2.7), we have

(2.39) 
$$\boldsymbol{Q}(0;t_j) = \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_0^T(\boldsymbol{x}) \boldsymbol{\varphi}_j(\boldsymbol{x}).$$

The time derivative of (2.38) is

$$\partial_{t}\boldsymbol{Q}(t;t_{j}) = \int_{\Omega} d\boldsymbol{x} \left[ \partial_{t}\boldsymbol{\psi}^{T}(t+\tau)\boldsymbol{\psi}(t+t_{j}+\tau,\boldsymbol{x}) + \boldsymbol{\psi}^{T}(t+\tau)\partial_{t}\boldsymbol{\psi}(t+t_{j}+\tau,\boldsymbol{x}) \right] \\ \stackrel{(2.1)}{=} \int_{\Omega} d\boldsymbol{x} \left\{ \left[ -\mathcal{L}\boldsymbol{\psi}(t+\tau,\boldsymbol{x}) + \boldsymbol{f}(t+\tau,\boldsymbol{x}) \right]^{T} \boldsymbol{\psi}(t+t_{j}+\tau,\boldsymbol{x}) + \boldsymbol{\psi}^{T}(t+\tau,\boldsymbol{x}) \left[ -\mathcal{L}\boldsymbol{\psi}(t+t_{j}+\tau,\boldsymbol{x}) + \boldsymbol{f}(t+t_{j}+\tau,\boldsymbol{x}) \right] \right\} \\ + \boldsymbol{\psi}^{T}(t+\tau,\boldsymbol{x}) \left[ -\mathcal{L}\boldsymbol{\psi}(t+t_{j}+\tau,\boldsymbol{x}) + \boldsymbol{f}(t+t_{j}+\tau,\boldsymbol{x}) \right] \right\}$$

$$(2.40) \qquad \qquad = \int_{\Omega} d\boldsymbol{x} \left\{ \boldsymbol{f}^{T}(t+\tau,\boldsymbol{x})\boldsymbol{\psi}(t+t_{j}+\tau,\boldsymbol{x}) + \boldsymbol{\psi}^{T}(t+\tau,\boldsymbol{x})\boldsymbol{f}(t+t_{j}+\tau,\boldsymbol{x}) \right\} ,$$

where we used that  $\mathcal{L}$  is skew-adjoint. Integrating in t and evaluating at t = 0 we get

$$Q(0;t_j) = \int_{-\infty}^{0} dt \int_{\Omega} d\boldsymbol{x} \left\{ \boldsymbol{f}^T(t+\tau,\boldsymbol{x})\boldsymbol{\psi}(t+t_j+\tau,\boldsymbol{x}) + \boldsymbol{\psi}^T(t+\tau,\boldsymbol{x})\boldsymbol{f}(t+t_j+\tau,\boldsymbol{x}) \right\}$$
$$= \int_{-\tau}^{\infty} \int_{\Omega} \boldsymbol{f}^T(-t',\boldsymbol{x})\boldsymbol{\psi}(t_j-t',\boldsymbol{x})d\boldsymbol{x}dt'$$
$$(2.41) \qquad + \int_{-\tau-t_j}^{\infty} \int_{\Omega} \boldsymbol{\psi}^T(-t_j-t'',\boldsymbol{x})\boldsymbol{f}(-t'',\boldsymbol{x})d\boldsymbol{x}dt'',$$

where we made the change of variables  $t + \tau = -t'$  and  $t + t_j + \tau = -t''$ . Since the source is supported in time in the interval  $(-t_s, t_s)$  and  $\tau \ge t_s$ , we observe from definition (2.3) that (2.42)

## REDUCED ORDER MODELING FOR INVERSE SCATTERING

the right-hand side in (2.41) equals the matrix  $D_j = A(t_j) + A^T(-t_j)$  defined in (2.35). The proof of (2.36) follows from (2.39).

Next, we show that the mass matrix is data driven. Writing its definition (2.22) block by block we get, for  $0 \le j \le l \le n_t - 1$ , that

$$egin{aligned} \mathbb{M}_{j,l} &= \int_\Omega doldsymbol{x} \, oldsymbol{arphi}_j^T(oldsymbol{x}) oldsymbol{arphi}_l(oldsymbol{x}) \ &= \int_\Omega doldsymbol{x} \, oldsymbol{arphi}_l^T(oldsymbol{x}) e^{-(t_l-t_j)\mathcal{L}} oldsymbol{arphi}_0(oldsymbol{x}) \ &= \int_\Omega doldsymbol{x} \, oldsymbol{arphi}_0^T(oldsymbol{x}) e^{-(t_l-t_j)\mathcal{L}} oldsymbol{arphi}_0$$

Here we used that  $e^{-t\mathcal{L}}$  is a unitary semigroup, since  $\mathcal{L}$  is skew-adjoint. It is obvious from the definition (2.22) that  $\mathbb{M}$  is symmetric, so the blocks below the diagonal are

(2.43) 
$$\mathbb{M}_{j,l} = (\mathbb{M}_{l,j})^T, \quad 0 \le l < j \le n_t - 1.$$

The stiffness matrix is also data driven: Starting from definition (2.23), we get

(2.44)  
$$\begin{split} \mathbb{S}_{j,l} &= \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_{j}^{T}(\boldsymbol{x}) \mathcal{P} \boldsymbol{\varphi}_{l}(\boldsymbol{x}) \\ &\stackrel{(2.12)}{=} \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_{j}^{T}(\boldsymbol{x}) \boldsymbol{\varphi}_{l+1}(\boldsymbol{x}) \\ &= \boldsymbol{D}_{l+1-j} \end{split}$$

for  $0 \le j \le l \le n_t - 1$ . Unlike the mass matrix,  $\mathbb{S}$  is not symmetric. However, we can calculate its remaining blocks, indexed by  $0 \le l < j - 1$ , with  $j = 2, \ldots, n_t - 1$ , as follows:

(2.45)  

$$\begin{split} \mathbb{S}_{j,l} &= \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_{j}^{T}(\boldsymbol{x}) \mathcal{P} \boldsymbol{\varphi}_{l}(\boldsymbol{x}) \\ &= \int_{\Omega} d\boldsymbol{x} \, [\mathcal{P}^{T} \boldsymbol{\varphi}_{j}(\boldsymbol{x})]^{T} \boldsymbol{\varphi}_{l}(\boldsymbol{x}) \\ &= \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_{j-1}^{T}(\boldsymbol{x}) \boldsymbol{\varphi}_{l}(\boldsymbol{x}) \\ &= \left[ \int_{\Omega} d\boldsymbol{x} \, \boldsymbol{\varphi}_{l}^{T}(\boldsymbol{x}) \boldsymbol{\varphi}_{j-1}(\boldsymbol{x}) \right]^{T} \\ &= \boldsymbol{D}_{j-1-l}^{T}. \end{split}$$

To prove the data interpolation relations (2.37), we deduce from (2.25) and (2.30) that

(2.46) 
$$\boldsymbol{R} = \left(\boldsymbol{\varphi}_0^{\text{ROM}}, \dots, \boldsymbol{\varphi}_{n_t-1}^{\text{ROM}}\right)$$

Since  $\boldsymbol{R}$  is the block Cholesky square root of  $\mathbb{M}$ , we have

(2.47) 
$$\boldsymbol{D}_{j} \stackrel{(2.42)}{=} \mathbb{M}_{0,j} = \boldsymbol{i}_{0}^{T} \mathbb{M} \boldsymbol{i}_{j} = \boldsymbol{i}_{0}^{T} \boldsymbol{R}^{T} \boldsymbol{R} \boldsymbol{i}_{j} = (\boldsymbol{\varphi}_{0}^{\text{ROM}})^{T} \boldsymbol{\varphi}_{j}^{\text{ROM}}$$

for  $j = 0, ..., n_t - 1$ , as stated in (2.37).

