A simulation method for the computation of the effective P-wave velocity in heterogeneous rocks

Ángel Javier Omella1 · Julen Alvarez-Aramberri2,3 · Magdalena Strugaru2 · Vincent Darrigrand4 · David Pardo1,2,5 · Héctor González5 · Carlos Santos6

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Abstract
We propose a set of numerical methods for the computation of the frequency-dependent effective primary wave velocity of heterogeneous rocks. We assume the rocks’ internal microstructure is given by micro-computed tomography images. In the low/medium frequency regime, we propose to solve the acoustic equation in the frequency domain by a finite element method (FEM). We employ a perfectly matched layer to truncate the computational domain and we show the need to repeat the domain a sufficient number of times to obtain accurate results. To make this problem computationally tractable, we equip the FEM with non-fitting meshes and we precompute multiple blocks of the stiffness matrix. In the high-frequency range, we solve the eikonal equation with a fast marching method. Numerical results confirm the validity of the proposed methods and illustrate the effect of density, porosity, and the size and distribution of the pores on the effective compressional wave velocity.

Keywords Effective P-wave velocity · Finite element method · Fast marching method

Mathematics Subject Classification 86-08 · 65N30 · 74Q05

1 Introduction
In geophysical applications, it is of paramount importance to characterize the effective velocity of an elastic wave traveling through the Earth’s subsurface. This information enables to identify gas saturated rocks as well as the porosity and other key petrophysical properties of the subsurface, and it is critical for an initial assessment of a reservoir.

According to the frequency of operation, we distinguish three different measurement acquisition systems for the characterization of subsurface elastic properties: (a) seismic data (typically below 100 Hz), (b) logging sonic measurements (from 2 kHz up to 300 kHz), and (c) core samples (analyzed at 300 kHz–2 MHz). After proper interpretation of the results via advanced numerical methods (see [9,39,51]) we obtain an Earth map with its macro-scale velocities. Unfortunately, maps obtained with measurements acquired at dissimilar frequencies are essentially different since a given heterogeneous rock exhibits disparate effective velocities at different frequencies; see e.g., [12,30,32,36,37,59,60]. This undesired phenomena occurs due to the nature of wave propagation in heterogeneous rocks [42].

Biot’s theory [8] describes the wave propagation phenomena over a porous rock. However, it ignores the microscopic level and assumes that all the minerals of the rock have the same bulk and shear moduli [40]. Moreover, the application of this theory using elastic or poro-elastic models is computationally expensive. In here, we focus on estimating the effective P-wave velocity using the acoustic equation and without incurring in a prohibitive computational cost. Hence, we are interested in the first arriving compressional (P) wave that propagates along heterogeneous rocks in the excitation direction. Specifically, we focus only in the first wavefront travel-time, neglecting errors in the amplitude values. Thus,
although compressional-to-shear (P-to-S) and S-to-P energy conversions may occur, they may be ignored, and an acoustic approximation of elastic waves is valid in this case, overcoming the limitations exposed in [11].

We need to analyze the structure of a given porous rock and estimate its effective P-wave velocities at different frequencies. With X-ray micro-CT technology (see [19] for a review), it is possible to characterize the internal structure of rock samples at pore scale, identifying with precision the spatial distribution of its constituents. The current resolution of micro-CT available at laboratories of oil companies provides a set of around 1500 images of 1200 × 1200 pixels per core sample. This allows us to identify the material of each voxel in three dimensions (3D) with sub-pore resolution.

After producing a micro-CT scan, we need to analyze its effective velocities at different frequencies. The high-quality requirements for the cores destined to ultrasonic testing makes expensive the laboratory measurements and often can only be reliably estimated at high frequencies (above 500 kHz) to avoid undesired reflections. Some geometrical recommendations to properly analyze cores for ultrasonic testing are available in [2].

On the other hand, the use of relatively simple bounds and “averaging” formulas is extended in the industry for computing the stiffness tensor and the effective velocity from the single properties of each constituent. Some averaging formulas are the so-called Voigt [62] and Reuss [50] bounds, Voigt-Reuss-Hill average [31], Hashin-Shtrikman bounds [28, 29], Kuster-Toksöz formulation for low-porosity rocks [34], Backus-average [3, 6, 54], Gassmann’s Equation [7, 18, 25], Wyllie time average [20, 53, 63], Raymer’s [49] and Gardner’s [24] relations. These analytical and semi-analytical formulas omit the specific spatial distribution of the rock constituents. In a layered 1D media perpendicular to the direction of propagation, the Backus average is exact in the low-frequency limit, while the Wyllie time-average drives the high-frequency regime. However, when it comes to realistic two-dimensional (2D) and three-dimensional (3D) heterogeneous rocks, all aforementioned theories fall short to provide accurate effective velocities at different frequencies.

There also exist multiple effective media theories, see [17, 23, 44]. For example, Differential Effective Medium (DEM) [43] considers different pore-type inclusions. Models for cracked medium are available in [13, 16, 22, 27, 33, 61]. There also exist a plethora of multi-scale methods for heterogeneous materials (see e.g., [10, 15, 21] or [26, 38] for a review). While some multi-scale methods are difficult to implement for industrial applications [1], others are unsuitable for high-frequency computations where it is crucial to determine the location of the micro-constituents in the rock at pore-scale. To the best of our knowledge, existing homogenization techniques often fail to solve the problem in the wide range of frequencies, as needed by our application.

Herin, we propose a set of simple-to-implement numerical methods that are capable of handling different frequencies and are suitable for the oil industry needs. These methods produce accurate approximations of the first P-wave arrival corresponding to heterogeneous rocks.

The numerical results presented throughout this work exhibit the need of repeating the rock several times in the low-frequency regime. This increases the size of the problem (information of thousands of millions of pixels in 3D problems with possibly different material properties) and the computational cost, becoming the problem computationally untractable via conventional numerical methods. Moreover, since this is a wave propagation problem over an open domain, truncating the computational domain becomes a great challenge that should be carefully treated to preserve the accuracy of the homogenized velocities. Finally, it is also challenging to estimate effective velocities from a given (simulated) wave propagation solution.

