Discrete Radon Transform and the Bounding Effective Properties of Periodical Isotropic Two-Phase Thermal Materials

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Abstract: This work is related to bounding the effective conductivity of an isotropic two-phase fibrous periodical composite. These well known bounds are classically obtained for any inclusion shape by the fourier method. So, they can be expressed only in the Fourier space. A real formulation of the solution of the periodical conductivity problem based on the discrete Radon transform has been recently proposed. The use of this framework leads us here to a simple and explicit real bounds for effective properties. The effect of the microstructure is hence more evidenced. It is also shown here that the obtained bounds coincide with the classical Hashin Shtrikmann bounds when the microstructure has some specific symmetry.

Key words: Homogenization, finite radon transform, Hashin-Shtrikman bounds, periodical media, symmetric, heterogeneous conductivity, fibrous media.

1. Introduction

Analyzing the effective behavior of heterogeneous structure is a difficult task. This is due to the numerical and mathematical difficulties to be tackled by Bensoussan [1], Nemat-Nasser [2], Milton [3], Suquet [4]. However, bounding this effective behavior appeared from the work of Hashin-Shtrikman [5], Wiener bounds (1912) to be more interesting than giving some empirical formula. Also bounding the effective properties in some exact ways is used to validate the obtained numerical solutions. On the other hand and for periodical structures the bounds proposed in the literature are based on the Fourier formalism. So the influence of the microstructure is not explicit because of the writing in the Fourier space. We purpose here to formulate the classical variational upper and lower bounds in a real space by using the expression proposed by Boukour and EL Omri (BE). The numerical calculus is based on the DRT (discrete radon transform) and Matus and Flusser [6]. This is the analogous discrete formulation of the solution obtained by Boukour and EL Omri (BE) [7] for the continuous case. The later is based on the Hill projectors [8] and the DRT proposed by Gelfand [9]. In Section 2 and after having presented the problem of a heterogeneous conductivity fibrous structure, the solution given by Boukour and EL Omri [7] is recalled for a two-phase composite. The case of symmetrical structure is then depicted to compare the bound hence obtained with the (HS) bounds. The third section is dedicated to the numerical algorithm used for the calculation of the finite radon transform. At last and in the fourth section, an illustration of this formalism is given for a hexagonal repartition of square fiber to check the validity of the analytical results here obtained.

2. Problem Position

2.1 Equations

Let us consider a periodical heterogeneous medium consisting in different phases with different
conductivities. In this case the problem to solve on some RVEs (representative volume elements) is:

\[
\begin{align*}
\text{div } j &= 0 \\
n &= C e \\
\vec{e} &= \vec{0} \\
\n\end{align*}
\]

where \( T, e \) and \( j \) denote respectively the field soft temperature, gradient temperature and heat current. \( C(x) \) denotes the conductivity tensor of the material occupying the position. \( \langle f \rangle \) is the mean of \( f \) over the RVE \( \Omega \) and the tilde means:

\[
\tilde{f} = f - \langle f \rangle
\]

2.2 The General Solution

Different propositions to solve this problem could be used. For complex microstructures, the Fourier method is well known to be simple in its numerical implementation. It leads to an iterative algorithm as insuquet [4] or to the inversion of a system of equations using FFTW (Fastest Fourier Transform in the West) performed by Frigo [10]. The solution proposed by Boukour and El Omri was based on the Hill projectors and the discrete Fourier transform is formulated in the real space. It is an analogous discrete form which has been proposed by (BE):

\[
\begin{align*}
\vec{e} &= \vec{E} - \sum_{n \in N} \Gamma^n \cdot \delta C \cdot \vec{e}^n \\
\end{align*}
\]

with

\[
\Gamma^n = (\mathbb{m}.C_r) m = \n \otimes n \odot C = C(x) - C_0
\]

where \( \otimes \) denotes a tensorial product, \( C(x) \) and \( C_0 \) denote the conductivity tensor in the RVE and in a reference medium.

\( \vec{e}^n \) is the DRT (Appendix) in a direction \( n \) belonging to the set:

\[
N = \{n = \cos \theta e_1 + \sin \theta e_2; \tan \theta \in \mathbb{Q}\}
\]

\( e_1, e_2 \) are a unit vector.

