Numerical experiments with digital twins of core samples for estimating effective elastic parameters

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- Motivation
- Description of the method
- Numerical implementation
- Examples of numerical calculations
- Conclusion and road map

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Motivation

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Motivation

Physical characteristics of the core samples are mainly determined by expensive laborintensive experiments, which result in a risk of damaging a sample.

Fortunately recently there have appeared and are intensively developing alternative approaches, based on 3D Computer Tomography (CT). This approaches give the possibility of providing a three-dimensional high-resolution digital representation of the internal structures of rock samples and make possible to numerically evaluate the desired physical properties.

The development of numerical methods for evaluating various properties of core samples from the CT images is one of important parts in the Digital rock physics.

Motivation

Digital rock physics includes a whole range of studies:

- Digital tomographic images of the core;
- Filtration and segmentation images;
- Two-dimensional images are collected in a three-dimensional cube (the geometry of the structure of microscale heterogeneities);
- Algorithms for calculating various properties of the sample (porosity, permeability, effective elastic moduli, wave velocities, etc.).

We propose the new numerical algorithm for evaluating elastic properties of the rock core samples by 3D CT digital images.

Effective physical properties

There are a number of approaches for determining the effective elastic parameters, including the methods based on:

- based on the analysis of inclusions [Kristinsen];
- wide range of homogenization methods [Aboudi];
- statistical approaches [Bajuk];
- based on the principle of the equivalence of energy deformations [Zhang, 2007] This approach was originally developed for composite materials to predict the effective elastic properties of media with periodic structures.

Zhang, W., Dai, G., Wang F., Sun S., Bassir H.: Using strain energy-based prediction of effective elastic properties in topology optimization of material microstructures. Acta Mechanica Sinica **23**(1), 77-89 (2007)

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Effective physical properties

The average pressures and stresses are determined by the formulas:

$$\overline{\sigma}_{ij} = \frac{1}{V} \int_{V} \sigma_{ij} dV, \quad \overline{\varepsilon}_{ij} = \frac{1}{V} \int_{V} \varepsilon_{ij} dV,$$



$$\overline{\sigma}_{ij} = c_{ijkl}^* \overline{\varepsilon}_{kl}, \quad \overline{\varepsilon}_{ij} = s_{ijkl}^* \overline{\sigma}_{kl}$$

Here C_{ilkl}^{*} and S_{ilkl}^{*} are the components of the fourth rank tensors, which are by definition the effective stiffness tensor C* and the effective compliance tensor S*.

The method is based on the property of homogeneous boundary conditions. They can be either kinematic or static and are defined in such a way that, when applied to the boundary S of a homogeneous elastic body with volume V, it causes uniform stresses and deformations in it.

In particular, the homogeneous kinematic boundary conditions are boundary conditions with displacements specified on the boundary in the form of linear functions:

$$u_i(S) = \varepsilon_{ij}^0 x_j$$

and the homogeneous static boundary conditions are the boundary conditions with constant stresses on the boundary:

$$t_i(S) = \sigma_{ij}^0 n_j$$

where $\sigma_{ij}^0, \varepsilon_{ij}^0$ are some constant stresses and deformations, n is the vector of the outer normal to the boundary of S.

The energy equivalence principle method is based on a theorem asserting that the homogeneous static (kinematic) boundary conditions applied to the boundary S of a non-homogeneous representative volume V generate such a stress (strain), that its averaging over the volume V is equal to the value of the constant stress (strain) σ_{ij}^0 applied to the boundary:

$$\overline{\sigma}_{ij} = \sigma^0_{ij}$$

where

$$\frac{1}{V}\int \sigma dV = \bar{\sigma}$$



It can be shown that the potential energy of deformations

$$U = \frac{1}{2} \int_{V} \sigma_{ij} \varepsilon_{ij} dV$$

when homogeneous static boundary conditions with σ_{ij}^0 are applied to an inhomogeneous elastic body, can be presented in the following form

$$U = \frac{1}{2} s_{ijkl}^* \sigma_{kl}^0 \sigma_{ij}^0 V$$

Thus, if the value of the potential energy U of the elastic body under the action of homogeneous boundary conditions (static stresses σ_{ij}^0) is known, then the equation can be used to find the components of the effective compliance tensor $S_{ijkl}^* = (C_{ijkl}^*)^{-1}$