In the low-medium frequency range, we solve the frequency-dependent wave equation by a FEM. To avoid undesired reflections from the domain boundary, we implement a perfectly matched layer (PML). At low frequencies, we observe that this PML adversely affects the results. Thus, we need to extend virtually the original domain by repeating it multiple times. This increases dramatically the problem size. Traditional FEM employ fitting meshes in which material properties are continuous within each element. The large number of pixels attached to the necessity of the rock repetition leads to a prohibitive computational cost when using this technique, especially in 2D and 3D. To overcome this challenge, we propose the use of non-fitting meshes [14], which reduces dramatically the number of degrees of freedom when the domain is large. However, this technique needs to be carefully employed to preserve the accuracy of the results. The repetition of the original domain allows to precompute blocks in FMMthe stiffness matrix in order to reduce the integration and assembling time.

After simulating the complex-valued pressure field in the frequency domain, we apply two methods to estimate the effective compressional wave velocity: (a) Prony’s method [46], which provides an accurate value of effective compressional wave velocity at low frequencies, but it diverges at large ones, and (b) counting the number of wavelengths, which provides valid (although sometimes exhibiting low accuracy) approximations of the effective velocities across the entire frequency spectrum.

In the high-frequency limit, we solve the eikonal equation to approximate the travel time of the wave by a fast marching method (FMM) [56]. Results in 1D heterogeneous rocks match with those obtained by the application of the Wyllie Time-Average [63]. This confirms the accuracy of our proposed method. Thus, we apply it to estimate the high-frequency P-wave velocity limit in 2D and 3D problems,
where analytical methods are unavailable for general porous rocks.

The remainder of the manuscript is organized as follows. Section 2 introduces the theoretical bounds in layered media for the P-wave velocity. Section 3 describes the acoustic formulation in time and frequency. Then, we explain the physical need to repeat the rock, and we introduce two techniques to accelerate the computations: non-fitting meshes and precomputed block matrix. After that, we describe two methods to obtain the effective compressional wave velocity. To conclude this section, we analyze the high-frequency range, in which we propose to solve the eikonal equation to estimate the effective velocity. Section 4 focuses on the numerical results. The first four considered experiments analyze numerically the techniques presented for low-medium frequencies; experiments 5-8 show the influence of the main physical quantities (density, porosity, the size of the pore, and the distribution in the sizes of the pores) in the effective velocities. Experiment 9 shows the effective velocity profile computed in non-periodic vertical transversely isotropic (VTI) rocks. Experiment 10 describes the necessity to extend the domain in the perpendicular dimension of the P-wave propagation direction. Experiment 11 illustrates the method scalability in higher dimensions. Experiment 12 shows the results for horizontal transversely isotropic (HTI) rocks. Finally, experiment 14 describes numerical results obtained from images of real rocks acquired in the laboratory via micro-CT. The last section is devoted to conclusions.

2 Theoretical bounds in layered media

We consider a heterogeneous rock composed of various materials. Backus [3] showed that a stratified medium composed of VTI layers behaves like a homogeneous VTI media in the long-wavelength limit. To determine it, we search for “a global” fourth-order stiffness tensor $C_{\text{eff}}$ that allows to treat the multi-material body as a homogenized effective one. The Backus homogenized $c_{ijkl}^{*}$ components of $C_{\text{eff}}$ are defined by relations among the components of $C$, and by using the volumetric weighted average defined as $\{\cdot\}$.

Attending to this homogenization, the vertically propagating P-wave velocity [35] is:

$$v_{P,v} = \sqrt{\frac{c_{3333}^{*}}{\rho^{*}}},$$  

(1)

where $c_{3333}^{*} = \left(c_{3333}^{-1}\right)^{-1}$, and $\rho^{*} = \{\rho\}$ is the volumetric weighted average of the densities.

Given a VTI layered rock, we consider known some information about each $i$-constituent (or layer): the volume fraction $(\phi_i)$, and some physical properties as density $(\rho_i)$ and compressional wave velocity $(v_i)$). Following (1), we use the Backus average to obtain the effective P-wave velocity $v_{B,eff}^{*}$:

$$v_{P,v} = v_{eff} = \sqrt{\frac{c_{3333}^{*}}{\rho^{*}}}, \quad \text{where} \quad \frac{1}{c_{3333}^{*}} = \sum_{i=1}^{n} \frac{\phi_i}{\rho_i v_i^2}.$$  

(2)

Wyllie time-average [63] describes the effective velocity in high-frequency regimes $v_{TA,eff}^{*}$ as:

$$\frac{1}{v_{TA,eff}^{*}} = \sum_{i=1}^{n} \frac{\phi_i}{v_i}.$$  

(3)

Figure 1 shows a schematic representation of the effective velocity with respect to the frequency. Specifically, we represent (a) the Backus average zone, where the effective velocity tends to $v_{B,eff}^{*}$; (b) the time-average zone where the effective velocity approximates $v_{TA,eff}^{*}$; and (c), the transition zone that occurs between the two aforementioned zones. The frequency limits in this transition zone are unclear and an analytical expression for the effective velocity is unknown. Indeed, within this transition zone, the behavior of the effective velocity with respect to the frequency is often not even monotonic [60].
3 Mathematical model and solution method

In this section, we consider a rock with heterogeneous density and we first focus on the low/medium frequency range. We introduce the mathematical model, followed by the FEM adopted to solve it. Next, we discuss the need to repeat virtually the original domain several times until it becomes at least n-wavelengths long, where n is typically between two and four. To make these problems computationally tractable, we consider a FEM with non-fitting meshes and precomputed stiffness matrices. Then, we use the solution obtained with FEM to evaluate the effective velocity via two different techniques, both based on the post-processing of the solution computed stiffness matrices. Then, we use the solution obtained we consider a FEM with non-fitting meshes and precompressed sample at multiple points. To conclude this section, we focus on the high-frequency regime. Specifically, we introduce the eikonal equation and a fast marching method (FMM) to solve it.

