Exact and Approximate Solid Substitution Transforms

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Summary

Using volume averaging we generalize Gassmann's (1951) isotropic equation for fluid-filled porous media to solid-filled porous media with disconnected pores. This exact equation can be used as an analog of Gassmann's fluid substitution transform for solid-filled porous media, since it predicts the change in effective moduli upon solid substitution, depending *only* on porosity, elastic stiffness of frame and pore-solids, and initial effective stiffness. This solid substitution transform is *exact* if induced pore-stress field during a specific experiment is homogeneous. For all other cases, this equation is just an approximation, and has also been suggested by Ciz and Shapiro (2007). We note that this approximation does not *always* fall within rigorous solid substitution bounds, but under specified conditions, it is a *strict bound* on solid substitution. We therefore discuss the factors which govern the accuracy and applicability of this approximation. We also present a general solid substitution approximation which requires, in addition to porosity, at least one of the following: ultrasonic fluid filled un-drained modulus, saturated modulus with a hypothetical solid or crack porosity.

Introduction

Gassmann's equation (1951) is known as a fluid substitution equation, as it predicts the change in effective elastic response of a fluid-saturated porous medium by replacing one pore-fluid with another. It makes this prediction without detailed knowledge of pore geometry, except for porosity and the necessary condition of homogeneous pore-pressure. Gibiansky and Torquato (1998) proved that Gassmann's equation is, in fact, a strict lower bound on the change in bulk modulus upon fluid substitution and suggested an improved upper bound, tighter than the corresponding HS upper bound (Hashin and Shtrikman, 1963). For solid-filled porous media, Berryman and Milton (1988) have suggested rigorous bounds on the change in effective elastic properties due to solid substitution (referred here as BM bounds). Although these bounds are tighter than HS bounds, they still provide only a wide range of possible solutions for solid substituted composites. Ciz and Shapiro (2007) generalized Gassmann's equation for solid-filled porous media with a heuristic effective compressibility parameter. Approximating this parameter, Ciz and Shapiro proposed an approximate solid substitution equation. Recently, Saxena et al., (2012, personal communication) generalized *two-phase* Gassmann's relations for linear elastic solid filled porous media using volume averaging (Whitaker, 1999) for effective bulk modulus. We present the corresponding effective shear modulus equation. Details of the derivation will be presented elsewhere. We discuss necessary conditions for an exact substitution and illustrate where the additional stiffness parameter originates, and how it affects the uniqueness and accuracy of the solid substitution process. Since the condition for exact substitution is very restrictive, we discuss the validity of approximate solid substitution.

Theory and Derivation

Following the thermodynamic study presented by de la Cruz et al. (1993) and subsequent work by Hickey et al. (1995) and Spanos (2009), we derive the macroscopic equations of motion for an isotropic composite with solids *A* (pore-solid) and *B* (frame-solid). Next, we obtain transforms which relate two effective moduli of the composite media, one each for effective bulk and shear. Both transforms have the same functional form:

$$\xi_{ud} = \frac{\eta^A\left(\frac{1}{\xi^B}-\frac{1}{\xi^A}\right)+\left(\frac{1}{\xi^B}-\frac{1}{\xi_{bc}}\right)}{\frac{\eta^A}{\xi_{bc}}\left(\frac{1}{\xi^B}-\frac{1}{\xi^A}\right)+\frac{1}{\xi^B}\left(\frac{1}{\xi^B}-\frac{1}{\xi_{bc}}\right)} \quad (1)$$

where η^A is the volume fraction (porosity) of solid *A*. ξ_{ud} is the effective solid-filled or un-drained elastic modulus. When ξ is replaced by K or μ we refer to bulk or shear equations, respectively. $K^{A,B}$ (when $\xi = K$) are the elastic bulk moduli of solids *A* and *B*, respectively. $\mu^{A,B}$ (when $\xi = \mu$) are the elastic shear moduli of solids *A* and *B*, respectively.