If we calculate the potential energy U_0 for a homogeneous sample with properties determined by the effective stiffness tensor C^* , then we obtain the expression:

$$U_0 = \frac{1}{2} s_{ijkl}^* \sigma_{kl}^0 \sigma_{ij}^0 V$$

If we compare U_0 with potential energy of an inhomogeneous elastic body

$$U = \frac{1}{2} s^*_{ijkl} \sigma^0_{kl} \sigma^0_{ij} V$$

It follows that the Energy method can be regarded as a method based on the equivalence principle of the potential energies for inhomogeneous and homogeneous samples, which are "equivalent":

$$U = U_0$$

We modify this approach for the rock core samples:

 The strain energy is calculated for the whole 3D CT digital volume without any periodic boundary conditions; 1 sample



- Only the stress components are calculated and used to find the strain energy;
- The static homogeneous boundary conditions (with specified stresses) instead of kinematic ones are used as boundary conditions for a series of static elasticity problems, because they most accurately correspond to the conditions for carrying out laboratory experiments with various external stresses applied to a sample;
- Parallel implementation scheme based on MPI + OpenMP.

The effective elastic stiffness tensor in 2D is written in the matrix form as

$$\begin{bmatrix} \overline{\sigma_{11}} \\ \overline{\sigma_{22}} \\ \overline{\sigma_{12}} \end{bmatrix} = \begin{bmatrix} C_{1111}^H & C_{1122}^H & C_{1112}^H \\ * & C_{2222}^H & C_{2212}^H \\ * & * & C_{1212}^H \end{bmatrix} \begin{bmatrix} \overline{\varepsilon_{11}} \\ \overline{\varepsilon_{22}} \\ \overline{\gamma_{12}} \end{bmatrix}$$

The effective elastic compliance tensor

$$\begin{bmatrix} \overline{\varepsilon_{11}} \\ \overline{\varepsilon_{22}} \\ \overline{\gamma_{12}} \end{bmatrix} = \begin{bmatrix} S_{1111}^H & S_{1122}^H & S_{1112}^H \\ * & S_{2222}^H & S_{2212}^H \\ * & * & S_{1212}^H \end{bmatrix} \begin{bmatrix} \overline{\sigma_{11}} \\ \overline{\sigma_{22}} \\ \overline{\sigma_{12}} \end{bmatrix}$$

Strategy to find S_{1111}^H



The numerical simulation of a series of laboratory experiments with various external stresses applied to a sample.

Strategy to find S_{1111}^H

1. Define fixed homogeneous static boundary conditions :

$$\sigma_{11}^{0}\Big|_{a} = 1, \quad \sigma_{22}^{0}\Big|_{b} = 0, \quad \sigma_{12}^{0}\Big|_{a,b} = 0$$

2. Find the solution of the boundary-value problem of the static theory of elasticity :

$$\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} = 0$$
$$\frac{\partial \sigma_{12}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} = 0$$
$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} = C_{ijkl} u_{k,l}$$

3. Calculate the potential energy of deformations :

$$U = \frac{1}{2} \int_{V} \sigma_{ij} \varepsilon_{ij} dV$$

$$U = \frac{1}{2} s^*_{ijkl} \sigma^0_{kl} \sigma^0_{ij} V$$

4. From the principle of the equivalence of potential energy, we find the components of the compliance tensor

$$U^{(1)} = \frac{1}{2} s^*_{1111} V, \qquad s^*_{1111} = 2U^{(1)} / V$$

Strategy to find S_{2222}^{H}



$\left[\overline{\varepsilon_{11}}\right]$	S_{1111}^{H}	S_{1122}^{H}	S_{1112}^{H}	$\left[\overline{\sigma_{11}}\right]$
$\overline{\varepsilon_{22}} =$	*	S_{2222}^{H}	S_{2212}^{H}	$\overline{\sigma_{22}}$
$\left[\overline{\gamma_{12}}\right]$	*	*	S_{1212}^{H}	$\overline{\sigma_{12}}$