It remains to prove the algebraic structure of the propagator ROM. We use (2.46) and the iteration (2.31). If we denote the  $n_{\mathcal{E}} \times n_{\mathcal{E}}$ , no-zero blocks of  $\mathbf{R}$  by  $\mathbf{R}_{j,l}$ , for  $0 \le j \le l \le n_t - 1$ , we get from (2.31) evaluated at j = 0 that the first column of blocks of  $\mathcal{P}^{\text{ROM}}$  satisfies

$$\boldsymbol{\varphi}_{1}^{\text{ROM}} = \begin{pmatrix} \boldsymbol{R}_{0,1} \\ \boldsymbol{R}_{1,1} \\ \boldsymbol{0} \\ \vdots \\ \boldsymbol{0} \end{pmatrix} = \boldsymbol{\mathcal{P}}^{\text{ROM}} \boldsymbol{\varphi}_{0}^{\text{ROM}} = \begin{pmatrix} \boldsymbol{\mathcal{P}}_{0,0}^{\text{ROM}} \\ \boldsymbol{\mathcal{P}}_{1,0}^{\text{ROM}} \\ \boldsymbol{\mathcal{P}}_{2,0}^{\text{ROM}} \\ \vdots \\ \boldsymbol{\mathcal{P}}_{n_{t}-1,0}^{\text{ROM}} \end{pmatrix} \boldsymbol{R}_{0,0}$$

Assumption 1 ensures that  $\mathbb{M}$  and therefore  $\mathbf{R}$  are invertible, which makes all the diagonal blocks of  $\mathbf{R}$  invertible. Thus, we have

$$\mathcal{P}_{l,0}^{\text{ROM}} \boldsymbol{R}_{0,0} = \boldsymbol{0} \quad \rightsquigarrow \quad \mathcal{P}_{l,0}^{\text{ROM}} = \boldsymbol{0}, \qquad 2 \le l \le n_{t-1},$$

and

$$\mathcal{P}_{1,0}^{\text{ROM}} \boldsymbol{R}_{0,0} = \boldsymbol{R}_{1,1} \quad \rightsquigarrow \quad \mathcal{P}_{1,0}^{\text{ROM}} \neq \boldsymbol{0}.$$

Now proceed inductively for  $j \ge 1$ , under the hypothesis that for j = 0, ..., J, with  $J \le n_t - 2$ , we have  $\mathcal{P}_{j+1,j}^{\text{ROM}} \neq \mathbf{0}$  and

(2.48) 
$$\mathcal{P}_{l,j}^{\text{ROM}} = \mathbf{0}, \qquad j+2 \le l \le n_{t-1}.$$

Then, (2.31) evaluated at j = J gives

$$\boldsymbol{\varphi}_{J+1}^{\text{ROM}} = \begin{pmatrix} \boldsymbol{R}_{0,J+1} \\ \boldsymbol{R}_{1,J+1} \\ \vdots \\ \boldsymbol{R}_{J+1,J+1} \\ \boldsymbol{0} \\ \vdots \\ \boldsymbol{0} \end{pmatrix} = \begin{pmatrix} \mathcal{P}_{0,J}^{\text{ROM}} \\ \mathcal{P}_{1,J}^{\text{ROM}} \\ \mathcal{P}_{2,J}^{\text{ROM}} \\ \vdots \\ \mathcal{P}_{n,t-1,J}^{\text{ROM}} \end{pmatrix} \boldsymbol{R}_{J,J} + \sum_{l=0}^{J-1} \begin{pmatrix} \mathcal{P}_{0,l}^{\text{ROM}} \\ \mathcal{P}_{1,l}^{\text{ROM}} \\ \mathcal{P}_{2,l}^{\text{ROM}} \\ \vdots \\ \mathcal{P}_{l+1,l}^{\text{ROM}} \\ \boldsymbol{0} \\ \vdots \\ \boldsymbol{0} \end{pmatrix} \boldsymbol{R}_{l,J}.$$

Equating the entries in the *l*th rows, with l > J + 1, and using that  $\mathbf{R}_{J,J}$  is invertible, we deduce that the induction hypothesis equation (2.48) extends to J, as well. We also have that

$$\mathcal{P}_{J+1,J}^{\text{ROM}} \boldsymbol{R}_{J,J} = \boldsymbol{R}_{J+1,J+1} \quad \rightsquigarrow \quad \mathcal{P}_{J+1,J}^{\text{ROM}} \neq \boldsymbol{0}.$$

The induction argument terminates at  $j = n_t - 2$  and proves that  $\mathcal{P}^{\text{ROM}}$  has unreduced block upper Hessenberg structure.

*Remark* 2.3. Definition (2.35) shows that if there is reciprocity in the response of the medium, i.e., if A is symmetric, then the data matrices  $D_j$  are symmetric and we can drop the transpose in (2.45). We show in section 3 that reciprocity holds in the case of acoustic waves.

Remark 2.4. The second term in definition (2.35) contributes only at the very early time instants  $t_j \leq 2t_s$ , due to causality. Indeed, at later instants, satisfying  $t_j > 2t_s$ , we have  $\psi^T(-t_j - t, \mathbf{x}) = \mathbf{0}$  in the integral, because  $-t_j - t \in (-t_j - t_s, -t_j + t_s)$  does not intersect the time interval  $(-t_s, \infty)$  where the wave is supported.

**2.5.** Properties of the ROM. The calculations above reveal two important aspects of the ROM that account for the action of the unitary semigroup  $e^{-t\mathcal{L}}$  generated by  $\mathcal{L}$ :

1. The mass matrix  $\mathbb{M}$  is symmetric, with block Toeplitz structure. Its main diagonal contains the initial data matrix  $D_0$ , which is symmetric by (2.36) evaluated at j = 0. The other diagonals contain the data matrices  $D_j$  for  $j = 1, \ldots, n_t - 1$ , respectively. The stiffness matrix  $\mathbb{S}$  is also block Toeplitz, but its diagonals are shifted. The initial data blocks  $D_0$  appear in the first subdiagonal, the main diagonal contains the data matrix  $D_1$ , and the remaining upper diagonals have the blocks  $D_j$  for  $j = 2, \ldots, n_t$ .

2. The ROM propagator  $\mathcal{P}^{\text{ROM}}$  preserves the unitary structure of the true wave propagator operator  $\mathcal{P} = \exp(-\Delta t \mathcal{L})$ . To see this, let us write the iteration (2.12) backward in time, using that  $\mathcal{P}$  is unitary,

(2.49) 
$$\boldsymbol{\varphi}_{j}(\boldsymbol{x}) = \mathcal{P}^{T} \boldsymbol{\varphi}_{j+1}(\boldsymbol{x}), \qquad j \ge 0$$

The Galerkin approximation of this equation, in the same space used before, has the snapshots

(2.50) 
$$\boldsymbol{\varphi}_{j}^{\text{GAL},-}(\boldsymbol{x}) = \boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{g}_{j}^{-}, \qquad j \ge 0,$$

where the superscript "-" reminds us that the stepping is backward in time and the coefficient matrices  $g_i^-$  satisfy, similar to (2.20),

(2.51) 
$$\int_{\Omega} d\boldsymbol{x} \boldsymbol{V}^{T}(\boldsymbol{x}) [\boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{g}_{j}^{-} - \mathcal{P}^{T}\boldsymbol{\Phi}(\boldsymbol{x})\boldsymbol{g}_{j+1}^{-}] = \boldsymbol{R}\boldsymbol{g}_{j}^{-} - (\boldsymbol{\mathcal{P}}^{\text{ROM}})^{T}\boldsymbol{R}\boldsymbol{g}_{j+1}^{-} = \boldsymbol{0}, \qquad j \ge 0.$$

Here we used the Gram–Schmidt equation (2.16) and the identity

(2.52) 
$$\int_{\Omega} d\boldsymbol{x} \boldsymbol{V}^{T}(\boldsymbol{x}) \mathcal{P}^{T} \boldsymbol{V}(\boldsymbol{x}) = \left[ \int_{\Omega} d\boldsymbol{x} \boldsymbol{V}^{T}(\boldsymbol{x}) \mathcal{P} \boldsymbol{V}(\boldsymbol{x}) \right]^{T} \stackrel{(2.34)}{=} (\boldsymbol{\mathcal{P}}^{\text{ROM}})^{T}.$$

The ROM snapshots for the backward iteration are

(2.53) 
$$\boldsymbol{\varphi}_{j}^{\text{ROM},-} = \boldsymbol{R}\boldsymbol{g}_{j}^{-}, \qquad j \ge 0,$$

and they evolve according to the transpose of the ROM propagator matrix

(2.54) 
$$\boldsymbol{\varphi}_{j}^{\text{ROM},-} = (\boldsymbol{\mathcal{P}}^{\text{ROM}})^{T} \boldsymbol{\varphi}_{j+1}^{\text{ROM},-}, \qquad j \ge 0.$$

This is the (ROM) algebraic form of (2.49).