3.1 Acoustics

When the density varies with position [5], the strong formulation of the acoustic problem in a fluid domain Ω is governed by the time-dependent wave equation,

$$\nabla \cdot \left( \frac{1}{\rho} \nabla \hat{u} \right) - \frac{1}{\rho c^2} \frac{\partial^2 \hat{u}}{\partial t^2} = \hat{f} \quad \text{in} \quad \Omega,$$

(4)

where \( \hat{u} \equiv \hat{u}(x, t) \) is the sound pressure, \( c \equiv c(x) \) is the propagation velocity of the sound wave in the fluid, \( \rho \equiv \rho(x) \) is the material density, and \( \hat{f} \equiv \hat{f}(x, t) \) is the volumetric stationary source term. In order to have unicity in the solution, we consider a Sommerfeld radiation condition [55,58], which imposes proper decay conditions at infinity:

$$\lim_{r \to \infty} \left( r \left( \frac{\partial \hat{u}}{\partial r} + \frac{1}{c} \frac{\partial \hat{t}}{\partial t} \right) \right) = 0,$$

(5)

where \( r \) denotes the radial component in the spherical coordinate system.

3.2 Low-medium frequencies analysis

3.2.1 Mathematical model

Applying a Fourier transform in time to equation (4), we obtain the following hyperbolic partial differential equation in the frequency domain:

$$\nabla \cdot \left( \frac{1}{\rho(x)} \nabla u(x, \omega) \right) + \frac{k^2(x)}{\rho(x)} u(x, \omega) = f(x, \omega) \quad \text{in} \quad \Omega,$$

(6)

where \( u \) and \( f \) stand for the Fourier transforms in time of \( \hat{u} \) and \( \hat{f} \) respectively, and \( k(x) = \frac{\omega}{\rho(x)c} \) is the medium wavenumber at angular frequency \( \omega \). In addition, the Sommerfeld radiation condition in spherical coordinates becomes:

$$\lim_{r \to \infty} \left( r \left( \frac{\partial u}{\partial r} - ik u \right) \right) = 0.$$

3.2.2 Finite element method (FEM)

To solve Eq. (6) using a FEM, we first introduce a polygonal domain \( \Omega_h \), over which we generate the mesh \( T_h = \{K\} \).

Then, we define the space of finite elements \( V_h \) where

$$V_h \equiv \{ v_h \in H^1(\Omega_h) \mid v_h|_K \in P_p(K), \forall K \in T_h, \text{and} v_h|_{\partial \Omega_h} = 0 \},$$

where \( P_p(K) \) is the space of polynomial functions of order \( p \).

We then rewrite (6) as a discrete variational problem:

$$\begin{align*}
\text{Find } u_h & \in V_h, \quad \text{such that:
- } -\int_{\Omega_h} \frac{1}{\rho} \nabla u_h \cdot \nabla v_h + \int_{\Omega_h} \frac{k^2}{\rho} u_h v_h &= \int_{\Omega_h} f v_h, \\
& \text{for all } v_h \in V_h,
\end{align*}$$

(8)

where \( u_h \) is the approximated solution of \( u(x, \omega) \) that appears by solving a system of linear equations.

Repetition Strategy. We first execute simulations at low frequencies –inside the Backus regime– and we observe incorrect values of the effective velocity. This occurs because the PML avoids boundary reflections, while in this application we seek for the homogenized velocities when the rock is repeated multiple times in the subsurface. This problem also affects laboratory experiments and partially explains the difficulties encountered when analyzing rocks at low frequencies. To overcome it in numerical simulations, we repeat the rock domain sample several times until we obtain a computational domain in which the effective velocity is unaffected by a surrounding (homogeneous slower) media. Experiments 3, 4 and 10 in Sect. 4 illustrate this strategy.

Non-fitting Meshes. The standard FEM employs fitting meshes to assemble the bilinear form associated with the material. In particular, it assumes that density \( \rho \) and wavenumber \( k \) are sufficiently smooth within each cell \( K \). However, this assumption makes the resulting simulator prohibitively expensive in our case since it would force us to consider thousands of millions of elements. For the sake of simplicity, we focus on the diffusive term of (8), and we write for a single element \( S \):
the number of sub-cells (elements) grouped into a macro-
ties, into a single macro-element $K$ over two or more cells, with possibly different material proper-
ties. Notice that we employ a standard FEM with non-fitting
meshes. We do not employ multiscale basis functions.

By using non-fitting meshes, we select larger macro-
elements and perform exact integration. This reduces the
number of unknowns in the finite element model and the cor-
responding computational requirements (time and memory).
For more details about this technique, we refer the reader
to [14].

**Precomputed Matrix.** We consider an original master
domain $\Omega_0$ discretized by the master mesh $T_0 = \{K_1^0, K_2^0, \ldots, K_m^0\}$. We often repeat $\Omega_0$ in space $n$-times to gener-
ate the entire domain $\Omega = \bigcup_{i=1}^n \Omega_i$, along with the
mesh $T$ that discretizes the domain $\Omega$. $T = \bigcup_{i=1}^n T_i = \{K_1, K_2, \ldots, K_{m,n}\}$, where $T_i$ is the discretization of each
$\Omega_i$.

\begin{equation}
\int_{S} \frac{k^2}{\rho} \phi_j \phi_i = \text{area}(S) \frac{k^2}{\rho S} \int_{S} \hat{\phi_j} \hat{\phi_i}, \quad (9)
\end{equation}

where $\phi_i$ is the $i$-th shape function associated with the ele-
ment $S$, and $\hat{\phi_i}$ is the $i$-th shape function corresponding to
the reference element $\hat{S}$.

The key ingredient in non-fitting meshes [14] is to group
two or more cells, with possibly different material proper-
ties, into a single macro-element $K$ (see Fig. 2). Let $s$ be
the number of sub-cells (elements) grouped into a macro-
element: $K = \bigcup_{l=1}^s S_l$, where $S_l, l = 1, \ldots, s$. Assuming
that the material properties are constant inside each sub-cell
$S_l$, we rewrite equation (9) for non-fitting meshes as:

\begin{equation}
\int_{K} \frac{k^2}{\rho} \phi_j \phi_i = \sum_{l=1}^{s} \int_{S_l} \frac{k^2}{\rho} \phi_j \phi_i = \sum_{l=1}^{s} \text{area}(S_l) \frac{k^2_{K,j}}{\rho_{K,l}} \int_{S_l} \hat{\phi_j} \hat{\phi_i}, \quad (10)
\end{equation}

where $\hat{S}_l$ is the sub-cell associated with the reference macro-
element $\hat{K}$, and as before, $\phi_i$ is the $i$-th shape function associated
with the macro-element $K$, and $\hat{\phi_i}$ is the $i$-th shape function corresponding to the reference macro-element $\hat{K}$. Notice that we employ a standard FEM with non-fitting
meshes. We do not employ multiscale basis functions.