$$s_{2222}^* = 2U^{(2)}/V$$

Strategy to find S_{1212}^H



$\left[\overline{\varepsilon_{11}}\right]$	S_{1111}^{H}	S_{1122}^{H}	S_{1112}^{H}	$\left[\overline{\sigma_{11}}\right]$
$\overline{\varepsilon_{22}} =$	*	S^{H}_{2222}	S_{2212}^{H}	$\overline{\sigma_{22}}$
$\left[\overline{\gamma_{12}}\right]$	*	*	S_{1212}^{H}	$\left[\overline{\sigma_{12}}\right]$

$$s_{1212}^* = 2U^{(3)} / V$$

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Strategy to find S_{1122}^H

$\overline{\varepsilon_{11}}$	S_{1111}^{H}	S_{1122}^H	S_{1112}^{H}	$\left[\overline{\sigma_{11}}\right]$
$\overline{\varepsilon_{22}} =$	*	S^{H}_{2222}	S_{2212}^{H}	$\overline{\sigma_{22}}$
$\overline{\gamma_{12}}$	*	*	S_{1212}^{H}	$\overline{\sigma_{12}}$

This boundary conditions are a linear combination of boundary conditions case 1 and 2. Therefore we use linearity property of the elasticity problem and calculate U with the use of results of the previous considerations.

$$U^{(4)} = \frac{1}{2} \int_{V} \sigma_{ij}^{(4)} \varepsilon_{ij}^{(4)} dV = \frac{1}{2} \int_{V} (\sigma_{ij}^{(1)} + \sigma_{ij}^{(2)}) (\varepsilon_{ij}^{(1)} + \varepsilon_{ij}^{(2)}) dV =$$
$$= U^{(1)} + U^{(2)} + U^{(1,2)}$$

No need to solve the problem for this case !!!



In the three-dimensional case, the algorithm for finding the components of the compliance tensor is analogous to 2D. The compliance tensor is written down in the form:





					*
Table 1. The boundary	conditions fo	r finding the	components	of	S_{ijkl}

	Faces a	Faces b	Faces c	Value s^*_{ijkl}
1	$\sigma_{33} = \sigma_{13} = \sigma_{23} = 0$	$\sigma_{22} = \sigma_{12} = \sigma_{23} = 0$	$\sigma_{11} = 1, \sigma_{12} = \sigma_{13} = 0$	$s_{1111}^* = 2U^{(1)}/V$
	$\sigma_{33} = \sigma_{13} = \sigma_{23} = 0$	$\sigma_{22} = 1, \sigma_{12} = \sigma_{23} = 0$	$\sigma_{11} = \sigma_{12} = \sigma_{13} = 0$	$s_{2222}^* = 2U^{(2)}/V$
9	$\sigma_{33} = 1, \sigma_{13} = \sigma_{23} = 0$	$\sigma_{22} = \sigma_{12} = \sigma_{23} = 0$	$\sigma_{11} = \sigma_{12} = \sigma_{13} = 0$	$s_{3333}^* = 2U^{(3)}/V$
4	$\sigma_{23} = 1, \sigma_{33} = \sigma_{13} = 0$	$\sigma_{23} = 1, \sigma_{22} = \sigma_{12} = 0$	$\sigma_{11} = \sigma_{12} = \sigma_{13} = 0$	$s_{2323}^* = 2U^{(4)}/V$
LL J	$\sigma_{13} = 1, \sigma_{33} = \sigma_{23} = 0$	$\sigma_{22} = \sigma_{12} = \sigma_{23} = 0$	$\sigma_{13} = 1, \sigma_{11} = \sigma_{12} = 0$	$s_{1313}^* = 2U^{(5)}/V$
6	$\sigma_{33} = \sigma_{13} = \sigma_{23} = 0$	$\sigma_{12} = 1, \sigma_{22} = \sigma_{23} = 0$	$\sigma_{12} = 1, \sigma_{11} = \sigma_{13} = 0$	$s_{1212}^* = 2U^{(6)}/V$