Note that the ROM snapshots for the forward and backward iterations coincide at the first time instants because the same reasoning that leads to (2.25) applies to the Galerkin approximation (2.50). We get

(2.55) 
$$\boldsymbol{g}_{j}^{-} = \boldsymbol{g}_{j} = \boldsymbol{i}_{j} \quad \rightsquigarrow \quad \boldsymbol{\varphi}_{j}^{\text{ROM}} = \boldsymbol{\varphi}_{j}^{\text{ROM},-}, \qquad j = 0, \dots, n_{t} - 1,$$

so the ROM propagator behaves as a unitary matrix for the first  $n_t$  snapshots. More explicitly, if we substitute (2.31) into (2.54) and use (2.55), we get

$$\begin{bmatrix} \boldsymbol{I}_{n_t n_{\mathcal{E}}} - \boldsymbol{\mathcal{P}}^{\text{ROM}T} \boldsymbol{\mathcal{P}}^{\text{ROM}} \end{bmatrix} \begin{pmatrix} \boldsymbol{R}_{0,0} & \boldsymbol{R}_{0,1} & \boldsymbol{R}_{0,2} & \dots & \boldsymbol{R}_{0,n_t-2} \\ \boldsymbol{0} & \boldsymbol{R}_{1,1} & \boldsymbol{R}_{1,2} & \dots & \boldsymbol{R}_{1,n_t-2} \\ & \vdots & & \\ \boldsymbol{0} & \boldsymbol{0} & \dots & \boldsymbol{0} & \boldsymbol{R}_{n_t-2,n_t-2} \\ \boldsymbol{0} & \boldsymbol{0} & \dots & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} = \boldsymbol{0} \in \mathbb{R}^{n_t n_{\mathcal{E}} \times (n_t-1)n_{\mathcal{E}}}.$$

Because the diagonal blocks of  $\boldsymbol{R}$  are invertible, we deduce from this equation that the first  $n_t - 1$  columns of  $(\boldsymbol{\mathcal{P}}^{\text{ROM}})^T \boldsymbol{\mathcal{P}}^{\text{ROM}}$  equal those of the identity matrix.

**3.** Acoustic waves. In this section we specialize the ROM to acoustic waves, governed by the first order hyperbolic system

(3.1) 
$$\partial_t \boldsymbol{u}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) + \rho^{-1}(\boldsymbol{x}) \nabla p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = \frac{s(t)}{\sqrt{\zeta_o}} \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}),$$

(3.2) 
$$\partial_t p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) + K(\boldsymbol{x}) \nabla \cdot \boldsymbol{u}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = 0,$$

satisfied at  $\boldsymbol{x} \in \Omega$  and  $t \in \mathbb{R}$ , by the acoustic pressure  $p_{\boldsymbol{\epsilon}}$  and velocity  $\boldsymbol{u}_{\boldsymbol{\epsilon}}$ , indexed by  $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2) \in \mathbb{N}^2$  (see Figure 3.1). Here the medium is modeled by the variable and unknown density  $\rho$  and bulk modulus K, which determine the wave speed



**Figure 3.1.** Illustration of the acoustic setup for inverse scattering with polarized excitations  $F_{\epsilon}(x)$ . The inversion domain is shown in darker blue and is surrounded by a homogeneous reference medium. The sensors are placed above this domain and generate waves with d different polarizations (here d = 2).

(3.3) 
$$c(\boldsymbol{x}) = \sqrt{\frac{K(\boldsymbol{x})}{\rho(\boldsymbol{x})}}$$

and the wave impedance

(3.4) 
$$\zeta(\boldsymbol{x}) = \sqrt{K(\boldsymbol{x})\rho(\boldsymbol{x})}.$$

The reference values of the coefficients are the constants  $\rho_o, K_o, c_o$ , and  $\zeta_o$ , respectively. These model the homogeneous medium near the sensors in the array.

**3.1. Derivation of the first order system (2.1).** The theory in the previous section was done for arbitrary forcing. For its application to acoustics, we assume a separable force function, which is typical in phased array data acquisitions. Thus, the right-hand side in (3.1) consists of the pulsed signal s, supported at  $t \in (-t_s, t_s)$ , and

(3.5) 
$$\boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}) \approx \delta(\boldsymbol{x} - \boldsymbol{x}_{\epsilon_1})\boldsymbol{e}_{\epsilon_2},$$

where  $\boldsymbol{x}_{\epsilon_1}$  is the location of the  $\epsilon_1$ th sensor and  $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_d$  is the canonical orthonormal basis in  $\mathbb{R}^d$ . The approximation means that  $\boldsymbol{F}_{\boldsymbol{\epsilon}}$  is an  $\boldsymbol{L}^2(\Omega)$  function normalized by

(3.6) 
$$\int_{\Omega} d\boldsymbol{x} \, \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}) = \boldsymbol{e}_{\boldsymbol{\epsilon}_2},$$

and supported in a ball centered at  $x_{\epsilon_1}$ , with small radius with respect to the wavelength. The scaling of the force by  $\zeta_o^{-1/2}$  in (3.1) is to simplify the formulas below. We model the boundary of the domain as sound soft,

$$(3.7) p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = 0, t \in \mathbb{R}, \ \boldsymbol{x} \in \partial \Omega$$

and suppose that the medium is quiescent prior to the excitation,

(3.8) 
$$p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = 0, \quad \boldsymbol{u}_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = \boldsymbol{0}, \quad t \ll 0, \ \boldsymbol{x} \in \Omega.$$

The hyperbolic system (3.1)–(3.2) can be put in the desired form (2.1) by defining the following m = d + 1 dimensional wave field:

(3.9) 
$$\boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x}) = \sqrt{c_o} \left( \frac{\sqrt{\rho(\boldsymbol{x})} \boldsymbol{u}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x})}{\frac{1}{\sqrt{K(\boldsymbol{x})}} p_{\boldsymbol{\epsilon}}(t,\boldsymbol{x})} \right).$$

We obtain (2.1) with the skew-adjoint operator

(3.10) 
$$\mathcal{L} = \begin{pmatrix} 0 & \frac{1}{\sqrt{\rho(\boldsymbol{x})}} \operatorname{grad} \left[ c(\boldsymbol{x})\sqrt{\rho(\boldsymbol{x})} \cdot \right] \\ c(\boldsymbol{x})\sqrt{\rho(\boldsymbol{x})} \operatorname{div} \left[ \frac{1}{\sqrt{\rho(\boldsymbol{x})}} \cdot \right] & 0 \end{pmatrix}$$

and the force

(3.11) 
$$\boldsymbol{f}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x}) = s(t) \begin{pmatrix} \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}) \\ 0 \end{pmatrix}.$$

