Electrical and mechanical response of random media – Training Session

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1 Introduction

This training session is devoted to the study, using Fourier computations, of the local and effective properties of random composites. Emphasis is put, in particular, on the effect of:

- Contrast of properties;
- Volume fraction of heterogeneities;
- Comparison of numerical results with analytical bounds and estimates;
- Observation of the heterogeneous local fields.

2 Fourier tool for computing the heterogeneous response of random media

2.1 How to run computations

2.1.1 Electrical response

The electrical behavior of a composite discretized on a 64^3 grid is solved using the software "morphhom" with the command

./morphhom -3d 64 MICRO -cl 1e-4 -l λ_1 λ_2 -E 1 0 0 -save EJMPce

where "-cl 1e-4" specifies the convergence criterion and required precision, λ_1 and λ_2 are the conductivity in phases 1 and 2 resp., and "-E 1 0 0" is the applied macroscopic voltage, here in the $\mathbf{e}_x$ direction. "MICRO" is the random microstucture; some of the available models are given in Table (1).

NB: you first need to copy the executables in the directory of the training session; e.g. mkdir ts3; cp data/morphhom/morphhom data/morphhom/mstats ts3/; cd ts3.

In conductivity in 3D, the FFT tool produces the files

_M (original microstructure)

-hs 0.5	Centered sphere of volume fraction 50%
-bm 0.1 10	Boolean model of spheres of average volume fraction 10% and diameter 10 voxels
-bm 0.1 10 -xf 0.1 0.9 0.1	Do 9 computations with Boolean models of spheres of diameter 10 and total volume fractions 10%, 20%, ...90%
-2d 256 -bm 0.1 10 -xf .1 .9 .1	2D Boolean model of discs of average surface fraction 10%, 20%, ...90% and diameter 10 pixels
-2d 256 -brec0 100 2 .1	2D microstructure with discretization 256^2 pixels containing 100 fibers of width 2 pixels, length $0.1 * 256$

Table 1: Options for specifying the microstructure model

_Ex (x-component of the electrical field $E_x(x_1, x_2, x_3)$)

_Ey (y-component of the electrical field $E_y(x_1, x_2, x_3)$)

_Ez (z-component of the electrical field $E_z(x_1, x_2, x_3)$)

_Jx (x-component of the current field $J_x(x_1, x_2, x_3)$)

_Jy (y-component of the current field $J_y(x_1, x_2, x_3)$)

_Jz (z-component of the current field $J_z(x_1, x_2, x_3)$)

_Phi (periodic part of the potential $\Phi(x_1, x_2, x_3)$)

_c (text file; convergence criterion and first moments as a function of iterations)

_e (text file; volume fraction and effective response $\widetilde{\lambda}$ so that $\langle J_x \rangle = \widetilde{\lambda} \langle J_x \rangle$)

Most important is the last file _e which provides the effective response in a ready to use format. Any file that needs to be kept should be renamed so that it not overwritten during the next computation.

To run computations in 2D, use e.g. -2d 512 instead of -3d 64, and -E 1 0 instead of -E 1 0 0.

2.1.2 Mechanical response

To compute the elastic response of a heterogeneous material use the options -l and -m to specify the shear and bulk modulus and specify hydrostatic strain loading conditions with -press. For instance in 2D:

./morphhom -2d 1024 MICRO -cl 1e-4 -l μ_1 μ_2 -m κ_1 κ_2 -press -save EJMPce

where (μ_1, κ_1) and (μ_2, κ_2) are elastic shear and bulk moduli of phases 1 and 2 respectively. The phases local response is isotropic. The effective bulk modulus can be plotted as a function of the surface fraction of discs using the data in the file _e as for the effective conductivty. The third column in the file gives the effective shear modulus $\widetilde{\mu}$ when shear strain loading is applied (-ss instead of -press).

The output files are _Epsilon_xx (likewise _Epsilon_xy etc.), _Sigma_xx and _U_x for the strain, stress and displacement vector fields.

2.2 How to visualize field maps

Full-field maps could be visualized using the post-processing tool mstats as

./mstats -2 -sl OUTPUT INPUT

The above generates an image with filename OUTPUT.ppm. The latter may be viewed with the program eog, e.g. eog OUTPUT.ppm. The x axis is vertical on the image, oriented top to bottom, whereas the y axis is horizontal oriented left-to-right. In 3D, the tool produces a set of image slides transverse to the z axis (use "-3" instead of "-2"). For microstructure images, add the option "-rm" to mstats.

The extreme values (and average) are shown on screen by mstats. It is sometimes necessary to threshold the fields between a minimum and maximum value. For this, use the options -min MIN -max MAX.

