Reflector-preserved lithological upscaling
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SUMMARY

By combining Percolation models with lithological smoothing, we arrive at a method for upscaling rock elastic constants that preserves reflections. In this approach, the Percolation model predicts sharp onsets in the elastic moduli of sand-shale mixtures when the shales reach a critical volume fraction. At that point, the shale inclusions form a connected cluster, and the macroscopic rock properties change with the power-law growth of the cluster. This switch-like nonlinearity preserves singularities, and hence reflections, even if no sharp transition exists in the lithology or if they are smoothed out using standard upscaling procedures.

PROBLEM STATEMENT

Equivalent medium theory that models specular reflections has been, and and probably still is, one of the main challenges in current-day rock physics. The reason for this challenge lies in the fact that equivalent medium theory generally derives from a spatial or ensemble averaging argument during which fine-scale medium variations are “averaged out”. This is problematic problematic because reflections are washed out as well.

While this type of averaging has made a major impact—not least thanks to Mike’s major contributions in describing the quasi-static behavior of waves, including anisotropy induced by fine-scale heterogeneity (Schoenberg and Muir, 1989) or of preferential-oriented cracks (Haugen and Schoenberg, 2000; Daley et al., 2006)—finding an averaging procedure that preserves specular reflections continues to be more illusive. The reason for this is that smoothing intrinsically mollifies singularities. Consequently, transitions where the derivative in the elastic medium properties becomes large are washed out and this explains why waves cease to reflect specularly in media that have been smoothed (using equivalent medium theory) to length-scales that are too close to the dominant wavelength. This observation was made early on by Folkstad and Schoenberg (1992) and proved extremely useful for the purpose of forward modeling. However, because the averaging-length scale required for the forward modeling needs to be approximately ten times finer than the dominant wavelength, it is perhaps a challenge to use these results to formulate an inverse problem.

One could argue that there are two possible remedies to address this issue. First, one may opt to replace linear windowed-equivalent medium averaging by an approach where the medium fluctuations are nonlinearly averaged. In mathematical terms, this means that we could nonlinearly approximate the medium fluctuations by increasing thresholds on the coefficients of the shift-invariant discrete wavelet transform. For the Haar wavelet, this approach is reminiscent of the nonlinear procedure known as “blocking”. Recent developments in the field of compressive sensing (see e.g. Herrmann et al., 2009), which achieve super resolution, could provide access to these large coefficients. However, despite the fact that these approaches preserve singularities, and hence, reflectivity, they lack a clear physical interpretation—i.e., it is somewhat to envision how this sort of thing would work for something as intricate as solving the upscaling problem. Therefore, we would like to explore another possibility and that one is related to the existence of critical phenomena in statistical mechanics. There, a system changes its behavior critically as a function of some order parameter (read ‘some volume fraction dependent on some spatial coordinate). An example of this type of behavior is the physical property of magnetization, which occurs when the density of aligned spins reaches a critical threshold. Below this threshold, the material is non-magnetic while above the critical point the degree of magnetization increases rapidly as a function of decreasing temperature that determines the density of aligned spins. Using a connectivity argument, Stauffer and Aharony (1994), and many others, developed Percolation theory, which explains this type of phenomenon. The argument is that there is a critical concentration at which the aligned spins form a connected cluster, and that point coincides with the critical point at which the material becomes magnetic. This model is not limited to magnetic materials and is known to describe the behavior of so-called transport properties that depend on connectivity, including electric conductivity, sustainability of shear, and the onset of permeability.

In this paper, we present an averaging method that incorporates these Percolation ideas. We do this by considering a rock consisting of a mixture of sand and shales, and we ask ourselves the question: Can we expect a critical point to occur as a function of the volume fractions, and hence can we predict the occurrence of a specular reflection, when the composition of bi-compositional reaches a point at which clusters of the stiffer property of magnetization, which occurs when the density of aligned spins reaches a critical threshold. Below this threshold, the material is non-magnetic while above the critical point the degree of magnetization increases rapidly as a function of decreasing temperature that determines the density of aligned spins. Using a connectivity argument, Stauffer and Aharony (1994), and many others, developed Percolation theory, which explains this type of phenomenon. The argument is that there is a critical concentration at which the aligned spins form a connected cluster, and that point coincides with the critical point at which the material becomes magnetic. This model is not limited to magnetic materials and is known to describe the behavior of so-called transport properties that depend on connectivity, including electric conductivity, sustainability of shear, and the onset of permeability.

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First, we will adapt the Percolation-based model introduced by the authors (Herrmann and Bernabé, 2004a; Bernabé et al., 2004) to model sand-shale mixtures. Second, we combine this model with an averaging method that acts on the lithology. This approach differs from current approaches where the elastic properties (e.g., bulk modulus) are typically averaged. Instead, we propose to average spatial variations in sand-shale volume fractions, and use our Percolation model to map these to the elastic properties. We will illustrate the behavior of this model with a synthetic lithology log.