**3.2. The data.** The variable coefficients in  $\mathcal{L}$ , written in terms of the wave speed c and density  $\rho$ , are the unknowns, to be determined from the measured array response matrix A. The entries (2.3) of this matrix are

$$(3.12) \qquad \mathbf{A}_{\boldsymbol{\epsilon}',\boldsymbol{\epsilon}}(t) \stackrel{(3.11)}{=} \int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \, s(-t') \begin{pmatrix} \boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x}) \\ 0 \end{pmatrix}^T \boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}) \\ \stackrel{(3.9)}{=} \int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \sqrt{c_o} \sqrt{\rho(\boldsymbol{x})} s(-t') \boldsymbol{F}_{\boldsymbol{\epsilon}'}^T(\boldsymbol{x}) \boldsymbol{u}_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}), \\ \approx \int_{-t_s}^{t_s} dt' \sqrt{\zeta_o} \boldsymbol{e}_{\boldsymbol{\epsilon}'_2}^T s(-t') \boldsymbol{u}_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}_{\boldsymbol{\epsilon}'_1}), \end{cases}$$

where the approximation is due to (3.5) and the assumption  $\rho(\boldsymbol{x}_{\epsilon_1}) = \rho_o$ . Thus, the array measures the velocity at the sensor locations. These measurements can be related to measurements of the pressure using the divergence theorem,

$$\int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \, s(-t') \, \operatorname{div} \, [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x})] p_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x})$$

$$= \int_{-t_s}^{t_s} dt' s(-t') \int_{\Omega} d\boldsymbol{x} \, \operatorname{div} \, [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x}) p_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x})]$$

$$- \int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \, [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x})]^T \, s(-t') \nabla p_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x})$$

$$\stackrel{(3.1)}{=} - \int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \, [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x})]^T \, s(-t') \left[ \frac{s(t-t')\rho_o}{\sqrt{\zeta_o}} \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}) - \rho(\boldsymbol{x})\partial_t \boldsymbol{u}_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}) \right]$$

$$(3.13) \qquad = \frac{\rho_o}{\sqrt{\zeta_o}} \left[ \frac{d}{dt} \boldsymbol{A}_{\boldsymbol{\epsilon}',\boldsymbol{\epsilon}}(t) - \int_{-t_s}^{t_s} dt' s(-t') s(t-t') \int_{\Omega} d\boldsymbol{x} \, [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x})]^T \, \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}) \right].$$

Here we used the boundary condition (3.7) and that  $\rho = \rho_o$  at the array. Note that the last term in the right-hand side of this equation vanishes when  $\epsilon'_1 \neq \epsilon_1$ , because the two forces have disjoint support. Note also that given our model (2.5) of the force, the derivative of the array response matrix gives approximately the components of the gradient of pressure at the array

(3.14) 
$$\int_{-t_s}^{t_s} dt' \int_{\Omega} d\boldsymbol{x} \, s(-t') \, \operatorname{div} \, [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x})] p_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}) \\ \stackrel{(3.5)}{\approx} \int_{\Omega} d\boldsymbol{x} \, \partial_{x_{\boldsymbol{\epsilon}'_2}} \delta(\boldsymbol{x}-\boldsymbol{x}_{\boldsymbol{\epsilon}'_1}) \int_{-t_s}^{t_s} dt' s(-t') p_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}) \\ = -\int_{-t_s}^{t_s} dt' s(-t') \partial_{x_{\boldsymbol{\epsilon}'_2}} p_{\boldsymbol{\epsilon}}(t-t',\boldsymbol{x}_{\boldsymbol{\epsilon}'_1}).$$

Suppose that the array is planar and that we measure the components of the velocity in the normal direction to the array. The calculation above says that this is basically the same as measuring the normal derivative of the pressure at the array. This is not enough information for solving the inverse problem, so we need to measure the velocity in the plane of the array, as well.

We end this section with the proof of reciprocity (symmetry of A), mentioned in Remark 2.3. Equation (3.13) shows that A is symmetric if the pressure field satisfies

(3.15) 
$$\int_{\Omega} d\boldsymbol{x} \operatorname{div} [\boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x})] p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = \int_{\Omega} d\boldsymbol{x} \operatorname{div} [\boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x})] p_{\boldsymbol{\epsilon}'}(t, \boldsymbol{x}) \qquad \forall \, \boldsymbol{\epsilon}, \boldsymbol{\epsilon}' \in \mathcal{E}$$

Equations (3.1)–(3.2) give that  $p_{\epsilon}$  satisfies the second order wave equation

(3.16) 
$$\partial_t^2 p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) - K(\boldsymbol{x}) \operatorname{div} \left[ \rho^{-1}(\boldsymbol{x}) \nabla p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) \right] = -c_o \frac{d}{dt} s(t) \operatorname{div} \left[ \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{x}) \right]$$

with homogeneous Dirichlet boundary condition at  $\partial \Omega$ . If we let G be the Green's function for the wave operator in this equation, we get that

(3.17) 
$$p_{\boldsymbol{\epsilon}}(t, \boldsymbol{x}) = c_o \frac{d}{dt} s(t) \star_t \int_{\Omega} d\boldsymbol{y} \, G(t, \boldsymbol{x}, \boldsymbol{y}) \, \operatorname{div} \left[ \boldsymbol{F}_{\boldsymbol{\epsilon}}(\boldsymbol{y}) \right],$$

where  $\star_t$  denotes convolution in time. It is known that G satisfies the reciprocity relation  $G(t, \boldsymbol{x}, \boldsymbol{y}) = G(t, \boldsymbol{y}, \boldsymbol{x})$  (see, for example, [24]). Therefore, (3.17) implies that (3.15) holds.

4. Multiparametric inversion. If we knew the wave field inside the domain  $\Omega$ , it would be easy to estimate c and  $\rho$ . This is precisely the point of hybrid (multiphysics) imaging modalities [2] that use one kind of wave to probe the medium and then measure the propagation of another wave. Hybrid methods require complex equipment and controlled measurement settings that cannot be implemented in general environments. Here we use the ROM to map the measurements at the array to a good approximation of the vectorial wave field inside  $\Omega$ .

The basic idea for obtaining such a map comes from the Gram–Schmidt equation (2.16), which factorizes the unknown snapshots contained in  $\boldsymbol{\Phi}$  in the data driven ROM snapshots, the block columns of  $\boldsymbol{R}$ , and the uncomputable orthonormal basis in  $\boldsymbol{V}$ . We know from Theorem 2.2 that the ROM snapshots satisfy the exact data fitting relation (2.37), just like the true snapshots. This means that all the information registered at the array is contained in the ROM snapshots. The uncomputable basis  $\boldsymbol{V}$  plays no role in the data fitting. Indeed, (2.16), (2.34), and (2.46) give

$$(4.1) \qquad \mathbf{D}_{j} = \int_{\Omega} d\mathbf{x} \, \boldsymbol{\varphi}_{0}^{T}(\mathbf{x}) \boldsymbol{\varphi}_{j}(\mathbf{x}) = \int_{\Omega} d\mathbf{x} \, [\mathbf{V}(\mathbf{x}) \boldsymbol{\varphi}_{0}^{\text{ROM}}]^{T} \, \mathbf{V}(\mathbf{x}) \boldsymbol{\varphi}_{j}^{\text{ROM}}$$
$$= (\boldsymbol{\varphi}_{0}^{\text{ROM}})^{T} \underbrace{\int_{\Omega} d\mathbf{x} \, \mathbf{V}^{T}(\mathbf{x}) \mathbf{V}(\mathbf{x})}_{I_{n_{t}n_{\mathcal{E}}}} \boldsymbol{\varphi}_{j}^{\text{ROM}} = (\boldsymbol{\varphi}_{0}^{\text{ROM}})^{T} \boldsymbol{\varphi}_{j}^{\text{ROM}}, \qquad j = 0, \dots, n_{t} - 1,$$

and the same result holds when replacing  $\boldsymbol{V}$  with any orthonormal basis. That is to say, if we define

(4.2) 
$$\widetilde{\boldsymbol{\varphi}}_{j}(\boldsymbol{x};\widetilde{c},\widetilde{\rho}) = \boldsymbol{V}(\boldsymbol{x};\widetilde{c},\widetilde{\rho})\boldsymbol{\varphi}_{j}^{\text{ROM}}, \qquad j = 0, \dots, n_{t} - 1,$$

with  $V(\cdot; \tilde{c}, \tilde{\rho})$  the orthonormal basis computed via the Gram–Schmidt procedure in the medium with search wave speed  $\tilde{c}$  and density  $\tilde{\rho}$ , we get, similar to (4.1), the exact data fit

