Simulation of the Bulk Modulus of Porous Media

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Summary

A simulation method is outlined for modeling elastic moduli of porous materials. Special attention is given to error estimation. The ratio of porous bulk modulus to non-porous bulk modulus is calculated for isotropic materials with a Poisson's ratio of ¼. Two cases are modeled: 1) The pores are non-overlapping but otherwise randomly distributed spheres. 2) The pores are randomly distributed (overlapping) spheres. In both cases the pores are empty and uniform in size. The results show that Norris' differential effective medium theory describes overlapping spheres well, and the Kuster-Toksöz model only slightly overestimates the modulus of non-overlapping spheres.

Introduction

A fundamental problem in processing data on reservoirs is understanding how elastic properties vary with porosity, as such information provides input to the Biot-Gassmann theories. A variety of theories have been developed to address this problem. The Kuster-Toksöz (Kuster, 1974) method based on scattering theory assumes that pores are dilute and non-overlapping. The differential effective medium (DEM) theory can also describe non-overlapping pores (Zimmerman, 1984) or overlapping pores (Norris, 1985). The simplest form of these theories is obtained for the case of spherical pores in isotropic media and these have been reviewed by Zimmerman (1991).

Comparison of various theories against experiment can be found in Berge *et al.* (1993) and Zimmerman (1991). In these studies, glass foam (with a bulk glass Poisson's ratio of $\sigma = .23$) is treated as having uniform spherical pores. Berge *et al.* find that the compressional velocity (V_p) of glass foam is intermediate between the Kuster-Toksöz model (equivalent in this case to the Hashin model [Hashin, 1962]) and Norris's DEM (although comparison with Zimmerman's DEM would be more appropriate, as glass foam consists of non-overlapping pores [Walsh, 1965]). Zimmerman finds similar results for the normalized bulk modulus. Such results are useful, but suffer from the drawback that one is dealing with errors both from theoretical approximations as well as from the incongruence of real substances with ideal pore models. Simulation is very helpful in this regard, as it allows one to assess theoretical results directly against pseudo-experimental data for the idealized pore models, with only well-controlled errors resulting from the simulation. Thus the purpose of this study is to carry out assessment of theory analogous to the above references (Berge, 1993; Zimmerman, 1991) but using simulation data instead of experimental data.

Such simulation methods, while not yet widely used in the rock physics community, are not new either. A number of workers in composite materials have carried out simulations of matter with spherical inclusions using a variety of simulation models, such as a point mass and spring lattice model (Day, 1992; Snyder, 1992), or the more general finite element method (Garboczi, 1995; Chen, 1995). Indeed, seismic wave propagation problems have also been studied using spring lattice methods (Krebes, 1987; Paranjape *et al.,* 1987; Scales, 2000). In the rock physics realm, Poutet *et al.* (1996) have performed a valuable simulation study on the physics of various pore arrangements. Thus there is a considerable history of application that can be adapted to rock physical problems.

Theory and Method

This study employs the point mass and spring lattice simulation model. While not as general as the finite element method, it is very simple and intuitive. Continuum matter is modeled as a collection of point masses connected by springs in a regular lattice. Various kinds of springs are possible, such as between nearest neighbours (denoted by a spring constant k_1), next-nearest neighbours (k_2), or next-next-nearest neighbours (k_3), etc. Certain conditions must be placed upon the springs in order for the lattice to model an elastic material. It can be demonstrated that any two of the above types of spring can be combined to represent an elastic Poisson solid ($\mu = \lambda$). For instance, Krebes (1987) and Paranjape (1987) employ k_1 and k_2 springs. This study employs k_1 and k_3 springs, which minimizes the number of springs.

Various workers (Montroll, 1947; Gazis, 1960; Krebes, 1987; Paranjape,1987) have implemented this model using a Lagrangian formulation. In this study it has been implemented by discretizing Newton's third law in a manner analogous to molecular simulation techniques (e.g., Allen and Tildesley, 1987). Periodic boundary conditions are applied to the simulation sample. Pore locations are generated from random numbers, and pores are created by removing point masses and springs in the pore region. To calculate the bulk modulus, a small compression is applied by rescaling the sample dimensions and the location of all point masses from their equilibrium positions. For non-zero porosity this results in unbalanced forces on the masses, and their positions are allowed to relax to equilibrium, which generally shrinks the pore regions further. Viscous forces are applied to the masses to approximate critical damping in the relaxation process. At equilibrium the bulk modulus is calculated from the change in energy via the relation $\delta E = \frac{1}{2} K (\delta V/V)^2$.

A vital aspect of such simulations is to provide an estimation of the error. Five sources of error were identified: 1) incomplete relaxation to equilibrium 2) non-linear responses 3) incomplete sampling of pore distributions 4) discrete grid representation of pore geometries 5) finite size of the total simulation sample. The first is controlled by requiring energy convergence to within a specified value. The second is easily controlled by making δV sufficiently small. The third error can be estimated from the scatter of results obtained using several different pore configurations. It is found in practice to be considerably smaller than the last two effects, which dominate the error in the results.