PERCOLATION FOR SAND-SHALE MIXTURES

Although the lithology of sedimentary crust is likely to be complex, we will assume here that, as far as modeling the elastic properties is concerned, we can use a simplified bi-compositional model with volume fractions that depend on the vertical coordinate only. We consider a region where only two lithologies are involved, namely sand and shale (see Fig 1, where the black inclusions refer to Shale). At the top of the co-existence region, the material exclusively consists of the weak
phase (LP). With increasing depth, inclusions of the stronger phase (HP) are progressively formed until only HP material remains. For the sake of simplicity, we assume that the volume fractions of HP and LP, \( p \) and \( q = 1 - p \), are linear functions of depth \( z \) (See Fig. 1 (a)). However, this assumption is non-essential and more complicated functions of \( z \) can be used as we will discuss below. At a critical depth \( z_c \), which corresponds to the percolation threshold \( p_c = p(z_c) \), an infinite, connected HP cluster is formed. It is important to note that, below \( z_c \), not all HP inclusions belong to the infinite cluster. Isolated HP inclusions can still be found, embedded in the remaining LP material and forming with it a mixture (\( M \)). In summary, above \( z_c \) we have a weak LP matrix containing randomly distributed, non-percolating, strong HP inclusions. Below \( z_c \), a strong HP skeleton is intertwined with the weaker, mixed material \( M \). Percolation theory predicts that, in the vicinity of the percolation threshold, the volume fraction \( p^* \) of HP material that belongs to the infinite cluster is zero for \( p < p_c \) (i.e., below \( z_c \)) and has a power-law dependence on \( (p - p_c) \) for \( p \geq p_c \) (Stauffer and Aharony, 1994). For convenience, we assume that this power-law extends to the bottom of the mixing region (i.e., \( p = 1 \)). Hence, \( p^* \) is given by:

\[
p^* = p \left( \frac{p - p_c}{1 - p_c} \right)^\beta,
\]

where the exponent \( \beta \) is a positive, real number, which in general, is considered to be “universal” (i.e., it only depends on dimensionality, but, for example, not on interconnection topology of the inclusions). Site Percolation theory predicts \( \beta = 0.41 \) in three-dimensional discrete lattices in the case of an isotropic, \( \delta \)-correlated, stochastic process (Stauffer and Aharony, 1994). However, universality of the Percolation exponents is unlikely to hold in the case of the sand-shale transitions. Indeed, the stochastic process responsible for inclusion emplacement should presumably display long-range, possibly anisotropic, spatial correlation owing to the elastic interaction of an inclusion with its surroundings (Kaganova and Roitburd, 1988). This causes a change of the exponent \( \beta \), especially since the inclusion connectivity problem belongs to continuum rather than lattice percolation (e.g., Isichenko (1992); Sahimi and Mukhopadhyay (1996)).

Below \( z_c \), the volume fractions for the mixed material \( M \) is, of course, given by \( q^* = 1 - p^* \). For modeling \( M \), we need the volume fractions of its LP and HP parts, \( q_M = (1 - p)/((1 - p) + (p - p^*)) \) and \( p_M = (1 - q_M) \), respectively. A simple calculation yields:

\[
p_M = 1 - \frac{q}{1 - p \left( \frac{p - p_c}{1 - p_c} \right)^\beta}.
\]

It is well-known in solid state physics and mechanical engineering that a binary mixture is elastically strong if its strong component forms a connected cluster and weak otherwise (e.g., Ledbetter et al. (1984); Gai et al. (1984); Deptuck et al. (1985); Turosov et al. (1986); Marion and Nur (1989); Favier et al. (1997); Novikov et al. (2001) for other applications of percolation theory to mechanics see de Gennes (1976), or Roux and Guyon (1985)). Thus a realistic elastic model of the coexistence region must take into account the connectivity (or lack of connectivity) of the HP phase.