(4.3)  
$$\int_{\Omega} d\boldsymbol{x} \, \widetilde{\boldsymbol{\varphi}}_{0}^{T}(\boldsymbol{x}; \widetilde{c}, \widetilde{\rho}) \widetilde{\boldsymbol{\varphi}}_{j}(\boldsymbol{x}; \widetilde{c}, \widetilde{\rho}) = (\boldsymbol{\varphi}_{0}^{\text{ROM}})^{T} \underbrace{\int_{\Omega} d\boldsymbol{x} \, \widetilde{\boldsymbol{V}}^{T}(\boldsymbol{x}; \widetilde{c}, \widetilde{\rho}) \boldsymbol{V}(\boldsymbol{x}; \widetilde{c}, \widetilde{\rho})}_{\boldsymbol{I}_{n_{t}n_{\mathcal{E}}}} \boldsymbol{\varphi}_{j}^{\text{ROM}} = (\boldsymbol{\varphi}_{0}^{\text{ROM}})^{T} \boldsymbol{\varphi}_{j}^{\text{ROM}} = \boldsymbol{D}_{j}, \qquad j = 0, \dots, n_{t} - 1.$$

The basis V maps the information registered at the array and contained in the ROM snapshots, from the algebraic (ROM) space to the physical space, at  $\boldsymbol{x} \in \Omega$ . Its computation requires knowing the medium. Thus, we define our approximation of the internal wave by (4.2), where the uncomputable V is replaced by the basis in our best guess of the medium, modeled by  $\tilde{c}$  and  $\tilde{\rho}$ . While this internal wave is consistent with the data, as shown above, it is not a solution of the hyperbolic system of equations. Assuming that the inverse problem is uniquely solvable [6], this would be the case only when  $\tilde{c}$  and  $\tilde{\rho}$  are equal to the true wave speed and density.

Therefore, our inversion approach seeks to minimize the discrepancy  $\mathcal{O}(\tilde{c},\tilde{\rho})$  between the estimated internal waves (4.2) and the solution of the wave equation, whose first  $n_t$  snapshots are gathered in  $V(\cdot;\tilde{c},\tilde{\rho})\mathbf{R}(\tilde{c},\tilde{\rho})$ , similar to (2.16). The objective function is

$$\mathcal{O}(\widetilde{c},\widetilde{\rho}) = \sum_{j=0}^{n_t-1} \int_{\Omega} d\boldsymbol{x} \| \widetilde{\boldsymbol{\varphi}}_j(\boldsymbol{x};\widetilde{c},\widetilde{\rho}) - \boldsymbol{\varphi}_j(\boldsymbol{x};\widetilde{c},\widetilde{\rho}) \|_F^2$$
  
$$= \int_{\Omega} d\boldsymbol{x} \| \boldsymbol{V}(\boldsymbol{x};\widetilde{c},\widetilde{\rho})\boldsymbol{R} - \boldsymbol{V}(\boldsymbol{x};\widetilde{c},\widetilde{\rho})\boldsymbol{R}(\widetilde{c},\widetilde{\rho}) \|_F^2$$
  
$$= \| \boldsymbol{R} - \boldsymbol{R}(\widetilde{c},\widetilde{\rho}) \|_F^2,$$

where  $\|\cdot\|_F$  is the Frobenius norm,  $\mathbf{R}$  without an argument is the data driven matrix containing the ROM snapshots, and  $\mathbf{R}(\tilde{c},\tilde{\rho})$  is the block Cholesky square root of the mass matrix computed in the guess medium with wave speed  $\tilde{c}$  and density  $\tilde{\rho}$ . The contribution of  $\mathbf{V}(\cdot;\tilde{c},\tilde{\rho})$ cancels out in (4.4) by the definition of the Frobenius norm and orthonormality. Thus, we are left with minimizing the misfit of the block Cholesky square root of the mass matrix.

Instead of working with (4.4), we minimize the objective function

(4.5) 
$$\mathcal{O}^{\text{ROM}}(\widetilde{c},\widetilde{\rho}) = \|\boldsymbol{R}(\widetilde{c},\widetilde{\rho})\boldsymbol{R}^{-1} - \boldsymbol{I}_{n_t n_{\mathcal{E}}}\|_F^2$$

This works better because by taking the inverse of  $\mathbf{R}$  we balance the contribution of the strong and weak echoes registered in the data  $\{\mathbf{D}_j\}_{j=0}^{n_t-1}$ .

**4.1. The inversion algorithm.** To formulate the algorithm, we need to specify the search space where  $\tilde{c}$  and  $\tilde{\rho}$  lie. We parameterize  $\tilde{c}$  and  $\tilde{\rho}$  as

(4.6) 
$$\widetilde{c}(\boldsymbol{x};\boldsymbol{\eta}) = c_o + \sum_{l=1}^N \eta_l \beta_l(\boldsymbol{x}), \qquad \widetilde{\rho}(\boldsymbol{x};\boldsymbol{\eta}) = \rho_o + \sum_{l=1}^N \eta_{l+N} \beta_l(\boldsymbol{x}),$$

where we recall that  $c_o$  and  $\rho_o$  are the known reference coefficients. Note that in (4.6) we use the same basis functions  $\{\beta_j\}_{j=1}^N$  for  $\tilde{c}$  and  $\tilde{\rho}$ , because we expect that the variations of the wave speed and density are related, since they model the same heterogeneous medium.

#### **REDUCED ORDER MODELING FOR INVERSE SCATTERING**

However, the inversion algorithm is not tied to using the same basis and the same number of parameters. One could use independent parameterizations for the two unknowns.

The objective function (4.5), for the parameterization (4.6), depends on the vector

$$\boldsymbol{\eta} = (\eta_1, \ldots, \eta_N, \eta_{N+1}, \ldots, \eta_{2N})^T,$$

so we simplify the notation as

(4.7) 
$$\mathcal{O}^{\text{ROM}}(\boldsymbol{\eta}) = \mathcal{O}^{\text{ROM}}(\widetilde{c}(\cdot;\boldsymbol{\eta}),\widetilde{\rho}(\cdot;\boldsymbol{\eta})), \qquad \boldsymbol{R}(\boldsymbol{\eta}) = \boldsymbol{R}(\widetilde{c}(\cdot;\boldsymbol{\eta}),\widetilde{\rho}(\cdot;\boldsymbol{\eta})).$$

The causality of the ROM, ensured by the Gram–Schmidt orthogonalization (2.16) and reflected in the causal (block upper triangular) structure of  $\mathbf{R}$ , can be used to estimate the medium in a layer stripping fashion: Denote by  $[\mathbf{R}]_k$  the upper left submatrix of  $\mathbf{R}$ , containing the first k blocks. This is defined by the early time data  $\mathbf{D}_j$ ,  $j = 0, \ldots, k-1$ , for  $k < n_t$ , which contain information about the medium sampled by the waves up to time  $t_{k-1}$ . Consequently, we can feed the data gradually, for increasing values of k, and estimate the medium in layers, by minimizing the subobjective functions

(4.8) 
$$\mathcal{O}_{k}^{\text{ROM}}(\boldsymbol{\eta}) = \left\| [\boldsymbol{R}(\boldsymbol{\eta})]_{k} ([\boldsymbol{R}]_{k})^{-1} - \boldsymbol{I}_{kn\varepsilon} \right\|_{F}^{2}.$$

As is the case with any inversion algorithm, the objective function must be complemented by a regularization penalty term. Any such regularization would work. We use the simplest, Tikhonov type penalty,

$$\mathcal{O}^{\text{Reg}}(\boldsymbol{\eta}) = \|\boldsymbol{\eta}\|_2^2$$

The minimization of the objective function (4.8) complemented by the regularization penalty can be carried out with any gradient based method. We choose the Gauss–Newton method.