K_{bc} is the effective bulk modulus with a constraint that the volume averaged incremental pore-pressure is kept zero with no constraint on the induced volume averaged pore-shear stress or point-by-point spatial deviation of pore-pressure. If for a specific pore-geometry, no point-by-point pore-shear stress is induced then K_{bc} can be approximated by un-relaxed frame bulk modulus (K_{sq}), suggested by Mavko and Jizba (1991). If the induced pore-pressure is homogeneous or zero everywhere in the pore solid, $K_{bc} = K_{zb}$. K_{zb} is exactly the undrained bulk modulus of a composite with the same geometry, solid frame and porosity but with a hypothetical solid of zero bulk modulus ($K^A = 0$) and finite shear modulus (μ^A). If no traction is induced at the pore-boundaries during the K_{bc} experiment, then $K_{bc} = K_{dry}$.

μ_{bc} is the effective *pure-shear* moduli with a constraint that the diagonal components of the volume averaged pore-stress tensor are kept zero, with no constraint on induced

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volume averaged shear stress or point-by-point spatial deviation of diagonal components of pore-stress tensor. Similar to the bulk modulus case, if no point-by-point pore-shear stress is induced then μ_{bc} can be approximated by Mavko and Jizba's un-relaxed frame shear modulus (μ_{sq}). If no traction is induced at the pore-boundaries during the μ_{bc} experiment, then, $\mu_{bc} = \mu_{dry}$. For convenience we will refer to Eqn. 1 as the following transform

$$\xi_{ud} = f(\xi_{bc}, \xi^{A}, \xi^{B}) \qquad (2)$$

For Eqn. 1 to be an exact solid substitution transform, starting with the un-drained effective modulus ($\xi_{ud}^{(1)}$) with pore-filling solid *A1* (K^{A1}, μ^{A1}) to predict the exact effective solid-filled modulus ($\xi_{ud}^{(2)}$) with pore-filling solid *A2* (K^{A2}, μ^{A2}), ξ_{bc} must remain invariant during the substitution process. This clearly, in general, requires homogeneity of the induced pore-stress field. The transform can be written as

$$\xi_{ud}^{(2)} = \Gamma\left(\xi_{ud}^{(1)}, \xi^{B}, \xi^{A1}, \xi^{A2}\right) \qquad (3)$$

For this study we assume that frame solid *B* is stiffer than pore-filling solids *A1* and *A2*, both in bulk and shear. Also we only consider cases with $(K^{A2} - K^{A1})/(\mu^{A2} - \mu^{A1}) > 0$.

Exact Solid Substitution

It is well known that exact substitution relations exist for any geometry corresponding to HS bounds, since an upper/lower bound with one pore-filling solid goes to another upper/lower bound with another pore-filling solid. These geometries are non-unique and various authors (Gibiansky and Sigmund, 2000) have discussed different geometric realizations of these bounds, such as coated spheres, matrix laminates, etc. All of these realizations have one common feature: if these structures are subjected to macroscopic confining pressure, stresses and strains are homogeneous and no shear stress is induced in the inclusion solid (solid *A* for upper bound and solid *B* for lower bound). This is a necessary condition for realizing HS bounds for effective bulk modulus.

For Eqn. 1 to be a consistent solid substitution equation for geometries that realize the HS upper and lower bulk modulus bounds, we must have $K_{bc} = K_{dry}$ and $K_{bc} = K_{zb}$, respectively, which can be checked by inverting K_{bc} from HS bounds for K_{ud}. This suggests

- Eqn. 1 for effective bulk modulus is an exact solid substitution equation for the upper HS bound. It is also an exact solid substitution equation for the lower HS bound, if and only if, the shear stiffness of the pore-solid does not change upon substitution.
- An exact solid substitution transform for effective bulk modulus can exist even if the pore-filling has a non-zero shear stiffness as long as the induced pore-pressure in the pore-solid is homogeneous during the K_{bc} experiment.

Similar to effective bulk, all geometries which realize the HS shear modulus bounds have one common feature: if subjected to pure shear, shear stress in the inclusion solid is homogeneous and no pressure is induced. Therefore, Eqn. 1 is also consistent with the upper HS shear modulus bound, since the conditions for realizing HS upper bound for effective shear and $\mu_{bc} = \mu_{dry}$ in Eqn. 1 are exactly the same. However, unlike the lower HS bulk modulus bound, Eqn. 1 cannot be used as an exact solid substitution transform for any geometry that realizes the lower HS shear modulus bound. Since the induced stress field in the pore-solid is not necessarily homogeneous during the μ_{bc} experiment, which does not guarantee invariance of μ_{bc} during solid substitution.