By using non-fitting meshes, we select larger macro-
elements and perform exact integration. This reduces the
number of unknowns in the finite element model and the cor-
responding computational requirements (time and memory).
For more details about this technique, we refer the reader
to [14].

**3.2.3 From the FEM solution to an effective velocity**

At low frequencies, a wave traveling through a heterogeneous
media behaves as a sum of plane waves. Figure 4 shows
the real part of the pressure computed by Equation (8). In
such scenarios, Prony’s method [45,46] accurately estimates
the effective velocity. From a uniform sampling of a sig-
Fig. 4 Real part of the solution at 1.27 kHz in a 1D rock with a porous size equal to 125 mm. The white background color indicates a material with \( v_{\text{solid}} = 4500 \text{ m/s} \); the gray background represents a material with \( v_{\text{fluid}} = 800 \text{ m/s} \). The density of both materials is 1000 Kg/m\(^3\).

Fig. 5 Real part of the solution at 48.3 kHz in 1D rock with 125 mm as size of the pore. The white background color indicates a material with \( v_{\text{solid}} = 4500 \text{ m/s} \); the gray background represents a material with \( v_{\text{fluid}} = 800 \text{ m/s} \). The density of both materials is 1000 Kg/m\(^3\).

However, at high frequencies, the wavelength is comparable to the size of the pores, and the solution behaves as piecewise plane waves, one inside each sub-domain. Figure 5 shows the real part of the pressure computed using (8). In this scenario, the plane wave assumption required by Prony’s method is invalid, and we need to estimate the effective velocities differently. For that, we propose a simple method based on counting the number of wavelengths of the solution over the whole domain. To do so, we sample the solution \( u_h \) as in the Prony’s method, and we compute the phase difference of the pressure from one receiver to the next. In this way, we approximate the number of wavelengths located between one receiver and the next. By repeating the process throughout all receivers, we obtain an estimate of the total number of wavelengths \( (k_{\lambda}) \) traveled by the wave. Then, we compute the velocity as:

\[
v_{\text{eff}} = \frac{L v}{k_{\lambda}},
\]

where \( v \) is the frequency in Hertz and \( L \) is the distance between the first and last receiver. Experiment 1 in Sect. 4 compares Prony’s method with the one based on counting the number of wavelengths.

### 3.3 High frequencies analysis

Approximation of high-frequency solutions by a FEM involves a prohibitive computational cost due to the need of considering several degrees of freedom per wavelength, which translates into large systems of equations. However, our application only requires to estimate the traveltime of the first arriving wave. To do so, we introduce the eikonal equation [48], which we solve with a FMM.

#### 3.3.1 Eikonal equation

We assume the solution of the wave Eq. (4) takes the following general form:

\[
p(t, x) = A(x) e^{-i \omega (T(x) + t)},
\]

where \( A \) is the amplitude, \( \omega \) is the angular frequency and \( T \) is a time function (the eikonal), which describes surfaces of constant phase (wavefronts) when \( T \) is constant.

Plugging the ansatz (13) into the wave equation (4), separating real and imaginary parts and using the high-frequency assumption \((\omega \to \infty)\) in the real part equation, we obtain the so-called eikonal equation:

\[
|\nabla T(x)|^2 = \frac{1}{c(x)^2} \quad \text{in} \ \Omega,
\]

where \( T \) is the traveltime evaluated at each point \( x \) of the domain \( \Omega \).

#### 3.3.2 Fast marching method (FMM)

A FMM is a finite difference scheme that solves boundary value problems with the unknown traveltime satisfying the eikonal equation:

\[
\begin{cases}
|\nabla T(x)|^2 = \frac{1}{c(x)^2} \quad \text{in} \ \Omega, \\
T(x) = f \quad \text{at least on a part of} \ \partial \Omega,
\end{cases}
\]

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where $f$ is typically 0.

We consider a front given by the initial condition, which is systematically updated in the propagation direction (one grid point at a time), in a downwind fashion from known upwind values. This entropy-satisfying strategy preserves stability in the presence of a wavefront discontinuity, as explained in [57]. The key ingredient of the method is to carefully select the order of traveltime evaluation based on the concept of traveltime in one end of the rock as:

$$(	ext{16})$$

where $c_{ijk}$ is the velocity at grid point $(i, j, k)$ and $D_{ijk}$ are first order finite difference operators given by:

$$(	ext{17})$$

and $\delta_x$, $\delta_y$, and $\delta_z$ are the grid spacings in $x$, $y$, and $z$ directions, respectively. We select a grid conforming with the spatial resolution given by the tomography:

$$(\text{18})$$

where subscript $(\cdot)$ denote the spatial component, and $N_{(\cdot)}$ and $L_{(\cdot)}$ denote the number of voxels obtained in the tomography, and the dimension of the rock, respectively. To initialize the narrow band, we compute analytically the traveltime in one end of the rock as:

$$(\text{19})$$

for $i \in 1, 2, \ldots, N_x$, $j \in 1, 2, \ldots, N_y$ and $k = 1$.

The FMM algorithm reads:

1. Generate the grid conforming to the voxels.
2. Initialize the narrow band using Eq. (19).
3. Do until all determining all traveltimes:

(a) Find the point with minimum traveltime in the narrow band.
(b) Update the narrow band.
(c) Update traveltimes at the points recently added to the narrow band and their neighbours using equation (16).
(d) Compute traveltimes on the bottom part of the domain using Eq. (19) with $k = N_z$.

Figure 6 illustrates the sequence 3(a)–3(b) in 2D. The first order scheme described above is unconditionally stable [56]. For more details on FMM, we refer the reader to [52].

In 1D, a FMM reduces to computing the traveltime from one point of the grid to the next one, using the spacing between the two points and the known velocity at the arrival point.