## Algorithm 1. (ROM based inversion).

**Input:** The data driven  $\mathbf{R}$ ; the number  $\ell$  of layers for layer stripping and the number q of iterations per layer; integer layer indices  $\{k_l\}_{l=1}^{\ell}$ , such that

$$1 \le k_1 \le k_2 \le \dots \le k_\ell = n_t.$$

Starting with the initial vector  $\boldsymbol{\eta}^{(0)} = \mathbf{0}$ , proceed: For  $l = 1, 2, \dots, \ell$ , and  $j = 1, \dots, q$ , set the update index

$$i = (l-1)q + j.$$

Compute  $\boldsymbol{\eta}^{(i)}$  as a Gauss-Newton update for minimizing the functional

(4.10) 
$$\mathcal{R}_{i}^{\text{ROM}}(\boldsymbol{\eta}) = \mathcal{O}_{k_{l}}^{\text{ROM}}(\boldsymbol{\eta}) + \mu_{i}\mathcal{O}^{\text{REG}}(\boldsymbol{\eta}),$$

linearized about  $\boldsymbol{\eta}^{(i-1)}$ . The penalty weight  $\mu_i > 0$  is chosen adaptively at each iteration, based on the decay of the singular values of the Jacobian of  $\mathcal{R}_i^{\text{ROM}}(\boldsymbol{\eta}^{(i-1)})$ . See [12] for the detailed description of the penalty weight computation. **Output:** The velocity and density estimates computed from equations (4.6), with the coefficients in  $\eta^{(\ell q)}$ .

**4.2. Regularization of the ROM computation.** So far we supposed that Assumption 1 holds, and thus the mass matrix  $\mathbb{M}$  is symmetric and positive definite. In reality this may not be true, especially for noisy data, so  $\mathbb{M}$  must be regularized before we can compute its block Cholesky square root.

It is easy to symmetrize the data driven mass matrix  $\mathbb{M}$  by taking  $(\mathbb{M} + \mathbb{M}^T)/2$ . This symmetrization is, in fact, the maximal likelihood estimator of a symmetric matrix given a noisy observation with additive Gaussian independent noise. We assume henceforth that  $\mathbb{M}$  is symmetric so it remains to map it to a positive definite matrix. This must be done carefully, in order to preserve the causality of the ROM, which is essential for a successful inversion. Here is one way to do it: Let

$$(4.11) \mathbb{M} = \mathbf{Z} \mathbf{\Lambda} \mathbf{Z}^T$$

be the eigendecomposition of  $\mathbb{M}$ , where Z is the orthogonal matrix of eigenvectors and  $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_{n_t n_{\mathcal{E}}})$  is the diagonal matrix of eigenvalues, sorted in descending order. We wish to filter out the smallest eigenvalues and the associated eigenvectors. Since the mass matrix has a block structure with  $n_{\mathcal{E}} \times n_{\mathcal{E}}$  blocks, we choose a number r such that  $1 \leq r < n_t$  and keep the  $rn_{\mathcal{E}}$  largest eigenvalues of  $\mathbb{M}$ . The corresponding leading orthonormal eigenvectors are the columns of

(4.12) 
$$\mathbf{Z}^{(r)} = [Z_{jk}]_{1 \le j \le n_t n_{\mathcal{E}}, 1 \le k \le r n_{\mathcal{E}}} \in \mathbb{R}^{n_t n_{\mathcal{E}} \times r n_{\mathcal{E}}}$$

and the projected mass matrix is

(4.13) 
$$\boldsymbol{\Lambda}^{(r)} = (\boldsymbol{Z}^{(r)})^T \mathbb{M} \boldsymbol{Z}^{(r)} = \operatorname{diag} (\lambda_1, \dots, \lambda_{rn_{\mathcal{E}}}).$$

The stiffness matrix S can also be projected,

(4.14) 
$$\mathbb{S}^{(r)} = (\mathbf{Z}^{(r)})^T \mathbb{S} \mathbf{Z}^{(r)} \in \mathbb{R}^{rn_{\mathcal{E}} \times rn_{\mathcal{E}}},$$

and the analogue of the ROM propagator defined in (2.32) is

(4.15) 
$$\mathbb{P}^{(r)} = (\mathbf{\Lambda}^{(r)})^{-1/2} \mathbb{S}^{(r)} (\mathbf{\Lambda}^{(r)})^{-1/2} \in \mathbb{R}^{rn_{\mathcal{E}} \times rn_{\mathcal{E}}}.$$

For a proper choice of r we have a well-conditioned projected mass matrix (4.13), at the cost of losing the block Toeplitz structure in (2.42)–(2.43) and the block upper Hessenberg structure of the ROM propagator. These structures reflect the causality of the ROM. To regain them, we use an additional orthogonal transformation, given by the block Arnoldi algorithm [35] applied to the matrix  $\mathbb{P}^{(r)}$ , with starting block

(4.16) 
$$(\mathbf{\Lambda}^{(r)})^{-1/2} (\mathbf{Z}^{(r)})^T \mathbf{i}_0^{(r)} \in \mathbb{R}^{rn_{\mathcal{E}} \times n_{\mathcal{E}}},$$

where  $i_0^{(r)} \in \mathbb{R}^{rn_{\mathcal{E}} \times n_{\mathcal{E}}}$  contains the first  $n_{\mathcal{E}}$  columns of the  $rn_{\mathcal{E}} \times rn_{\mathcal{E}}$  identity matrix. We give the algorithm in Appendix B. It produces an orthogonal matrix  $\boldsymbol{Q}^{(r)}$  such that  $(\boldsymbol{Q}^{(r)})^T \mathbb{P}^{(r)} \boldsymbol{Q}^{(r)}$ 

is block upper Hessenberg. Moreover,  $\boldsymbol{Q}^{(r)}$  enables the computation of the block Cholesky square root

(4.17) 
$$(\boldsymbol{Q}^{(r)})^T \boldsymbol{\Lambda}^{(r)} \boldsymbol{Q}^{(r)} = (\boldsymbol{\Pi}^{(r)})^T \mathbb{M} \boldsymbol{\Pi}^{(r)} = (\boldsymbol{R}^{(r)})^T \boldsymbol{R}^{(r)}, \qquad \boldsymbol{\Pi}^{(r)} = \boldsymbol{Z}^{(r)} \boldsymbol{Q}^{(r)}.$$

In inversion, we also need to compute the block Cholesky square root of the mass matrix  $\mathbb{M}(\boldsymbol{\eta})$  for the current search velocity and density parameterized as in (4.6). We make this calculation compatible with the regularization process (4.11)–(4.17), by using the same  $\mathbf{\Pi}^{(r)}$  defined in (4.17) to get

(4.18) 
$$(\mathbf{\Pi}^{(r)})^T \mathbb{M}(\boldsymbol{\eta}) \mathbf{\Pi}^{(r)} = \mathbf{R}^{(r)}(\boldsymbol{\eta})^T \mathbf{R}^{(r)}(\boldsymbol{\eta}).$$

The inversion Algorithm 1 works exactly the same, except that  $\mathbf{R}$  and  $\mathbf{R}(\boldsymbol{\eta})$  are replaced by  $\mathbf{R}^{(r)}$  and  $\mathbf{R}^{(r)}(\boldsymbol{\eta})$  defined above.

**4.3.** Numerical results. In this section we compare the performance of Algorithm 1 to conventional multiparameter full waveform inversion (MFWI). To make the comparison as close as possible, our implementation of MFWI uses the same data matrices as Algorithm 1, but instead of (4.10), it minimizes the objective function

(4.19) 
$$\mathcal{R}_{i}^{\scriptscriptstyle \mathrm{FWI}}(\boldsymbol{\eta}) = \mathcal{O}_{k_{l}}^{\scriptscriptstyle \mathrm{FWI}}(\boldsymbol{\eta}) + \mu_{i}\mathcal{O}^{\scriptscriptstyle \mathrm{REG}}(\boldsymbol{\eta}), \qquad \mathcal{O}_{k_{l}}^{\scriptscriptstyle \mathrm{FWI}}(\boldsymbol{\eta}) = \sum_{j=0}^{k_{l}} \|\operatorname{Triu}\left(\boldsymbol{D}_{j} - \boldsymbol{D}_{j}(\boldsymbol{\eta})\right)\|_{F}^{2},$$

where  $D_j(\eta)$  are the data matrices computed in the medium with search speed  $\tilde{c}$  and density  $\tilde{\rho}$ , parameterized by  $\eta$  as in (4.6). Since the noiseless matrices  $D_j$  are symmetric, we use the operation Triu to zero out the entries below the main diagonal.