When considering a heterogeneous medium consisting two isotropic phases material, \( \Phi_\chi \) and \( \Phi_r \), the relative conductivities are \( C_\chi = c_\chi \cdot I \) and \( C_r = c_r \cdot I \). These two phases occupy the volumic fractions \( f_\chi \) and \( f_r = 1 - f_\chi \). By taking \( \Phi_r \) as the reference media and the characteristic function of the \( \Phi_\chi \) phase,

\[
\chi(x) = \begin{cases}1 & \text{if } x \in \Phi_\chi \\0 & \text{if not} \end{cases}
\]

The general solution Eq. (6) writes:

\[
\vec{e} = \vec{E} - \xi \sum_{n \in N} \Gamma^n \vec{e}^n
\]

where \( \xi = \frac{c_\chi - c_r}{c_r} \) and

\[
\Gamma^n = (\mathbb{m} - m)^{-1}\begin{pmatrix}
\cos^2 \theta_n & \cos \theta_n \sin \theta_n & 0 \\
\sin \theta_n \cos \theta_n & \sin^2 \theta_n & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

2.3 DRT-Based Variational Bounds of First Order

Following the variational theorem of Hashin [11] an upper bound is obtained when the most conducting phase as reference medium and when the energy is uniform in this phase. The lower bound of complementary energy is obtained by taking as the most resistive phase. This theorem is universal and also valid in periodic homogenization, Huet [12].

\[
\begin{align*}
\chi_\chi &= 1 - \xi \sum_{n \in N} \Gamma^n \vec{e}^n \\
\chi_r &= 0
\end{align*}
\]

Using Eq. (9), a kinematic solution writes:

\[
\begin{align*}
\vec{e} &= \vec{E} - \xi \sum_{n \in N} \Gamma^n \vec{e}^n
\end{align*}
\]

Multiplying by \( \chi_\chi \) and averaging, the last equation becomes:

\[
\begin{align*}
\langle \chi_\chi \vec{e} \rangle &= \langle \chi_\chi \vec{E} \rangle - \xi \sum_{n \in N} \Gamma^n \vec{e}^n
\end{align*}
\]

The constant field in the \( \Phi_\chi \) is then:

\[
\begin{align*}
\vec{E}_\chi &= \frac{m_\chi - m_r}{m_r} \vec{E}_r
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The constant field in the \( \Phi_\chi \) is then:

\[
\begin{align*}
\vec{E}_\chi &= \frac{m_\chi - m_r}{m_r} \vec{E}_r
\end{align*}
\]
So, the homogenized law is:
\[
J = (f_\chi c_\chi E_\chi - c_r < (1 - \chi)e_r > \text{ (20)}
\]

With
\[
\text{J} = <J>; <(1 - \chi)e_r = (I - f_\chi A)E \text{ (21)}
\]
The homogenized conductivity \( C_{\text{Hom}} \), is finally given by
\[
C_{\text{Hom}} = c_r I + f_\chi (c_\chi - c_r)A \text{ (22)}
\]

### 2.4 Lower Bounding

Following the same procedure by evaluating the current \( J \), we obtain the homogenized resistivity \( M_{\text{Hom}} \)
\[
M_{\text{Hom}} = m_r I + f_\chi (m_\chi - m_r)B \text{ (23)}
\]
where \( M = C^{-1} \), the concentration tensor \( B \) is given by:
\[
B = (f_\chi I - \zeta \sum_{\delta N} K^\delta < \chi K^\delta >)^{-1}f_\chi \text{ (24)}
\]

### 2.5 Symmetrical Isotropic Inclusion

For fibrous microstructures with isotropic as shown in Fig. 1, constituent has the following symmetry:
\[
\chi(x, y) = \chi(-x, y) = \chi(x, -y) = \chi(-x, -y)
\]
Using the fact that:
\[
\sum_n < \chi K^n > = \sum_n < (\chi^n)^2 > = f_\chi (1 - f_\chi)
\]
It can be shown that:
\[
\tilde{\xi} \sum_n G^n \delta c < \chi K^n > = \tilde{\xi} \sum_n G^n \delta c < (\chi^n)^2 > \text{ (25)}
\]
The expression Eq. (23) becomes, putting
\[
\delta c = c_\chi - c_r \text{ and } c = \frac{c_\chi}{c_r}
\]
\[
c_{RD} = \frac{2f_r c_c}{Z + (c-1)(1-f_r)} + c_r \text{ (26)}
\]
To apply the same assumption to \( \Phi_r \) we find
\[
c_{RD}^+ = \frac{-2m c_c}{Z + (\frac{1}{c} - 1)(1-f_r)} + c_r \text{ (27)}
\]
which are nothing else than the classical Hashin-Shtrikman bounds.

