Computation of the physical response of random media – Training Session

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The purpose of this session is to estimate bounds of the thermal conductivity and of the elastic moduli of various random media. This can be made by means of three files that can be loaded (load 'FILE')in the GNUPLOT software:

- Bounds_Permittivity.plt for the dielectric permittivity (or similarly the thermal conductivity) of two-phase composites.

- Bounds_Elasticity.plt for the elastic moduli of two-phase composites.

- Bounds_Elasticity_Porous.plt for the elastic moduli of porous media.

The training session will be carried out on a linux virtual server. Go to the webpage https://rep.mines-paristech.fr/home and log in with your login/password, then choose "create session", "join running session" and "connect". Open a terminal (if not already present) using the bottom-left button, then "system tools" then "XTerm". The files needed for the training sessions are in the directory "data". We advise you to create a different directory for each training session, and copy the relevant files in each directory, e.g.: mkdir ts2, cp data/gnuplot/*gpt ts2/. You will find the bounds files in the gnuplot directory. After you have moved to the ts2 directory in a terminal (mv ts2), you can access the gnuplot shell by typing "gnuplot" in the terminal.

Tip To lower the screen resolution on the virtual server, and increase the font size, you can run /home/user/data/installScreenResolution.sh in a terminal, and then click on the bottom-left button, "Preferences", "Monitor Settings".

1 Third order bounds for the dielectric permittivity (resp. thermal conductivity)

The third order bounds are available from the file Bounds_Permittivity.plt, where we use the following notations:
e"model"" b" (E_1, E_2, p), where

- E_1 is the permittivity (resp. conductivity) of phase 1 with volume fraction p

- "b" is u (upper bound) or l (lower bound)

- "model" is the type (code) of model. The list of available models (in 3D) is given in Table 1.

For instance, the upper bound of the conductivity of a Boolean model of spheres where phase 1 (with volume fraction 0.5) has the conductivity 100, and phase 2 the conductivity 1, is available on the screen by typing:

print esbu(100,1,0.5)

The result given is 27.8311

To get a plot of the two bounds of a Boolean model of spheres with a changing volume fraction of phase 1, type:

plot esbu(100,1,x),esbl(100,1,x)

The two Hashin-Shtrikman bounds are given by ehsu(E_1, E_2, p) and ehsl(E_1, E_2, p).

Model (for phase 1)	Code
Boolean Spheres	sb
Complementary Boolean Spheres	sbc
Hard Core of Spheres ($p < 0.6$)	hc
Complementary Hard Core of Spheres ($p > 0.4$)	hcc
Mosaïc of Spheres	ms
Mosaïc of Plates	ma
Mosaïc of Needles	mn

Table 1: Codes for models of random media

It can also be useful to compare the bounds to the self-consistent estimate esc(E_1, E_2, p).

2 Third order bounds for the elastic moduli

The third order bounds are available from the file Bounds_Elasticity.plt, where we use the following notations:

"m""model""b" (K_1, G_1, K_2, G_2, p), where

- K_1 and K_2 are the bulk moduli of phase 1 (with volume fraction p), G_1 and G_2 the corresponding shear moduli.

- "m" is the type of modulus: k for the bulk modulus K, g for the shear modulus G, e for the Young's modulus E, and nu for the Poisson's modulus ν.

- "b" is u (upper bound) or l (lower bound)

- "model" is the type (code) of model. The list of available models (in 3D) is given in Table 1.

For instance, the upper bound of the Young's modulus of a Boolean model of spheres where phase 1 (with volume fraction 0.5) has the moduli $K_1 = 100, G_1 = 100$ and phase 2 has the moduli $K_2 = 15, G_2 = 5$, is available by typing:

  print esbu(100,100,15,5,0.5)

The result given is 64.4335

To get a plot of the two bounds of a Boolean model of spheres with a changing volume fraction, type:

  plot esbu(100,100,15,5,x),esbl(100,100,15,5,x)

The two Hashin-Shtrikman bounds are given by ehsu(K_1, G_1, K_2, G_2, p) and by ehsl(K_1, G_1, K_2, G_2, p).