Eshelby (1957) proved that the strain field within an ellipsoidal inclusion in an infinite elastic matrix is uniform and is linearly related to the applied external strain field. Therefore, for composites with identical stiff ellipsoidal inclusions, Eqn. 1 will be a very good approximation, since the stresses induced during ξ_{bc} will be quite homogeneous.

Approximate Solid Substitution and Inequalities

For any composite the value of ξ_{bc} depends on the details of interaction between the pore geometry and stiffness of the pore-filling solid. Therefore, changing pore-solid also changes ξ_{bc}, except for the cases discussed above. For solid substitution we need to replace ξ_{bc} with an effective modulus which remains invariant during the substitution process. Ignoring the contribution of tractions at the boundaries we can approximate ξ_{bc} with effective dry modulus, ξ_{dry} as,

$$\xi_{ud} \approx \xi_{ud}^{C-S\ approx.} = f\left(\xi_{dry}, \xi^{A}, \xi^{B}\right) \qquad (4)$$

Eqn. 4 is the approximate solid substitution equation suggested by Ciz and Shapiro (2007), hence we will refer to this equation as the *C-S approx.* throughout this paper. Since ignoring the effects of tractions can only make the modulus softer, we must have

$$\xi_{bc} \geq \xi_{dry} \qquad (5)$$

The approximate effective solid-filled modulus $\xi_{ud}^{C-S\ approx.}$ obtained from Eqn. 4 starting with dry bulk

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modulus ξ_{dry} will always be less than or equal to ξ_{bc} and thus will under predict the actual effective modulus ξ_{ud} bounded by the upper BM bound as

$$\xi_{ud} \epsilon \left[\max\{\xi_{ud}^{C-S\ approx.}, \xi_{ud}^{BM-}\}, \xi_{ud}^{BM+}\right] \quad (6)$$

where $\xi_{ud}^{BM\pm}$ are the BM bounds for ξ_{ud}. The predicted *C-S approx.* effective modulus $\xi_{ud}^{C-S\ approx.}$ will be within the BM bounds for ξ_{ud} if

$$\Gamma(\xi_{dry}, \xi^{B}, \xi^{A1} = 0, \xi^{A2}) \geq \xi_{ud}^{BM-} \qquad (7)$$

Eqn. 7 is always satisfied for any arbitrary geometry fluid-filled porous media, for which case $\xi_{ud}^{C-S\ approx.}$ is a strict lower bound for ξ_{ud}. For arbitrary geometry solid-filled composites, Eqn. 7 is not always satisfied. The corresponding condition if starting with the effective solid-filled modulus $\xi_{ud}^{(1)}$ to predict the modulus $\xi_{ud}^{(2)}$ is,

$$\Gamma\left(\xi_{ud}^{(1)}, \xi^{B}, \xi^{A1}, \xi^{A2}\right) \geq \xi_{ud}^{(2)BM-}$$

if $(K^{A2} \geq K^{A1})$ and $(\mu^{A2} \geq \mu^{A1})$, otherwise

$$\Gamma\left(\xi_{ud}^{(1)}, \xi^{B}, \xi^{A1}, \xi^{A2}\right) \leq \xi_{ud}^{(2)BM+} \qquad (8)$$

$\xi_{ud}^{(2)BM\pm}$ are the BM bounds for $\xi_{ud}^{(2)}$, respectively. Using Eqn. 8 bounds on $\xi_{ud}^{(2)}$ can be constructed.

Effect of initial effective stiffness on solid substitution

To illustrate the implications of Eqn. 7 we plot (see Figure 1) the minimum ξ_{dry} for which *C-S approx.* will give predictions falling within the HS bounds for ξ_{ud}. We note that for low porosities (less than 0.3), a significant portion of physically realizable ξ_{dry} does not satisfy Eqn. 7. Furthermore for a given porosity, this portion increases with increasing stiffness contrast between the substituted pore-solids. For comparison, we numerically compute all effective moduli for four granular pack geometries (as shown in Figure 2) and compare the numerically obtained ξ_{ud} with $\xi_{ud}^{C-S\ approx.}$. All four geometries obey Eqn. 7.