2.3 How to plot the effective properties

Bounds for the electrical conductivity of random media are provided in the file Bounds_Permittivity.plt (from the 'bounds" training session). Using gnuplot, the appropriate functions are loaded with load 'FILE'. Numerical FFT data for the effective properties could be plotted by loading the file "_e" in gnuplot, e.g. plot "e_10". To *save* plots into a file (for your report!) you can do one of

set term png; set output "out.png"; replot

set term postscript; set output "out.ps"; replot

Don't forget to reset your settings back to normal output with :

set term x11

3 Electrical conductivity

3.1 Boolean model of spheres

3.1.1 Highly conducting spheres

Compute the effective electrical conductivity $\widetilde{\lambda}$ of a Boolean models of spheres of conductivity $\lambda_2 = 100$ embedded in a matrix of conductivity $\lambda_1 = 10$, with varying sphere volume fractions: 10%, 20%, ..., 90%. Compare with the Hashin and Shtikman upper and lower bounds, with the third-order upper and lower bounds and with the self-consistent estimates. What do you observe?
Change the conductivity in the matrix to $\lambda_1 = 1$ and compare with the same bounds and estimates. Then with $\lambda_1 = 1$ and $\lambda_2 = 10^6$ (add -disc-w14 -ds to the command line to use an alternative algorithm to speed up computations). What's happening?

3.1.2 Insulating spheres

Set $\lambda_1 = 1$. Compute the effective electrical conductivity of Boolean models of insulating spheres at varying volume fractions. Use steps of 5%, and compare with the Hashin-Shtikman and third-order bounds, and with the self-consistent estimates (change the convergence criterion to -cl 1e-5 and use -network -ds in the command line to speed up the computations). What do you observe?

3.2 2D Boolean models

3.2.1 Discs

Compute the effective electrical conductivity $\widetilde{\lambda}$ of a Boolean models of discs of conductivity $\lambda_2 = 10^3$ embedded in a matrix of conductivity $\lambda_1 = 1$, with varying disc surface fractions: 10%, 20%, ..., 90% (change the convergence criterion to -cl 1e-5 and use -network -ds in the command line). Comment on the results you find.

3.2.2 Elongated fibers

Compute the effective electrical conductivity $\widetilde{\lambda}$ of a Boolean models of fibers with the number of fibers equal to 100, 300, 500 700 and 1000 (change the convergence criterion to -cl 1e-4 and use -network -ds in the command line). Compare with the Boolean model of discs. Interpret the results.

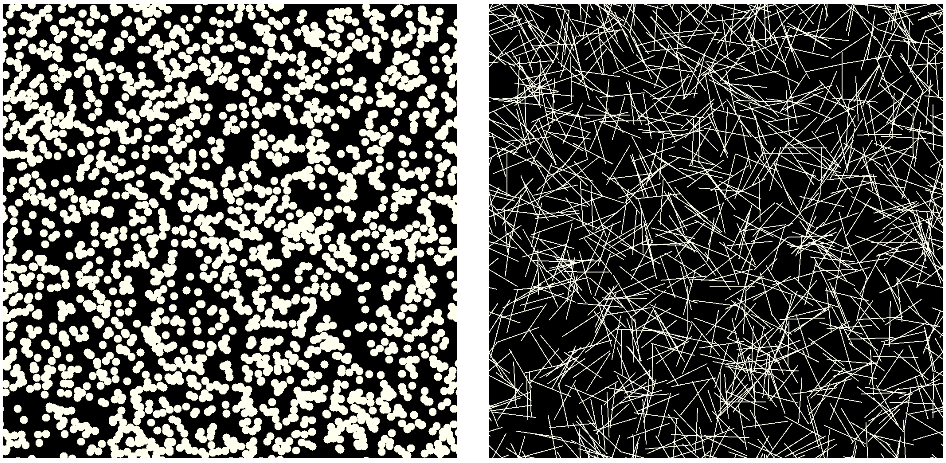

Figure 1: Boolean models of discs and cylinders with apsect ratio 100

4 Mechanical response of heteroegeneous media

4.1 Linear elasticity

Compute the effective bulk modulus $\widetilde{\kappa}$ for Boolean models of porous spheres with varying surface fraction f comprised between 10 and 60%. The bulk and shear moduli in the matrix is set to $\kappa_1 = \mu_1 = 1$. Compare the results with the Hashin and Shtrikman upper bounds for 2D media:

$$\widetilde{\kappa} \leq \kappa^{(HS)} = \kappa_1 + \frac{f}{\frac{1}{\kappa_2 - \kappa_1} + \frac{1-f}{2\kappa_1}} \tag{1}$$

Generate maps of the local mean stress and strain fields $\sigma_m = (1/2)(\sigma_{xx} + \sigma_{yy})$ and $\sigma_m = (1/2)(\sigma_{xx} + \sigma_{yy})$ for various surface fraction of discs (e.g. 10%, 20%, 30%). To visualize the field patterns, use a threshold between -1 and 1 with the command:

```
./mstats -2d 512 -sl OUTPUT -min -1 -max 1 -m INPUT_xx INPUT_yy
```

Comment on the field maps. Where are the stress concentration highest?