## 4 Numerical results

This section contains multiple numerical results. Experiments 1-4 consider 1D periodic and non-periodic formations, and assess the performance of the methods for different values of the involved parameters (e.g., number of rock repetitions and number of wavelengths needed in the domain). Experiments 5-8 show the influence of the principal physical quantities (e.g., density, porosity, the size of a pore, and different pore distribution) in the effective velocity. Experiment 9 describes the effective velocity profile computed for four non-periodic formations. Experiment 10 analyzes the lateral extension of the domain for a 2D rock. Experiment 11 exhibits a 2D VTI rock. It also shows the match
Table 1  Nomenclature associated to each one-dimensional pixel

| Graphical representation | Material state | Material properties |
|--------------------------|----------------|---------------------|
|                          | Solid (S)      | $v_{\text{solid}}$  $ho_{\text{solid}}$ |
|                          | Fluid (F)      | $v_{\text{fluid}}$  $ho_{\text{fluid}}$ |

Table 2  Nomenclature and porosity associated with two one-dimensional periodic formations

| Graphical representation | Nomenclature | Porosity |
|--------------------------|--------------|----------|
|                          | 1DP8(7S1F)   | 12.5%    |
|                          | 1DP8(3S1F)   | 25%      |

Table 3  Nomenclature and porosity of non-periodic one-dimensional formations

| Nomenclature    | Porosity  | Nomenclature    | Porosity  |
|-----------------|-----------|-----------------|-----------|
| 1D Rock 1       | 11.31%    | 1D Rock 3       | 21.36%    |
| 1D Rock 2       | 22.61%    | 1D Rock 4       | 25.85%    |

between the Time-Average formula and FMM in the high-frequency regime. Experiment 12 employs HTI rocks and shows the discrepancy between the Time-Average formula and the FMM. Then, experiment 13 further validates the FMM. Finally, experiment 14 applies the proposed methods to two real rocks.

4.1 Samples and modeling considerations

We consider samples composed of two materials. We identify solid (S) and fluid (F) pixels with white and black color, respectively (see Table 1).

We generate particular periodic samples by repeating a specific sequence of pixels several times. To refer to a periodical 1D synthetic rock, we introduce the following nomenclature: we first indicate that it is a one-dimensional (1D) periodic (P) rock with the abbreviation 1DP. Next, we write the number of total pixels that compose the sample and finally, inside brackets, the repeated sequence of pixels. Table 2 shows two periodic samples.

We additionally consider four large realistic non-periodic formations composed each of 1203 pixels. Table 3 summarizes the nomenclature and the porosity of each non-periodic formation.

Figure 7 describes the one-dimensional model of the formation and identifies the necessary geometric model parameters.

We denote the domain of the sample by $\Omega_0 = (a, b)$. To truncate the computational domain, we introduce a PML on the outer part of the domain. We automatically select its size

$$|a - a'| = |b - b'|$$

as the minimum between 10% of the domain of the sample and three times the size of the largest wavelength, i.e.:

$$|a - a'| = |b - b'| = \min (0.1(b - a), 3\lambda_{\text{fast}}),$$

where $\lambda_{\text{fast}}$ is the wavelength associated with the fastest material of the rock (in our case, the solid, i.e., $\lambda_{\text{fast}} = \lambda_{\text{solid}}$).

We often extend the analysis domain by repeating the sample. We can repeat the original rock only at one side (see Fig. 8a), or at both sides (see Fig. 8b).

We consider a domain $\Omega_0 = (-0.5, 0.5)^d$ meters, where $d$ is the spatial dimension. A rescaling to a different sample size is straightforward. We place the transmitter 0.05 m away from the closest boundary, and the receivers at least 0.10 away from any boundary, following a straight line. In the Finite Element experiments, we select the polynomial order of approximation $p = 2$.

We also generate a synthetic formation of 1200 x 1200 pixels that we denote as the labyrinth (see Fig. 9). In this formation, the fastest wave travels through the solid, circumventing the black fluid material.

Table 5 shows three types of 3D layered periodic formations. In the first formation with VTI symmetry, the normal vector of each layer points towards the direction of the main P-wave propagation direction ($z$-axis). The other two formations with HTI symmetry have the normal vector of each layer pointing perpendicularly to the main P-wave propagation direction. The subscript ($x$ or $y$) denotes the normal vector of the layers.
Table 4 Nomenclature and porosity associated with 2D periodic VTI and HTI formations

| Graphical representation | Nomenclature         | Porosity |
|--------------------------|----------------------|----------|
| 2DVTI 12x12(1F2S)       | 33.3%                |
| 2DHTI 12x12(1F3S)       | 25%                  |

Finally, we consider two heterogeneous real rock samples we analyzed in the laboratory with a micro-CT scan. The main P-wave propagation direction is along the last dimension (z-axis). The postprocessed data extracted from the micro-CT is a set of 1618 images of $1200 \times 1200$ pixels each. The domain is $\Omega_0 = 1.547 \times 1.547 \times 2.086$ cm. Each pixel of the micro-CT map corresponds to a square of 12.89 micrometers. To reduce the computational cost, we sample over one vertical cross-section of $1200 \times 1618$ pixels extracted from the samples.

(a) The first rock, denoted as 3D Rock 1, is composed of five materials. Table 6 summarizes the number assigned to each material, its volume fraction percentage, and properties.

(b) The second rock, denoted as 3D Rock 2, is composed of three materials. Table 7 summarizes the number assigned to each material, its volume fraction percentage, and properties.

Table 5 Nomenclature and porosity associated with 3D periodic formations

| Graphical representation | Nomenclature         | Porosity |
|--------------------------|----------------------|----------|
| 3DVTI 12x12x12(1F2S)    | 33.3%                |
| 3DHTI$_x$ 12x12x12(1F3S)| 25%                  |
| 3DHTI$_y$ 12x12x12(1F3S)| 25%                  |
Table 6 Material number, volume fraction, wave velocity and density of the 3D Rock 1 constituents

| Material number ($i$) | Volume fraction ($\phi_i$) | $c_i$ (m/s) | $\rho_i$ (kg/m$^3$) |
|-----------------------|----------------------------|-------------|---------------------|
| 1                     | 0.800185                   | 6041.98     | 2648.0              |
| 2                     | 0.034559                   | 2424.87     | 1373.0              |
| 3                     | 0.071186                   | 1513.27     | 1000.0              |
| 4                     | 0.046283                   | 2138.54     | 1298.4              |
| 5                     | 0.047787                   | 1493.02     | 1149.2              |

Table 7 Material number, volume fraction, wave velocity and density of the 3D Rock 3 constituents

| Material number ($i$) | Volume fraction ($\phi_i$) | $c_i$ (m/s) | $\rho_i$ (kg/m$^3$) |
|-----------------------|----------------------------|-------------|---------------------|
| 1                     | 0.619703                   | 6645.11     | 2710.0              |
| 2                     | 0.354040                   | 5161.60     | 2197.0              |
| 3                     | 0.026257                   | 1513.27     | 1000.0              |

Table 8 summarizes the simulation parameters used in each experiment.