The grid error results from the imperfect representation of the pore-skeleton interface, and is essentially proportional to the volume of the interface between the pores and the skeleton. It is estimated by the expression $a\,\phi\,dl\,/\,r$, where ϕ is the porosity, r is the pore radius, and a is a constant found empirically from trial calculations at different grid resolutions. One trick was found to be important in reducing the grid error. If the pore is obtained by removing all grid points within the radius of the pore, the change in modulus with grid size contains a strong systematic component, as the effective porosity is always higher than the target porosity. However if the value $r - 0.2\,dl$ is used as the radius for creating the pore, then the systematic component is effectively removed and the grid error is reduced by a factor of about twenty.

Finite size effects arise from the interaction of pores with their periodic replications. This error is proportional to $(\,r\,/\,l\,)^3$, where l is the length of the sample edge. The proportionality constant was estimated from the values of δE in a series of single pore simulations of fixed pore volume, but increasing sample volume.

From the expressions $(\phi\,dl\,/\,r)$ and $(\,r\,/\,l\,)^3$ it is clear that there is a competition between grid error and finite size error. For a fixed porosity and grid, the grid error is decreased by having fewer, larger pores, and the finite size error by more and smaller pores. At each porosity an optimal number of pores was estimated and employed in the simulations to minimize the total error.

Example
The simulations were carried out on a 160 X 160 X 160 grid. Typical runs required several hours on a modern Sun Workstation to achieve adequate energy convergence. The simulation samples were compressed by .04% in each dimension. The calculated bulk moduli are scaled by the pure bulk value, and are thus independent of the actual values of host density and moduli. The pores are in all cases spherical and uniform in size, and the Poisson's ratio is ¼. The results are shown in Figure 1 below:
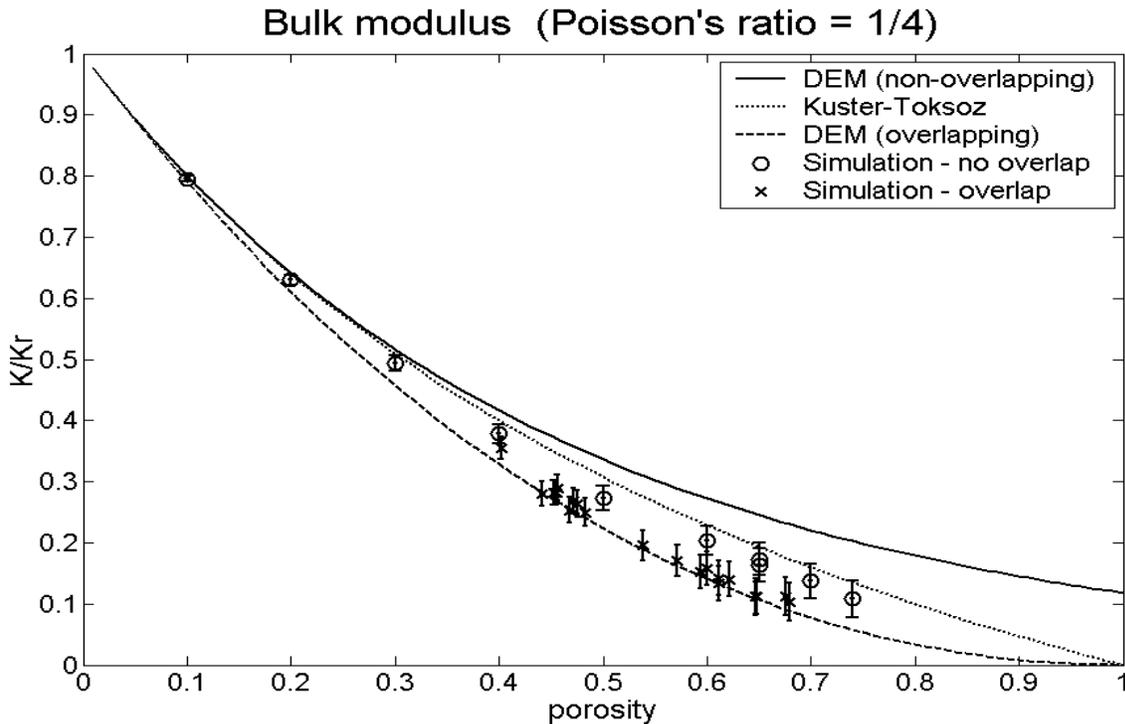
Figure 1. The dependence of bulk modulus on porosity. Theoretical results are shown by lines and simulation results by individual data points and error bars.

In Figure 1 one first notes that simulation exhibits behaviour similar to theory in that non-overlapping pores exhibit a higher modulus than overlapping pores. Furthermore, it appears that Zimmerman's DEM, intended to represent non-overlapping pores, is not as accurate as the simpler Kuster-Toksöz model. On the other hand, Norris's DEM, which represents overlapping pores, is quite accurate. One weakness of the Zimmerman DEM is that it does not vanish, even for $\phi = 1$, which is clearly unphysical. In fact, simulation results for non-overlapping spheres can only be carried out up to $\phi \approx .74$, which corresponds to the close packing of uniform spherical pores.

This first simulation study demonstrates that it is practical and feasible to conduct three-dimensional simulations of sufficient accuracy to be useful in assessing various theoretical approaches. Simulation can also be an aid in exploring more general pore models.

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