We begin by assuming that both the HP and LP phases are elastically isotropic and that the HP inclusions have a spherical shape so that the HP/LP mixture is locally (statistically) isotropic as well. Hashin and Shtrikman (1962) demonstrated that the elastic moduli of statistically isotropic, binary mixtures are tightly bounded by two quantities known as the Hashin-Shtrikman (HS) bounds. More importantly, it has been shown that the HS bounds can effectively be used to model the elastic properties of materials consisting of isolated spherical inclusions randomly distributed inside a continuous (connected) matrix (e.g., Mori and Tanaka (1973); Benveniste (1987)), even for non-dilute concentrations of inclusions (e.g., Luo and Weng (1987)). Note that the model accuracy increases with decreasing elastic contrast between the two components of the mixture. The upper HS bound must be used when the strong component forms the connected matrix while the lower one applies otherwise (e.g., Marion and Nur (1989); Favier et al. (1997); Novikov et al. (2001); Saidi et al. (2003)). Accordingly, the bulk modulus \( K \) of the co-existence region above \( z_c \) is given by the lower HS bound:

\[
K = K_{LP} \left( 1 + \frac{p(K_{HP} - K_{LP})}{q(K_{HP} - K_{LP})a_{ILLP} + K_{HP}} \right),
\]

where \( a_{ILP} = 3K_{LP}/(3K_{LP} + 4G_{LP}) \), and the subscripts LP and HP refer to the two lithologies involved in the transition. A similar relation is obtained for the shear modulus, except that \( a_{ILP} \) is replaced by \( b_{ILP} = 6(K_{LP} + 2G_{LP})/(5(3K_{LP} + G_{LP})) \). Below \( z_c \), we must switch to the higher HS bound:

\[
K = K_{HP} \left( 1 + \frac{q^*(K_{M} - K_{HP})}{p^*(K_{M} - K_{HP})a_{ILLP} + K_{HP}} \right),
\]

where \( K_{M} \) is the bulk modulus of the mixed material \( M \). Since the HP inclusions in \( M \) are isolated, \( K_{M} \) is calculated using the lower HS bound:

\[
K_{M} = K_{LP} \left( 1 + \frac{pM(K_{HP} - K_{LP})}{qM(K_{HP} - K_{LP})a_{ILLP} + K_{HP}} \right).
\]

Similar equations can be written for \( G \), where \( a_{ILP} \) and \( a_{ILH} \) are replaced by \( b_{ILP} \) and \( b_{ILH} \). Hence, we can calculate \( K \) and \( G \) for all values of \( p \) between 0 and 1.

**PERCOLATION-INDUCED REFLECTIVITY**

The above Percolation-based model predicts rapid changes in the transport properties as a function of the volume fractions of bi-compositional mixtures. For mixtures of two materials, e.g. one hard one soft, the behavior of such a mixture is well understood. Less well-known is the fact that the mixture undergoes an abrupt change when the volume fraction of the stronger material reaches a point where the inclusions connect. At that critical point, a fractional-order discontinuity is created in the elastic properties of the mixture.

So, we have a \( \beta \)-order singularity in the elastic bulk moduli as the critical depth \( z_c \) is approached from below. Thus, the fluctuations in the elastic bulk moduli with respect to a smoothly varying background obey the following power-law relation,

\[
\Delta(z) \propto \begin{cases} (z - z_c)^\beta & z \geq z_c \\ 0 & z < z_c \end{cases}
\]
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Figure 1: Site Percolation Model (SPM) (adapted from Herrmann and Bernabé, 2004b) of the coexistence region. (a) Depth-profile of the mixture density, \( \rho = \varphi_p p_{\text{LP}} + \varphi_H p_{\text{HP}} \), which does not behave singularly for a smoothly varying composition \( \varphi(z) \). (b) Schematic illustration of the phase transition by formation of the strong lithology (HP) inclusions in a weak lithology (LP) matrix. The HP inclusions (black) are assumed to be horizontal-oriented ellipsoids. At the critical depth \( z_c \) (dotted line) the HP inclusions percolate, form an infinite cluster containing long vertical dendrites of the LP matrix and some isolated HP inclusions. (c) Corresponding shear wavespeed profile (solid line) showing a singularity at \( z_c \). The singularity is clearly apparent in the derivative (dashed line). The magnitude of the singularity depends on the difference between the mixing laws (here Reuss and Voigt averages). The value for the singularity order was taken to be \( \beta = 0.30 \).

with \( 0 < \beta < 1 \) and where the symbol \( \Delta \) refers to fluctuations in the bulk modulus, \( \Delta K = K - K_0 \), or shear modulus, \( \Delta G = G - G_0 \), with the barred quantities representing (moving) averages such that \( \Delta K, \Delta G \ll 1 \). Notice that Eq. 6 implies divergence of the \( \alpha \)-order derivative at (with \( \alpha > \beta \)). Conversely, the lithology, as expressed by the volume fractions \( (\varphi_p \text{ and } \varphi_H) \) and the mixture density \( \varphi(z) = \varphi_p p_{\text{LP}} + \varphi_H p_{\text{HP}} \), varies smoothly. Since \( \beta \) cannot be theoretically constrained, we must instead use seismic waves to probe the singularity and estimate the exponent. Refer to Maysami and Herrmann (2008) where seismic data was used to constrain the exponent associated with the opal-A (Amorphous) to opal-CT (Cristobalite/Tridymite) transition in the North Sea near the Shetland Islands.