*Indicates that the corresponding field is a variable explained in its own experiment subsection.

–Indicates that such field is not applicable in the considered experiment.

### 4.2 Experiment 1: Prony versus count wavelength

In this experiment, we extend the domain at both sides of the original sample to guarantee $10 \lambda_{soli}$ at each side.

Figure 10 shows the theoretical effective velocities computed by Eqs. (2) and (3), and compares the profiles of compressional wave effective velocities obtained by the application of Prony’s method (red line) and counting the number of wavelengths (green line) for two periodic rocks. We observe that Prony’s method converges only in the low-frequency regime, which is the region where the solution is given by a sum of plane waves. The count wavelengths method properly estimates velocities at low frequencies, matching the results obtained by Prony’s method. It also performs adequately in the high-frequency regime and converges to the theoretical solution $v_{eff}$ given by the Wyllie time-average.

### 4.3 Experiment 2: Precomputed-matrix and fitting versus non-fitting meshes

In this experiment, we assess the accuracy of non-fitting meshes and precomputed matrix technique. We compute the compressional wave effective velocity using Prony’s method for the non-periodic formations displayed in Table 3, excited at a frequency of 10 Hz. We extend the domain at both sides of the original sample virtually to guarantee $1 \lambda_{Backus}$ at each side.
| Experiment number | Figure or table number | Formation nomenclature | $c_{\text{solid}}$ (m/s) | $\rho_{\text{solid}}$ (kg/m³) | $c_{\text{fluid}}$ (m/s) | $\rho_{\text{fluid}}$ (kg/m³) | Precomputed matrix | Fitting meshes |
|-------------------|------------------------|------------------------|--------------------------|---------------------------|--------------------------|---------------------------|----------------|--------------|
| 1                 | Figure 10a             | 1DP8(3S1F)             | 4500                     | 2800                      | 800                      | 1000                      | No             | No           |
|                   | Figure 10b             | 1DP8(7S1F)             |                          |                           |                          |                           | No             | No           |
| 2                 | Table 9                | 1D Rock 1-4            | 4500                     | 1000                      | 800                      | 1000                      | *              | *            |
|                   | Figure 11              | 1D Rock 4              |                          |                           |                          |                           | Yes            | Yes          |
| 3                 | Figure 12a             | 1DP8(3S1F)             | 4500                     | 2800                      | 800                      | 1000                      | No             | Yes          |
|                   | Figure 12b             | 1DP8(7S1F)             |                          |                           |                          |                           | Yes            | No           |
| 4                 | Figure 13a             | 1D Rock 1              | 4500                     | 1000                      | 800                      | 1000                      | Yes            | Yes          |
|                   | Figure 13b             | 1D Rock 2              |                          |                           |                          |                           | Yes            | No           |
| 5                 | Figure 14a             | 1DP8(3S1F)             | 4500                     | *                         | 800                      | *                         | Yes            | Yes          |
|                   | Figure 14b             | 1DP8(7S1F)             |                          |                           |                          |                           | Yes            | Yes          |
| 6                 | Figure 15a             | 1DP8(1S1F) 1DP8(3S1F) 1DP8(7S1F) | 4500                     | 2800                      | 800                      | 1000                      | Yes            | Yes          |
|                   | Figure 15b             |                          |                          |                           |                          |                           | Yes            | Yes          |
| 7                 | Figure 16a             | 1DP8(1S1F) 1DP80(1S1F) 1DP800(1S1F) | 4500                     | 2800                      | 800                      | 1000                      | Yes            | Yes          |
|                   | Figure 16b             |                          |                          |                           |                          |                           | Yes            | Yes          |
|                   | Figure 17a             | 1DP8(3S1F) 1DP80(3S1F) 1DP800(3S1F) |                          |                           |                          |                           | Yes            | Yes          |
|                   | Figure 17b             | 1DP8(7S1F) 1DP80(7S1F) 1DP800(7S1F) |                          |                           |                          |                           | Yes            | Yes          |
| 8                 | Figure 18a             | *                      | 4500                     | 2800                      | 800                      | 1000                      | Yes            | Yes          |
|                   | Figure 18b             |                         |                          |                           |                          |                           | Yes            | Yes          |
| 9                 | Figure 19              | 1D Rock 1-4            | 4500                     | 2800                      | 800                      | 1000                      | Yes            | Yes          |
| 10                | Figure 20              | 2DVTI 12x12 (1F2S)     | 4500                     | 1000                      | 800                      | 1000                      | Yes            | Yes          |
| 11                | Figure 22a             | 1DP12(1S1F) 2DVTI (1F2S) | 4500                     | 2800                      | 800                      | 1000                      | Yes            | Yes          |
|                   | Figure 22b             |                          |                          |                           |                          |                           | Yes            | Yes          |
|                   | Table 11               | 2D VTI (1F2S) 2D VTI (1F3S) 2D VTI (1F7S) 3D VTI (1F3S) |                          |                           |                          |                           |                  |              |
| 12                | Figure 23a             | 2DHTI (1F2S)           | 4500                     | 2800                      | 800                      | 1000                      | Yes            | Yes          |
|                   | Figure 23b             |                          |                          |                           |                          |                           | Yes            | Yes          |
|                   | Table 12               | 2D HTI (1F2S) 2D HTI (1F3S) 2D HTI (1F7S) 3D HTI (1F3S) |                          |                           |                          |                           |                  |              |
| 13                | Figure 24a             | Labyrinth              | 4500                     | –                         | 800                      | 1000                      | –              | –            |
| 14                | Figure 25              | 3D Rock 1              | *                        | *                         | *                        | *                        | Yes            | Yes          |
|                   | Figure 26              | 3D Rock 2              |                          |                           |                          |                           |                  |              |
Table 9 shows the effective velocity (in m/s) computed over the non-periodic formations defined in Table 3 using the three different methods listed below.