### 3. Numerical Algorithm

To deal with the numerical evaluation of Eqs. (15) and (16), let recall the finite radon transform by Mattus-Flusser \([6]\) of a matrix \( f(p \times p) \) representing a sampling form of a real function \( f(x) \).
\[
f(x) = f^0 + \sum_{m=0}^{p^2} \tilde{f}^m(x) \text{ (28)}
\]
With
\[
\tilde{f}^m(i, j) = \begin{cases} 
\frac{1}{p} \sum_{k=0}^{p-1} f([i + k]_p, [j + mk]_p) - f_0(i, j), & 0 \leq m < p \\
\frac{1}{p} \sum_{k=0}^{p-1} f(i, [j + mk]_p) - f_0(i, j), & m = p
\end{cases}
\]
and
\[
f_0(i, j) = \frac{1}{p^2} \sum_{k_l=1-p}^{p} f(k, l)
\]
where, \( p \) is prime and \([x]_p\) denotes \( x \mod p \).
Numerically this calculus could be performed more rapidly by Chandra \([13]\) by using the relationship between the FRT and the discrete Fourier transform:
For \( m = 0..p-1 \)
\[
\tilde{f}^m(k_1, k_2) = \begin{cases} 
\frac{p}{p} \sum_{r=0}^{p-1} f(0, r)e^{\frac{-2\pi irk_2}{p}} & \text{if } [k_1 + m k_2]_p = 0 \\
0 & \text{if not}
\end{cases}
\]
For \( m = p \)
\[
\tilde{f}^p(k_1, k_2) = \begin{cases} 
\frac{p}{p} \sum_{k=0}^{p-1} f(r, 0)e^{\frac{-2\pi r k_1}{p}} & \text{if } k_2 = 0 \\
0 & \text{if not}
\end{cases}
\]
By defining a new operator \( O^0 \),
For \( i = 0..p-1 \).
\[
O^0(k_1, k_2) = \begin{cases} 
1 & \text{if } [k_1 + ik_2]_p = 0 \\
0 & \text{if not}
\end{cases}
\]
For \( i = p \)
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\[ O^p(k_1, k_2) = \begin{cases} 1 & \text{if } [k_2]_p = 0 \\ 0 & \text{if not} \end{cases} \quad (33) \]

On other side we have:

\[ \hat{A} (k_1, k_2) = \hat{a}^l (k_1) O^l (k_1, k_2) \quad (34) \]

With

\[ \hat{a}^l (k_1) = \sum_{r=0}^{p-1} a(r, 0) e^{-2 \pi i r k_1} \quad (35) \]

By using the linearity of the DFT in Eqs. (21) and (27) it gives

\[ \hat{A} (k_1, k_2) = \sum a^l (k_1) O^l (k_1, k_2) \quad (36) \]

It can also be shown using the fact that \( p \) is prime:

\[ O^l (k_1, k_2) O^l (k_1, k_2) = \delta_{i,j} O^l (k_1, k_2) \quad (37) \]

\( \delta_{i,j} \) is the Kronecker symbol.

It comes

\[ \hat{A} (k_1, k_2) = O^l (k_1, k_2) \hat{A} (k_1, k_2) \quad (38) \]

So the FRT of \( A \) in the direction \( i \):

\[ \hat{\Lambda} (k_1, k_2) = F^{-1} \left( O^l (k_1, k_2) \hat{A} (k_1, k_2) \right) \quad (39) \]

where, \( F^{-1} \) is the Fourier transform inverse.

Remarking that \( G^l (k_1, k_2) = G^l (k_1, k_2) O^l (k_1, k_2) \) and using the linearity of the DFT let Eqs. (31) and (32), it gives us an interesting relationship:

\[ \sum G^l \hat{A} = F^{-1} (G \hat{A} (k_1, k_2)) \quad (40) \]

and

\[ G^l (k_1, k_2) = \sum_{i=0}^{p} G^l (k_1, k_2) \quad (41) \]

The solution Eq. (6) can then be used in a more useful form:

\[ \hat{e} (k_1, k_2) = \hat{E} (k_1, k_2) - \hat{G} \cdot \hat{\delta} \hat{e} (k_1, k_2) \quad (42) \]

where, \( \hat{E} (k_1, k_2) = \hat{\delta} (k_1, k_2), \hat{E} \).

The general continuous solution Eq. (9) reads now:

\[ \hat{e} (k_1, k_2) = \hat{E} (k_1, k_2) - \hat{G} \cdot \hat{\delta} \hat{e}_{\chi} \quad (43) \]

4. Results and Validation

To illustrate the formalism presented here, we will present here an evaluation of the homogenized properties and also the bounds obtained by considering a uniform fields in the phase \( \Phi_{\chi} \). The example considered here consists in a two-phase isotropic material compositing with a hexagonal repartition of square fibers in Fig. 2. The RVE could be taken as in Fig. 3. The corresponding conductivities are denoted by \( c_{\chi} \) and \( c_r \).

It can be seen from tables that the bounds obtained numerically and those obtained by (HS) are the same as expected by the present formalism.

Tables 1 and 2 summarize the result obtained for two different values of the contrast \( c = \frac{c_{\chi}}{c_r} \).

\[ \text{Fig. 2 Periodical and symmetrical hexagonal fiber structure.} \]

\[ \text{Fig. 3 Unit cell microstructure.} \]
Table 1  Upper and lower bounds given by Hashin-Schtrickman method an Radon Method for a contraste $c = 5$.