Table 2. The boundary conditions for finding the components of $\vec{s_{iikl}}$

Values s^*_{ijkl}				
$s_{1122}^* = U^{(1,2)}/V$	$s_{1123}^* = U^{(1,4)}/V$	$s_{1113}^* = U^{(1,5)}/V$	$s_{2313}^* = U^{(4,5)}/V$	$s_{3312}^* = U^{(3,6)}/V$
$s_{1133}^* = U^{(1,3)}/V$	$s_{2223}^* = U^{(2,4)}/V$	$s_{2213}^* = U^{(2,5)}/V$	$s_{1112}^* = U^{(1,6)}/V$	$s_{2312}^* = U^{(4,6)}/V$
$s_{2233}^* = U^{(2,3)}/V$	$s_{3323}^* = U^{(3,4)}/V$	$s_{3313}^* = U^{(3,5)}/V$	$s_{2212}^* = U^{(2,6)}/V$	$s_{1312}^* = U^{(5,6)}/V$

Similar to 2D case, we use the linearity property and the previous results to find the remaining 15 components without calculations (Table 2).



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Solution of static problems

The most time-consuming component of the approach from the standpoint of computation is the solution of a series of static problems in the elasticity theory with external stresses given at the boundaries.

The system of equations consists of the equilibrium equations:

$$\sigma_{ij,j}=0$$

and the Hooke law:

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} = C_{ijkl} u_{k,l}$$

On the boundary S we set the static boundary conditions:

$$t_i(S) = \sigma_{ij}^0 n_j$$

To solve them, both direct and iteration methods can be used. Direct methods, having certain advantages, in this case are not suitable for solving three-dimensional problems due to excessive demands for computer resources. Therefore, we have chosen iterative methods for determining effective parameters.

Solution of static problems

Let us describe the new iteration method based on the relaxation technique we propose to use. The solution of static problem is sought for by finding the steady-state solution of the dynamic problem of the elasticity theory in the formulation of the stress/displacement velocity with additional dissipative terms added to equations of motion:

$$\rho \dot{\upsilon}_{i} + \alpha \upsilon_{i} = \sigma_{ij,j}$$
$$\dot{\sigma}_{ij} = C_{ijkl} \dot{\varepsilon}_{kl} = C_{ijkl} \upsilon_{k,l}$$

with zero initial conditions for t = 0:

$$v_i = 0$$
 $\sigma_{ij} = 0$

and time-invariant boundary conditions on the boundary S:

$$t_i(S) = \sigma_{ij}^0 n_j$$

where $v_i = \dot{u}_i$ displacement velocity components.

Solution of static problems

Using the virial theorem (Landau and Lifshitz, 2001) it is possible to prove the convergence of dynamic problem with dissipative term to corresponding static problem under study. We "switch on" the relaxation parameter only after the generated waves have filled the whole calculation domain.



finite-difference scheme on staggered grids

Solution of static problem

To illustrate this method we consider the 2D solution of static problem for a homogeneous medium and boundary conditions in the form:

$$\sigma_{11}|_a = 1, \quad \sigma_{22}|_b = 0, \quad \sigma_{12}|_{a,b} = 0$$

This static homogeneous boundary conditions admit the unique exact solution:

$$\sigma_{xx}(x, y) = 1, \ \varepsilon_{xx}(x, y) = 1/(\lambda + 2\mu),$$



Convergence of relaxation method



Snapshots of component σ_{11} with an interval of 200 steps of the difference scheme with respect to time without dissipative term.

Convergence of relaxation method



Snapshots of component σ_{11} with an interval of 200 steps of the difference scheme with respect to time with dissipative term.

Convergence of relaxation method



- MPI
- MPI/OpenMP
- Coarray





MPI/OpenMP



History of Coarray Fortran

- Co-Array Fortran is defined by:
- R.W. Numrich and J.K. Reid, "Co-Array Fortran for Parallel Programming", ACM Fortran Forum, 17(2):1-31, 1998

• Integrated into Fortran 2008 standard (approved in 2010)

• Additional information on the web: - www.co-array.org - www.pmodels.org

What is Co-Array Syntax?

Co-Array syntax is a simple extension to normal Fortran syntax.

 It uses normal rounded brackets () to point to data in local memory.

 It uses square brackets [] to point to data in remote memory.