In summary, critical Percolation phenomena (Herrmann and Bernabé, 2004a; Bernabé et al., 2004) have profound implications on the interpretation of seismic discontinuities, which in this case can no longer be attributed to steep gradients in the composition. Instead the discontinuities are due to an intricate mechanism which, when well understood, provides (i) complementary information on the composition of the subsurface and (ii) a method to do lithological upscaling. Because of the “switch” at the critical point, upscaling by smoothing the lithology, e.g. by smoothing of the volume fractions of shale in sand-shale mixtures, no longer washes out the reflectivity, an unwanted effect of many equivalent-medium based upscaling techniques. Instead, reflectors will be preserved.

LITHOLOGICAL UPSCALING

To understand how to incorporate the Percolation switch in upscaling let us study the behavior of sonic wavespeeds as a function of the compliance \( K \) calculated from volume fraction \( \varphi \) that is a function of depth. From mixing theory, it is known that the compliance for any rock mixture lies within the Hashin-Shtrikman (HS) bounds (See Fig. 2). According to our model, the rock mixture follows for low volume fractions the lower-HS bound and as it reaches the critical point, the compliance displays a ‘cusp-like’ behavior departing the lower-bound, followed by a ramping up towards the upper bound (the red line in Fig. 2). As we will show, this ‘switch-like’ behavior will have a distinct impact on upcaled velocities, and in particular on reflectivity. This can be understood because reflectivity entails a differentiation with respect to the medium properties and this differentiation is sensitive to cusp-like singularities.

To illustrate upscaling according to our Percolation model, we study the lithology of the synthetic well-log plotted in Figure 3 (kindly provided by Dave Wilkinson). We use the volume fractions from this log to calculate the velocities with the model presented in this paper. We use published values for the bulk moduli of pure sand and pure Shale in the equations. The calculated velocities for the detailed synthetic well are plotted in Figure 4. Because the detailed lithology profile contains sharp transitions, we observe sharp transitions in the both velocity profiles. We also observe significant differences whenever the volume fraction profile passes through the critical volume fraction of \( \varphi_c = 0.32 \) (see Fig. 2). Even though both profiles contain sharp zero-order transitions (these correspond to scale exponent \( \beta = 0 \)), the profile yielded by our model contains additional singularities associated with the Percolation switch. The cross plots for these velocities included in Figure 5 reveals the presence of this smoother type of singularity reflected in the cusp-like feature that is not present in the velocity predictions using equivalent medium theory.

This subtle difference proves extremely important for upscaling when this is done by averaging the lithology instead of the density and elastic moduli as is commonly done. Mathematically, we can represent this upscaling to the scale \( \sigma \) via

\[
\varphi_{\sigma}^v(z) = P\left(\varphi + \varphi_{\sigma}\right)(z),
\]

with \( \varphi_{\sigma} \) a Gaussian bell shape with width \( \sigma \), \( p(z) \) the volume fraction profile, and \( P(...) \) represents the Percolation-switch model. Because we are interested in reflectivity (or in converted waves), we plot in Fig. 6 the derivatives for both velocity profiles for increasing upscalings (from left to right). As expected, the reflectivity obtained after equivalent medium averaging disappears as the scale increases. However, the presence of the switch in our model, preserves reflections at locations where the upscaled lithology log crosses the critical volume fraction.

CONCLUSIONS

We presented a upscaling methodology during which reflections are preserved that otherwise would have been washed out during conventional upscaling techniques. Our contribution lies in the combination of a nonlinear switch-like Percolation model with a linear smoothing procedure that acts on the spatial variations of volume fractions of sand-shale mixtures. This approach in interesting because it may give us access to the lithology by studying reflections.

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Figure 2: HS bounds for the elastic compliance (black) as a function of the lithology (volume fraction $p$) and the cusp-like behavior according to our critical percolation-based model (red).

Figure 3: A well with a synthetically generated lithology log for the volume fractions of shale as a function of depth.

Figure 4: Velocities calculated with conventional equivalent medium theory (blue) and our Percolation-based model (green). Notice that there are significant differences between the values. Also remark, that both logs contain edges because of the sharp edges present in the lithology log itself (cf. Fig. 3).

Figure 5: Cross plots calculates from the velocity logs plotted in Fig. 4. Notice, the presence of the cusp for the crossplot of the velocities calculated with the Percolation model (red).

Figure 6: Reflector-preserved lithological upscaling. (a) Upscaled reflection traces according to the classical upscaling based on equivalent medium theory. (b) The same but now from the Percolation model. Notice the vanishing of the reflectivity for coarser scales with the classical upscaling and the preservation of the events related to our nonlinear upscaling model.
REFERENCES