- Method 1 (M1) employs a FEM with a traditional fitting mesh technique.
- Method 2 (M2) uses a FEM with a non-fitting mesh with only one element in each repeated rock and without a precomputed matrix.
- Method 3 (M3) considers a FEM with a non-fitting mesh and a precomputed matrix.

This table also exhibits the Backus effective velocity $v_{eff}^B$ given by Eq. (2).

Table 9 reveals that the computation of the effective velocity through any of the aforementioned methods provides an excellent approximation to the Backus average velocity $v_{eff}^B$ (see equation 2). Moreover, the results obtained with methods two and three coincide. This validates the implementation of the precomputed matrix technique. The solution associated with a non-fitting mesh differs slightly from the one computed with a fitting mesh. To assess these discrepancies, Fig. 11 shows the velocity computed with non-fitting meshes against the number of subcells for different values of the fast material density, in the case of 1D Rock 4. For a large number of subcells per element, the error increases as function of the ratio between densities.

The optimal number of macro-elements to have the numerical error under control depends upon multiple parameters, including: (a) the user-selected tolerance error, (b) the frequency, (c) the ratio between densities, (d) the number of subcells in the original rock, and (e) the size of the original domain. For the cases showed in Fig. 11, we limit ourselves to $[(\rho_2/\rho_1)^{\rho_2/\rho_1}]$ macro-elements to discretize the original rock. Moreover, we consider a similar number of subcells for each macro-element.

Fig. 11 Influence of the number of subcells per element in the estimated effective compressional wave velocity solution. Non-periodic 1D Rock 4 sample excited at 10 Hz for multiple densities

4.4 Experiment 3: Rock-repetitions: one side versus two sides

We consider two periodic rocks. Figure 12 shows the effective velocity (obtained counting wavelengths) in the original rock, as well as the effect of repeating the rock at one or both sides of the original rock.

At low frequencies, the effective velocity is different from the Backus velocity $v_{eff}^B$ when considering only the original rock. But if we repeat it at one or both sides, then the two velocities match. A one-side repetition is computationally more efficient. At high frequencies, all simulations converge to $v_{eff}^T$.

The results of this experiment indicate we should repeat the rock at one side and guarantee a minimum number of wavelengths in the domain.

4.5 Experiment 4: Rock-repetitions: number of wavelengths

This experiment analyzes the number of times we should repeat the rock. For that, we use the samples 1D Rock 1 and 1D Rock 2.

Figure 13 studies the effect of the number of wavelengths contained in the domain on the effective velocity. We consider three cases: 10, 3, and 1 wavelengths of the solid. Aside from slight differences in the solution, all of them provide good approximations of the quantity of interest.

4.6 Experiment 5: Influence of density

At low frequencies, an increase in the density of the fast material diminishes the effective velocities (see Fig. 11). Figure 14...
investigates the effect of different density ratios $\rho_{\text{solid}}/\rho_{\text{fluid}}$ on the compressional wave velocity for two periodic rocks. The one-side repetition of the rock guarantees a domain size of $1\lambda_{\text{solid}}$.

We observe a decrease of the effective compressional wave velocity with the increase of the ratio $\rho_{\text{solid}}/\rho_{\text{fluid}}$ at low frequencies. The frequency that separates the Backus average zone and the transition zone takes smaller values when increasing this ratio. At high frequencies, the value of the compressional wave velocity is independent of the densities. These two observations agree with the theoretical limits discussed in Sect. 2.

**4.7 Experiment 6: Influence of porosity**

We consider the samples 1DP8(1S1F), 1DP8(3S1F) and 1DP8(7S1F) with porosities equal to 50%, 25%, and 12.5%, respectively. We repeat the rock at one-side to guarantee a domain size of $1\lambda_{\text{solid}}$. Figure 15 shows a decrease on the effective compressional wave velocity when the porosity diminishes. The three curves display a qualitatively similar profile—in terms of oscillations and frequency limits—in the transition zone. The frequency that separates the Backus average zone from the transition zone increases when augmenting the porosity.
4.8 Experiment 7: Influence of the size of the pore

In this experiment, we repeat the rock on one-side to guarantee \( 1 \lambda_{\text{solid}} \). Figure 16 illustrates the behavior of the effective velocity in three synthetic rocks: 1DP8(1S1F), 1DP8(1S1F) and 1DP8(1S1F), all of them of porosity 50% and size of the pores \((d_{\text{fluid}})\) equal to 125, 12.5, and 1.25 millimeters, respectively.

Figure 17a considers the synthetic rocks 1DP8(3S1F), 1DP8(3S1F) and 1DP8(3S1F) with porosity 25%. Figure 17b employs the rocks 1DP8(7S1F), 1DP8(7S1F) and 1DP8(7S1F) with porosity 12.5%.

In all case of Figs. 16 and 17 we observe a shift of the curves on frequency as the size of the pore decreases. We conclude the shift is independent of the porosity and density. These results agree with the theoretical 1D results (see Fig. 1): the Backus average zone appears when the ratio between the wavelength and the size of the pore is greater than one. When this ratio is much smaller than one, we are in the time average zone.
### 4.9 Experiment 8: Influence of the distribution of the sizes of the pore

We consider rocks with a specific size of the pore distribution by joining the rocks 1DP400(150T50F) with 1DP400(3T1F)–porosity equal to 25%—, and 1DP400(350T50F) with 1DP400(7T1F)–porosity equal to 12.5%—.

Figure 18 illustrates how the transition zone between low and high frequencies is wide if there are pores with different sizes in the same rock. In this case, the frequency that indicates the change from the Backus average zone to the transition zone is related to the largest size of the pore, whereas the frequency from the transition zone to the time average zone is associated with the smallest size of the pore.

### 4.10 Experiment 9: 1D Non-periodical formations

Figure 19 displays the effective velocity profiles over the rocks displayed in Table 3. The profiles converge to the theoretical bounds at low and high frequencies.
To assess FMM’s efficiency, we compare its effective velocities with the Wyllie time average $v_{\text{TA}}^e$. Table 10 shows that the two methods deliver equivalent results in 1D.