Clearly, the *C-S approx.* does not yield good estimates for soft porous media, regardless of the pore geometry. Furthermore, Eqns. 4 and 8 also suggest that the *C-S approx.* will underestimate the magnitude of change in effective modulus due to solid substitution. Better approximations can be achieved if we approximate the effective modulus ξ_{bc} with ξ_{sq} instead of ξ_{dry} as

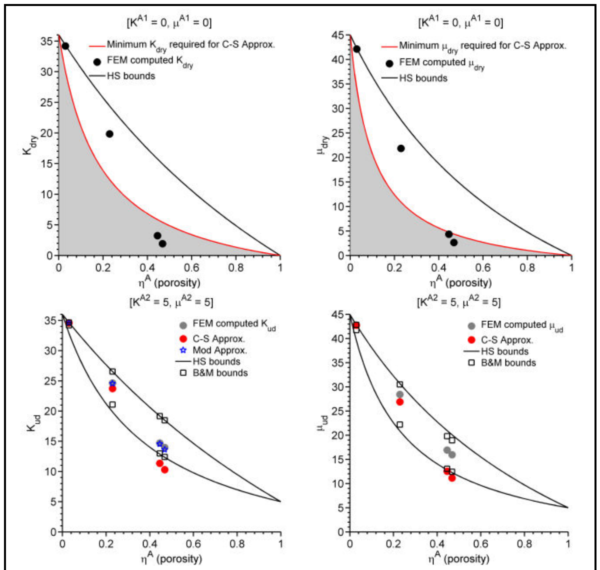

Figure 1: Top: minimum required dry modulus (bulk: left; shear: right) for C-S approx. to be within bounds for solid-filled bulk modulus with pore-solid A2 (Quartz frame: bulk 36 (GPa) and shear 45 (GPa)). FEM computed dry moduli shown in black circles. Bottom: FEM computed effective solid-filled bulk (left) and shear (right) moduli (grey circles) compared with C-S approx. solid-filled moduli (red circles). Modified approx provides better estimates for bulk modulus. All units in GPa.

$$\xi_{ud} \approx \xi_{ud}^{Mod\ approx.} = f\left(\xi_{sq}, \xi^{A}, \xi^{B}\right) \qquad (9)$$

This approximation requires additional knowledge of the pore-geometry, for example crack density, etc, or ultrasonic measurements. Specifically, for the effective bulk modulus when the pore-solid shear stiffness is large, the modified approximation instead takes the form

$$K_{ud} \approx K_{ud}^{Mod\ approx.} = f(K_{zb}, \xi^{A}, \xi^{B}) \qquad (10)$$

This is so because K_{zb} contains the contributions of shear tractions as in K_{bc} and only ignores the heterogeneity of induced pore-pressure. Therefore, Eqn. 3 will provide very good estimates if the pore shear stiffness does not change during solid substitution since K_{zb} will be invariant for a given pore geometry.

Effect of pore geometry on solid substitution

Next, we consider four stiff pore geometries, grouped in two sets. All four geometries obey the necessary condition in Eqn. 7. The first set includes two geometries: spherical pores and arbitrary shape pores whereas the second set includes the same geometries as in the first set but with added flat tetrahedron shape cracks (Figure 3).

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Exact and Approximate Solid Substitution

We note that the difference between the numerically calculated ξ_{ud} and $\xi_{ud}^{C-S\ approx.}$ generally increases with pore-filling stiffness contrast and crack porosity (Figure 4). The difference ξ_{ud} and $\xi_{ud}^{C-S\ approx.}$ is an order of magnitude larger for arbitrary shape pore geometry as compared to the spherical pore geometry, although both geometries have similar dry moduli and porosity. This is mainly due to non-ellipsoidicity of arbitrary shape pore geometry since both geometries have disconnected pores and are devoid of cracks.

The goal of this section was to highlight how pore geometry affects the accuracy of solid substitution transforms with controlled simulation parameters, and although the difference between numerically calculated ξ_{ud} and $\xi_{ud}^{C-S\ approx.}$ is relatively small for the four stiff geometries considered here, in practical situations this difference will be governed by the extent of pore disconnectedness, pore shape, crack density, contrast in elastic properties of the substituted solids and initial effective elastic properties of the composite, as shown in the previous section. While in extreme cases this difference may be substantial, for the four geometries the C-S approx. is reasonably good.