Syntactic and semantic rules apply separately but equally to () and [].

real :: s[*]
real :: a(n)[*]
complex :: z[*]



Declaring and allocating Fortran co-arrays

```
REAL, DIMENSION(:,:) :: A ! Private array.
REAL, DIMENSION(:,:)[*] :: B ! Co-array
```

```
ALLOCATE ( A( M, N ), STAT = IERR ) ! Allocating private array
ALLOCATE ( B( M, N )[*], STAT = IERR ) ! Allocate co-array.
```

```
A(1) = B(2)[7] ! All images load B(2) from image 7 into their A(1).

A(5) = B(3) ! All images load their B(3) into their A(5).
```

CAF Memory Model





Domain Decomposition

MPI	Coarray
<pre>real :: u(0:N+1, 0:M+1) call mpi_isend(u(1,1:M), M, mpi_real, top(myid), tag1,) call mpi_irecv (u(N+1,1:M), M, mpi_real,bottom(myid), tag1,) call mpi_isend(u(N,1:M), M, mpi_real,bottom(myid), tag2,) call mpi_irecv (u(0,1:M), M, mpi_real, top(myid), tag2,) call mpi_isend(u(1:N,M), N, mpi_real, right(myid), tag3,) call mpi_irecv (u(1:N,0), N, mpi_real, left(myid), tag3,) call mpi_isend(u(1:N,1), N, mpi_real, left(myid), tag4,) call mpi_irecv (u(M+1,1:N), N, mpi_real, right(myid), tag4,) call mpi_irecv (u(M+1,1:N), N, mpi_real, right(myid), tag4,) call mpi_waitall()</pre>	real :: u(0:N+1, 0:M+1)[pN,*] u(N+1,1)[top(1),top(2)] = u(1,1:M) u(0,1:M)[bottom(1),bottom(2)] = u(N,1:M) u(1:N,0)[right(1),right(2)] = u(1:N,M) u(1:N,M+1)[left(1),left(2)] = u(1:N,1) sync all



Strong scaling speedup on CPU Intel Xeon E5-2697A v4.

Weak scaling efficiency on CPU Intel Xeon E5-2697A v4.

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Numerical Examples

The proposed method was verified using different synthetic samples with specified properties. First we estimate the accuracy for 3D homogeneous isotropic samples. In this case, the effective parameters must coincide with the original sample properties (Table 1).

Exact values	Calculated values
$\lambda + 2\mu = c_{1111}^* = c_{2222}^* = c_{3333}^* = 271518000000;$	$\lambda + 2\mu = c_{1111}^* = c_{2222}^* = c_{3333}^* = 271518000633164;$
$\mu = s_{2323}^* = s_{1313}^* = s_{1212}^* = 82895280000;$	$\mu = s_{2323}^* = s_{1313}^* = s_{1212}^* = 82895279858.3661;$
$\lambda = c_{1122}^* = c_{1133}^* = c_{2233}^* = 105727440000;$	$\lambda = c_{1122}^* = c_{1133}^* = c_{2233}^* = 105727440302.816;$
the rest of values $c_{ijkl}^* = 0$.	the rest of values $c_{ijkl}^* \approx 10^{-1}$.

Table 1 Comparison of exact and calculated values of elastic moduli for a 200³ digital cube sample of homogeneous isotropic steel.

Numerical Examples

The next series of numerical experiments was carried out for the samples with a varying number of thin parallel interlayers with clay parameters. The results were compared to the effective parameters found by the Schoenberg averaging method for the case of a system of thin parallel layers.



Numerical Examples



Fig. 3. The different layered models of media (a-b) and the segmented digital model of core sample (c).

The size of the models was varied along the interlayers, across, the number of layers and their incline was changed and so on. A comparison was made between the results of the proposed method and the Schoenberg averaging method. The difference decreased with increasing size along the interlayer and for size of 500*500*500 was $\approx 2\%$.

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Conclusion and road map

We propose the new numerical technique to estimate effective elastic parameters of a core sample from their 3D CT images.

We assume that the volume under study has an irregular distribution of inhomogeneities without any periodic or quasi-periodic structure.

Our method is based on the energy equivalence principle and the new approach to solve **3D** static elasticity problem by the solution of the corresponding dynamic elasticity problem with some relaxation mechanisms providing the convergence to a static problem.

We implement MPI, MPI+OpenMP, CAF parallel techniques in order to speed up our computations.

Numerical results have shown a good accuracy of calculations.

This approach with minor modifications can be used to find the frequency-dependent effective elastic parameters.