We refer to Appendix A for the details of the numerical simulations, the model of noise added to the data, and the choice of the regularization parameter r. The remainder of the section is dedicated to presenting numerical results. In all the simulations we start the optimization with  $\eta = 0$ . The number of iterations for the MFWI and ROM algorithms is chosen to be the same, so that for both of them, the last updates are of the order of  $10^{-2} ||c_0||_{\infty}$  and  $10^{-2} ||\rho_0||_{\infty}$  of the sup norm  $|| \cdot ||_{\infty}$  of the wave speed and density, respectively.

From various numerical experiments, we observed that the time step  $\Delta t$ , the aperture size, and the number of sensors affect the quality of the inversion. The effect of  $\Delta t$  and the sensor separation on the approximation of the internal wave was already investigated in the scalar acoustic case in [13], and it is similar here. Roughly, the results say that the optimal choice is for  $\Delta t \leq 1/(2\nu)$  and sensor separation of the order of half the wavelength. Here, we make the additional observation that the estimation of the density benefits from having a large aperture. The choices made in the experiments below follow these observations.

4.4. Disjoint inclusions. The objective of the first numerical experiment is to assess the amount of cross-talk between the two acoustic parameters. The medium has two disjoint rectangular inclusions, one with a contrast in c and the other one with a contrast in  $\rho$  in a homogeneous background with  $c_o = 1 \text{km/s}$  and  $\rho_o = 1 \text{g/cm}^3$ . The inclusion contrasts are 1.5 for both c and  $\rho$ . The domain is  $\Omega = [0, 3 \text{km}] \times [0, 2 \text{km}]$ . The array has  $n_s = 35$  sensors at depth of 1 km, chosen to minimize the effect of the boundary on this experiment. The data



**Figure 4.1.** Two disjoint inclusions. Top row: true velocity and density; middle row: ROM based estimates; bottom row: MFWI estimates. Source locations are yellow crosses. Axes are in km. The colorbar shows the contrast i.e., ratios of c and  $\rho$  with the reference values  $c_o$  and  $\rho_o$  of the medium near the array.

are noiseless. The optimization search space has dimension  $2N = 2(30 \times 20) = 1200$  with velocity and density parameterized as in (4.6).

We display in Figure 4.1 the model and the estimates obtained with MFWI and our ROM algorithm. For both approaches we take 15 iterations. Given the simplicity of the model, we do not use layer stripping in this experiment i.e.,  $\ell = 1$ ,  $k_1 = n_t$ , and q = 15 in Algorithm 1.

We observe that the results of the ROM based inversion are better than those of MFWI. Both the shape and contrasts of the inclusions are recovered well. The cross-talk from c to  $\rho$  is minimal. The cross-talk from  $\rho$  to c is more visible, but small. MFWI does a worse job in recovering the inclusions and minimizing the cross-talk. In particular, the cross-talk from  $\rho$  to c is almost as strong as the recovered c inclusion.



**Figure 4.2.** Two-coefficient Marmousi model. Top row: true velocity and density; middle row: ROM based estimates; bottom row: MFWI estimates. Source locations are yellow crosses. Axes are in km. The colorbar shows the contrast.

**4.5.** Marmousi model. The objective of this experiment is to assess how the ROM inversion mitigates cycle skipping, which is the main cause of the spurious local minima of the conventional (MWFI) objective function. We consider a section of the two-coefficient Marmousi model [31] in the domain  $\Omega = [0, 6\text{km}] \times [0, 3.75\text{km}]$ . An array of  $n_s = 30$  sensors is placed at the depth of 150m. No noise is added to the data. The inversion is carried out in six layers, i.e.,  $\ell = 6$  in Algorithm 1. The optimization search space has dimension  $2N = 2(50 \times 40) = 4000$ , with velocity and density parameterized as in (4.6).

The results of the second numerical experiment are shown in Figure 4.2. We display both MFWI and ROM based estimates obtained after 50 iterations. We took 8 iterations for the first five layers and 10 iterations in the last layer. As expected, MFWI gets stuck in a local minimum and the result has multiple artifacts in the estimated velocity and a mostly nonsensical density estimate. In contrast, the ROM based estimates of c and  $\rho$  capture the true medium, except for some artifacts in the density close to the (reflective) sides of the domain.

**4.6.** Models with cracks. In the third experiment we test the effect of noise on the inversion. See Appendix A for the noise model, with standard deviation quantified by the dimensionless parameter b.

We consider two models with crack like features, embedded into smooth backgrounds. Both models occupy the domain  $\Omega = [0, 2.5 \text{km}] \times [0, 1.2 \text{km}]$  with variable background velocity ranging from 1km/s to 1.5km/s and background density in the  $1 - 1.2 \text{g/cm}^3$  range. The velocity inside the cracks is 2km/s while the density is  $1.5 \text{g/cm}^3$ . The difference between the two models is that the crack features of c and  $\rho$  are interchanged.

We invert for both the background and the cracks, i.e., only the reference values  $c_o$  and  $\rho_o$  of the medium near the array are assumed known. The array of  $n_s = 25$  sensors is placed at the depth of 100m. The inversion is carried out with both noiseless and noisy data, with noise level  $b = 10^{-2}$  and  $b = 3 \cdot 10^{-2}$  for the first and the second model, respectively. The optimization search space has dimension  $2N = 2(30 \times 20) = 1200$ , with velocity and density parameterized as in (4.6). For both models we perform 40 iterations of MFWI and the ROM based inversion. We do not display MFWI results with noise, because they are not so different from the noiseless ones (MFWI is known to be robust with respect to additive Gaussian noise). The results of the ROM based inversion with noisy data are shown after 30 iterations. A single layer ( $\ell = 1$ ) is used in all the cases.

The results for the first model are in Figure 4.3. The bottom branch of the crack feature in c is difficult to recover, because most of the energy is reflected back to the array by the top branch. MFWI gives a worse recovery of this branch and also introduces an artifact in the density estimate. The ROM based estimate from noisy data is qualitatively similar to that of MFWI, which implies that the information about the deeper part of the model is masked by the noise and is discarded during the regularization process.

The results of the experiments for the second model with cracks are shown in Figure 4.4. This model is easier to recover due to the fork-like crack being in the density part of the model rather than in the velocity part. Thus, we observe that the cracks are estimated well by the ROM based inversion both with noisy and noiseless data. MFWI gives a worse estimate of the density crack even from the noiseless data.

5. Summary. We introduced a data driven reduced order model (ROM) for a general first order hyperbolic system of equations that governs the evolution of all linear types of waves (acoustic, electromagnetic, and elastic) in a lossless medium occupying some domain  $\Omega$ . We derived an exact time stepping scheme for the hyperbolic system, on a uniform time grid. This scheme maps the wave field snapshots from one instant to the next, using a unitary operator called the wave propagator. The ROM is defined as an orthogonal, Galerkin projection of the time stepping scheme on the space spanned by the wave snapshots. We are interested in a ROM that can be used to solve inverse wave scattering problems, where the snapshots are unknown almost everywhere in  $\Omega$ . The ROM is called data driven, because it can be computed from inverse scattering data, i.e., measurements of the snapshots at a few sensor locations which probe the medium in  $\Omega$  with short signals (pulses) and record the generated,



**Figure 4.3.** First crack model. Top row: true velocity and density; second row: ROM based estimates from noiseless data; third row: ROM based estimates from noisy data with  $b = 10^{-2}$ ; bottom row: MFWI estimates from noiseless data. Source locations are yellow crosses. Axes are in km. The colorbar shows the contrast.

backscattered waves. The mapping between these measurements and the ROM is nonlinear, but we show that it can be computed using efficient techniques from numerical linear algebra.