For the case of a porous medium where the volume fraction of the solid phase is given by p, the third order upper bound is given by "m""model" (K, G, p) and the Hashin-Shtrikman upper bound is given by "m"hs(K, G, p).

3 Exercises on bounds of the thermal conductivity of composites

3.1 Mosaïc models

Compare the third order bounds of the mosaïc models (sphere, needles, plates) to the Hashin-Shtrikman bounds for two phase composites with the following properties ($\lambda_1 = 100$, $\lambda_2 = 10$), ($\lambda_1 = 100$, $\lambda_2 = 1$). For each contrast, plot the bounds obtained for the full range of volume fractions (p varying between 0 and 1) on a single figure.

3.2 AlN materials

Two images of AlN materials (*S_B_13.bmp* and *T_B_21.bmp*) are present in the folder data/images . The conductivity of the black phase (AlN) is equal to 100 W.m^{-1}.K^{-1} and of the white phase is equal to 10 W.m^{-1}.K^{-1}.

For the full range of volume fractions (p varying between 0 and 1), compare the third order bounds obtained for the two types of microstructures corresponding to these materials to the Hashin-Shtrikman bounds. Which type of microstructure (and for which range of volume fraction of AlN) yields the highest conductivity? Compare these bounds to the self-consistent estimate for conductivity.

3.3 Hard-core model of spheres

Compare the third order bounds for the Hard-core model of spheres, and for its complementary set, to the Hashin-Shtrikman bounds for two phase

composites with the following properties: $\lambda_1 = 100, \lambda_2 = 10$, then $\lambda_1 = 100$, $\lambda_2 = 1$. For each contrast, plot the bounds obtained as functions of p.

4 Exercises on bounds of the elastic moduli of composites

4.1 Mosaïc models

Compare the third order bounds of the elastic moduli (K, G, E, ν) of the mosaïc models (sphere, needles, plates) to the Hashin-Shtrikman bounds for two phase composites with the following properties: $\{K_1 = 273333$ MPa$, G_1 = 164000$ MPa$, K_2 = 91667$ MPa$, G_2 = 42308$ MPa$\}$ and $\{K_1 = 273333$ MPa$, G_1 = 164000$ MPa$, K_2 = 9166$ MPa$, G_2 = 4230$ MPa$\}$. For each contrast, plot the bounds obtained as functions of the volume fraction of phase 1.

4.2 AlN materials

We assume that the black phase has the following elastic moduli: $K_1 = 273333$ MPa$, G_1 = 164000$ MPa, and that the white phase has the following moduli: $K_2 = 91667$ MPa$, G_2 = 42308$ MPa. Give the third order bounds of the materials corresponding to the two studied images, and compare them to the Hashin-Shtrikman bounds.

For the full range of volume fractions (p varying between 0 and 1), compare the bounds obtained for the two types of microstructures corresponding to these materials to the Hashin-Shtrikman bounds. Which type of microstructure (and for which range of volume fraction of AlN) yields the highest moduli?

4.3 Hard-core model of spheres

Compare the third order bounds for the Hard-core model of spheres, and of its complementary set, to the Hashin-Shtrikman bounds for two phase composites with the following properties: $\{K_1 = 273333$ MPa$, G_1 = 164000$ MPa$, K_2 = 91667$ MPa$, G_2 = 42308$ MPa$\}$, then $\{K_1 = 273333$ MPa$, G_1 = 164000$ MPa$, K_2 = 9166$ MPa$, G_2 = 4230$ MPa$\}$. For each contrast, plot the bounds obtained as functions of the volume fraction of phase 1.

4.4 Porous media

In the case of the AlN materials, replace the white phase by pores. Estimate the corresponding upper bounds of the elastic moduli of the two materials. Compare them to porous media with the same volume fraction of pores, modelled by a Hard-core model of spheres, then by its complementary set.