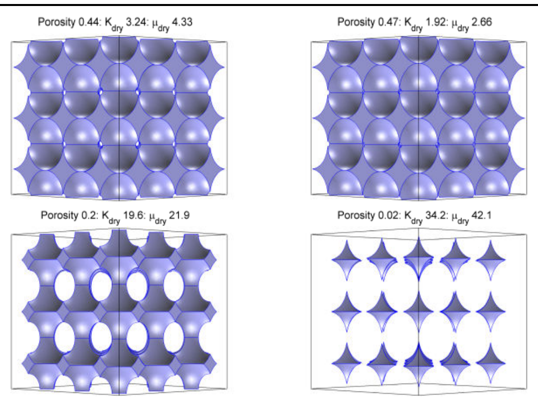

Figure 2: Four pore geometries for FEM calculations shown in Figure 1. Quartz frame is transparent.

Conclusions

We have generalized Gassmann's equation for porous media with solid-filled disconnected pores using volume averaging, Eqn. 1 in this paper. This generalized equation can be used as an exact solid substitution equation if the induced stress field is homogeneous during the experiment ξ_{bc} , which is satisfied by Eshelby's ellipsoidal inclusions and by any arbitrary geometry realizing HS bounds, except for the lower HS shear modulus bound.

We note that the *C-S approx*. does not always fall within rigorous bounds (Eqns. 7 and 8). Furthermore, it underestimates the change in magnitude of effective solid-filled modulus due to solid substitution. Nevertheless, C-S approximation generally provides good estimates for composites with stiff ellipsoidal pores and requires porosity as the only geometric input. We find that the accuracy of this approximate equation negatively correlates with: crack density, pore-disconnectedness, non-ellipsodicity of pores, contrast in stiffness of initial and substituted pore-filling solids, and initial effective stiffness of the porous media.

We present tighter solid substitution bounds (Eqns. 6 and 8) valid under specified conditions, and general approximate solid substitution equations (Eqns. 9 and 10) which requires additional measurements. In certain cases, ultrasonic/un-relaxed fluid saturated un-drained measurements are more useful than dry measurements for solid substitution.

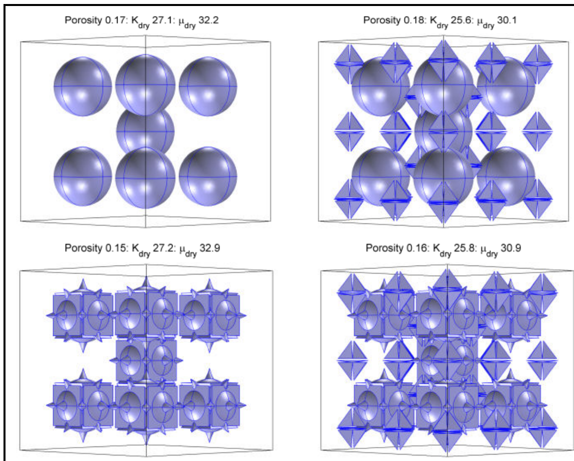

Figure 3: Four pore geometries for FEM calculations shown in Figure 4. Quartz frame is transparent.

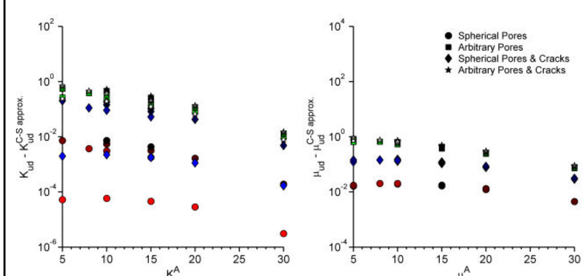

Figure 4: Difference between FEM computed solid-filled effective modulus and C-S approx.predicted modulus. Effective bulk (left) and shear (right) colorcoded with pore-filling solid's shear and bulk moduli, respectively. The colorcoded pore-filling shear modulus varies between 0 and 15 GPa for the effective bulk modulus plot and viceversa for effective shear modulus. Quartz frame and all units in GPa.

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