The definition of the ROM respects the causality of wave propagation: The matrix of ROM snapshots is block upper triangular and the ROM propagator, the Galerkin projection of the propagator operator, is a block upper Hessenberg matrix. The size of the blocks of these matrices is given by the number of wave excitations. The block algebraic structure reflects the causal dependence on the data: The top left k blocks are determined by the measurements

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**Figure 4.4.** Second crack model. Top row: true velocity and density; second row: ROM based estimates from noiseless data; third row: ROM based estimates from noisy data with  $b = 3 \cdot 10^{-2}$ ; bottom row: MFWI estimates from noiseless data. Source locations are yellow crosses. Axes are in km. The colorbar shows the contrast.

up to the kth time instant. This is essential not only because the ROM captures correctly the physics of wave propagation, but also because we can use it to solve the inverse problem in a layer peeling fashion.

While the definition of the ROM is general, we specialize its application to inverse scattering with acoustic waves. The wave field consists of the acoustic pressure and velocity and the medium in  $\Omega$  is modeled by the unknown and variable wave speed c and density  $\rho$ . We use the ROM to approximate the mapping from the data to the vectorial wave field at inaccessible points in  $\Omega$ , a.k.a. the internal wave. This wave is computed for the best guess of c and  $\rho$ , and it fits the data by design. However, it is not a solution of the hyperbolic system of equations unless the guess of the medium is right. This motivates the formulation of the inverse problem as a minimization of the discrepancy between the approximated wave field and the solution of the hyperbolic system of equations. Carefully designed numerical simulations show that this formulation consistently outperforms the minimization of the nonlinear least squares data misfit objective function, used by the existing inverse scattering methodology.

The ROM construction and inversion methodology is specialized to the time domain formulation of wave propagation. There are ROMs for frequency domain formulations, with array measurements of time harmonic waves at multiple frequencies. Examples of such ROMs are in [10] for parabolic equations and in [11] for waves in lossy one-dimensional media. The construction of these ROMs is different and they do not enjoy the useful causality properties of the ROMs built in the time domain. The frequency domain formulation is important for dealing with dispersive and lossy media, which motivates future work.

Appendix A. Setup for the numerical simulations. The numerical simulations are carried out in a two-dimensional (d = 2) rectangular domain  $\Omega$  with sound soft boundary condition (3.7). We use  $n_{\mathcal{E}} = 2n_s$  excitations  $F_{\epsilon}(\mathbf{x})$  of the form (3.5) with sources located at  $\mathbf{x}_{\epsilon_1}$ ,  $\epsilon_1 = 1, \ldots, n_s$ , and with two polarizations  $\epsilon_2 \in \{1, 2\}$  at each location. The probing pulse is

(A.1) 
$$s(t) = \mathbb{1}_{[-t_s, t_s]}(t) \frac{d}{dt} \left( \cos(2\pi\nu t) \exp\left[ -\frac{(2\pi B)^2 t^2}{2} \right] \right)$$

with central frequency  $\nu = 6$ Hz and bandwidth B = 4Hz. Here  $1_{[-t_s,t_s]}(t)$  is the indicator function of the interval  $[-t_s,t_s]$ , where  $t_s = 1.5/(\nu + B) = 150$ ms. The noiseless data (2.12) are generated by solving numerically (2.9) using an exponential integrator<sup>4</sup> based on [1] with a time step  $\tau_f$  defined below. The operator (3.10) is discretized using a finite difference scheme with two-point first order discretization of all the partial derivatives. The initial state (2.8) is calculated using a backward Euler scheme with the same time step  $\tau_f$  as in the exponential integrator. The data are sampled at intervals  $\Delta t = 1/[2.3(\nu + B)] = 43.5$ ms. The numerical time integration step is  $\tau_f = \Delta t/10$ .

It remains to describe the noise model. Consider the noise signal  $\mathfrak{N}(t) \in \mathbb{R}^{n_{\mathcal{E}} \times n_{\mathcal{E}}}$  with  $t \in [-t_s, t_{\max} + t_s]$  discretized on a uniform time grid with step  $\tau_f$ , where  $t_{\max} = (n_t - 1)\Delta t$ . The entries of  $\mathfrak{N}(t)$  are identically distributed, Gaussian, with mean zero and standard deviation chosen so that

(A.2) 
$$\left( \int_0^{t_{\max}} dt \, \|\mathfrak{N}(t)\|_F^2 \right)^{1/2} = b \left( \int_0^{t_{\max}} dt \, \left\| \widetilde{\boldsymbol{A}}(t) \right\|_F^2 \right)^{1/2},$$

for a user defined noise level b, where

(A.3) 
$$\widetilde{\boldsymbol{A}}_{\boldsymbol{\epsilon}',\boldsymbol{\epsilon}}(t) = \int_{\Omega} d\boldsymbol{x} \begin{pmatrix} \boldsymbol{F}_{\boldsymbol{\epsilon}'}(\boldsymbol{x}) \\ 0 \end{pmatrix}^{T} \boldsymbol{\psi}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x}) \stackrel{(3.9)}{\approx} \sqrt{\zeta_{o}} \boldsymbol{e}_{\boldsymbol{\epsilon}'_{2}}^{T} \boldsymbol{u}_{\boldsymbol{\epsilon}}(t,\boldsymbol{x}_{\boldsymbol{\epsilon}'_{1}}).$$

 $^{4}$ The derivation of the ROM uses that the wave field is a time-dependent flow, as stated in (2.10). This is why we used a forward solver that preserves this property.

The noisy data  $\boldsymbol{D}_{i}^{\mathfrak{N}}$  are

(A.4) 
$$D_j^{\mathfrak{N}} = D_j + \int_{-t_s}^{t_s} dt \,\mathfrak{N}(t_j - t) s(-t), \quad j = 0, \dots, n_t - 1,$$

where the integrals in (A.2) and (A.4) are computed numerically using the trapezoidal rule on the same grid on which  $\mathfrak{N}(t)$  is defined.

The regularization parameter r can be determined with a trial-and-error approach: One can start with a large r and then see how the results improve or deteriorate if we decrease it. This is sufficient in the examples addressed in this paper. A more systematic approach can be based on estimating the noise level from the deviation of the data from the reciprocity relation. We refer to Appendix F in [12] for a description of such an approach.

Appendix B. The block Arnoldi iteration. The following algorithm computes the orthogonal transformation that puts the regularized ROM propagator in the causal, block upper Hessenberg form. We write it for a generic matrix X with  $m \times m$  blocks.

Algorithm 2. (block Arnoldi iteration).

Input: The matrix  $\mathbf{X} \in \mathbb{R}^{mn \times mn}$  and the starting block  $\mathbf{y} \in \mathbb{R}^{mn \times m}$ . Compute  $\mathbf{q}_0 = \mathbf{y}(\mathbf{y}^T \mathbf{y})^{-1/2} \in \mathbb{R}^{mn \times m}$ ; For k = 1, ..., n - 1: - Set  $\mathbf{w} = \mathbf{X} \mathbf{q}_{k-1} \in \mathbb{R}^{mn \times m}$ ; - Orthogonalize  $\mathbf{w} = \mathbf{w} - [\mathbf{q}_0, ..., \mathbf{q}_{k-1}] ([\mathbf{q}_0, ..., \mathbf{q}_{k-1}]^T \mathbf{w})$ ; - Normalize  $\mathbf{q}_k = \mathbf{w}(\mathbf{w}^T \mathbf{w})^{-1/2} \in \mathbb{R}^{mn \times m}$ .

**Output:** Orthogonal matrix  $\boldsymbol{Q} = [\boldsymbol{q}_0, \dots, \boldsymbol{q}_{n-1}] \in \mathbb{R}^{mn \times mn}$  such that  $\boldsymbol{Q}^T \boldsymbol{X} \boldsymbol{Q} \in \mathbb{R}^{mn \times mn}$  is block upper Hessenberg.

To obtain  $(\boldsymbol{w}^T \boldsymbol{w})^{-1/2}$ , we use the unique, symmetric positive definite matrix square root computed via the spectral decomposition of the Grammian  $\boldsymbol{w}^T \boldsymbol{w}$ .

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