**Fig. 18** Effective compressional wave velocities computed counting wavelengths in samples with different size of the pore ($d_{\text{fluid}}$)

**Fig. 19** Effective compressional wave velocities computed counting wavelengths for the non-periodic rocks

**4.11 Experiment 10: Lateral extension**

This experiment analyzes the importance of the domain size in the perpendicular direction to the main P-wave propagation direction (controlled by the parameter $M$). For this, we test the sample 2DVTI 12x12(1F2S). We postprocess the solution over one vertical line located at the center of the rock.

Figure 20 reveals that at low frequencies, the domain should be repeated along its lateral dimension (perpendicular direction to the main P-wave propagation direction). In the remaining experiments, we will select $M$ to guarantee at least one $\lambda_{\text{solid}}$.

It is possible to repeat infinite times the rock in the perpendicular directions to the source. To do so, it is sufficient to mirror the original rock once in 2D (or four times in 3D) and impose periodic boundary conditions (see Fig. 21). While this is a viable venue, we did not explore it in this work.
Notice, however, that a similar alternative does not exist in the propagation direction due to the presence of the source.

4.12 Experiment 11: VTI rocks

This experiment compares the solution for the VTI Rock 2DVTI 12x12 (1F2S) defined in Table 4 with the solution computed for the Rock 1DP12(1F2S). We post-process the solution over one vertical line located at the center of the rock.

Figure 22 shows similar results for 1D and 2D. However, in the case of a large contrast between the two densities, the 2D solution exhibits additional oscillations in the transition zone before reaching the high-frequency velocity limit.

Table 11 shows a match between the velocity computed with the FMM and with the Wyllie time-average formula (3).
4.13 Experiment 12: HTI rocks

Figure 23 shows the effective P-wave velocity for the periodic rock 2DHTI 12x12(1F2T) defined in Table 4. In this case, the choice of the analysis line is crucial for the accurate computation of the effective velocity.

The effective compressional wave velocity computed by FMM matches with the value of the fast material, regardless the porosity (see Table 12). On the other hand, the velocity computed by the Wyllie time-average formula (3) is much lower. This result confirms that the use of the Wyllie time-average formula is invalid outside of VTI symmetries, as physically expected.

4.14 Experiment 13: The Labyrinth

In this experiment, we consider the labyrinth depicted in Fig. 9. At high frequencies, the first arriving wave circumvents the fluid by following the solid red line in Fig. 24a. Its effective velocity is approximately \( \frac{c_{\text{solid}}}{2} \).

Figure 24b displays the effective velocity computed with the FMM at the bottom of the domain as a function of space. These results confirm that the FMM is trustworthy and provides physically consistent velocities at all arriving points in a non-trivial domain.

4.15 Experiment 14: Real rocks

Figures 25 and 26 show the effective P-wave velocity average analyzed along five lines in a cross-section of 3D Rock1 (see Table 6), and 3D Rock 2, respectively.

Table 13 collects the values computed with FMM for the full 3D rocks as well as some of their cross-sections. As expected, the effective compressional wave velocity computed in the high-frequency regime for the 3D rock is in between the one computed for the cross-section and the sound velocity of the fastest material.

5 Conclusions

We propose a set of numerical methods to estimate the effective compressional wave velocity of heterogeneous rocks. At low frequencies, the PML pollutes the values of the computed effective compressional wave velocity. Thus, we extend the domain through rock repetition in order to guarantee at least two wavelengths in the propagation direction. To make the resulting problem computationally tractable, we employ non-fitting meshes, which introduce some controlled numerical errors. When carefully implemented, the resulting effective velocities exhibit acceptable accuracies. The Prony’s post-processing method provides accurate values of the effective compressional wave velocity in the Backus average zone, but the method diverges in the transition zone, where the behav-

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Table 12 Effective P-wave velocities computed with Time-Average and FMM. \( c_{\text{solid}} = 4500 \text{ m/s} \)

| Nomenclature | Porosity | \( \nu_{\text{eff}}^T \) (m/s) | FMM (m/s) |
|--------------|----------|------------------------------|-----------|
| 2D HTI (1F2S)* | 33.3% | 1770.49 | 4500.00 |
| 2D HTI (1F3S)* | 25% | 2086.96 | 4500.00 |
| 2D HTI (1F7S)* | 12.5% | 2541.18 | 4500.00 |
| 3D HTI_x (1F3S)** | 25% | 2086.96 | 4499.99 |
| 3D HTI_y (1F3S)** | 25% | 2086.96 | 4499.99 |

*Size of 1200 \times 1200 pixels
**Size of 100 \times 100 \times 100 voxels

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\( \nu_{\text{eff}}^T \) is the time-average effective compressional wave velocity.
Numerical results, in accordance with the existing theory, indicate the following: (a) an increase in the density of the fast material decreases the value of the effective compressional wave velocity at low frequencies. On the other hand, effective velocities at high frequencies become unaltered by these density changes, as predicted by the theory; (b) an increase in the porosity produces a decrease in the value of the effective compressional wave velocity. This decrease is more pronounced at high frequencies; (c) the presence of different sizes of the pore produces a widening of the transition zone since the most significant size of the pore is related to the frequency regime in which the Backus average is valid, while the smallest size of the pore characterizes the frequency for which the time average holds; (d) the Wyllie time-average formula fails outside of VTI rocks.

At high frequencies, the computation of the effective velocity by FMM matches with the theoretical limit expected in VTI rocks. We show the validity of this numerical method in higher spatial dimensions.

Table 13  Effective P-wave velocities computed by FMM and faster constituent sound velocity

| Formation      | $v_{eff}^{FMM\_2D}$ (m/s) | $v_{eff}^{FMM}$ (m/s) | $c_{fast}$ (m/s)  |
|----------------|---------------------------|-----------------------|------------------|
| 3D Rock 1      | 5946.94                   | 6031.15               | 6041.98          |
| 3D Rock 2      | 6415.495                  | 6607.81               | 6645.11          |

Fig. 24 Sketch of the labyrinth domain and the computed effective velocity at the bottom of the core by the FMM

Fig. 25 Average of effective P-wave velocity for a cross-section of 3D Rock 1

Fig. 26 Average of effective P-wave velocity for a cross-section of 3D Rock 2
Possible extensions of this work include the use of parametric solvers like the one presented in [41] for the low frequency spectrum to analyze simultaneously a group of rocks, and multilevel methods [47] for the medium frequency spectrum.

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