<table>
<thead>
<tr>
<th>$f_1$</th>
<th>HS-</th>
<th>HS+</th>
<th>RD-</th>
<th>RD+</th>
<th>EXACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1.142</td>
<td>1.249</td>
<td>1.147</td>
<td>1.275</td>
<td>1.153</td>
</tr>
<tr>
<td>0.2</td>
<td>1.307</td>
<td>1.521</td>
<td>1.311</td>
<td>1.527</td>
<td>1.327</td>
</tr>
<tr>
<td>0.3</td>
<td>1.500</td>
<td>1.818</td>
<td>1.510</td>
<td>1.834</td>
<td>1.548</td>
</tr>
<tr>
<td>0.4</td>
<td>1.727</td>
<td>2.142</td>
<td>1.739</td>
<td>2.159</td>
<td>1.825</td>
</tr>
<tr>
<td>0.5</td>
<td>2.000</td>
<td>2.500</td>
<td>2.000</td>
<td>2.500</td>
<td>2.236</td>
</tr>
<tr>
<td>0.6</td>
<td>2.333</td>
<td>2.894</td>
<td>2.315</td>
<td>2.874</td>
<td>2.739</td>
</tr>
<tr>
<td>0.7</td>
<td>2.750</td>
<td>3.333</td>
<td>2.725</td>
<td>3.309</td>
<td>3.228</td>
</tr>
<tr>
<td>0.8</td>
<td>3.285</td>
<td>3.823</td>
<td>3.273</td>
<td>3.813</td>
<td>3.766</td>
</tr>
<tr>
<td>0.9</td>
<td>4.000</td>
<td>4.375</td>
<td>3.977</td>
<td>4.358</td>
<td>4.335</td>
</tr>
</tbody>
</table>

Table 2  Upper and lower bounds given by Hashin-Schtrickman method an Radon Method for a contraste $c = 20$.

<table>
<thead>
<tr>
<th>$f_1$</th>
<th>HS-</th>
<th>HS+</th>
<th>RD-</th>
<th>RD+</th>
<th>EXACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1.198</td>
<td>2.047</td>
<td>1.204</td>
<td>2.077</td>
<td>1.224</td>
</tr>
<tr>
<td>0.2</td>
<td>1.441</td>
<td>3.204</td>
<td>1.447</td>
<td>3.228</td>
<td>1.501</td>
</tr>
<tr>
<td>0.3</td>
<td>1.745</td>
<td>4.489</td>
<td>1.763</td>
<td>4.561</td>
<td>1.898</td>
</tr>
<tr>
<td>0.4</td>
<td>2.134</td>
<td>5.925</td>
<td>2.155</td>
<td>5.99</td>
<td>2.534</td>
</tr>
<tr>
<td>0.5</td>
<td>2.652</td>
<td>7.540</td>
<td>2.652</td>
<td>7.541</td>
<td>4.610</td>
</tr>
<tr>
<td>0.6</td>
<td>3.375</td>
<td>9.277</td>
<td>3.333</td>
<td>9.277</td>
<td>7.964</td>
</tr>
<tr>
<td>0.7</td>
<td>4.454</td>
<td>11.46</td>
<td>4.384</td>
<td>11.343</td>
<td>10.557</td>
</tr>
<tr>
<td>0.8</td>
<td>6.241</td>
<td>13.87</td>
<td>6.195</td>
<td>13.82</td>
<td>13.336</td>
</tr>
<tr>
<td>0.9</td>
<td>9.769</td>
<td>16.681</td>
<td>9.627</td>
<td>16.597</td>
<td>16.348</td>
</tr>
</tbody>
</table>

5. Conclusion

In this work, the conductivity bounds for a two-phase fibrous material are presented. The analytical form, here obtained, is the analogous real form of those obtained by Fourier method. Its simplicity leads us to deal some special symmetrical cases. In fact, and for the symmetry (cf 2.5) the obtained bounds are shown to be the same as the HS classically known as the optimal bounds [5]. Using the relation with the DFT, the complexity of the presented algorithm is also the same as the algorithm using Fourier method. All this encourages the use of the presented algorithm to deal with other situations as the non-linear cases or the systematic theory of Kröner [14] related to statistical description of heterogeneous structures.

References


DRT (Discrete Radon Transform)

Theorem: if a function $f(x_1, x_2)$ is supported on the unit square $0 < x_1, x_2 < 1$ then:

$$f(x_1, x_2) = f_0 + \sum_n \hat{f}_n(x_1, x_2)$$

With

$$\hat{f}_n(x) = \sum_{m=-\infty}^{\infty} \int_{\Omega} f(x') \delta(x', k\rho - m) dx'$$

$\rho = x \cdot n; \ f_0 = < f >_{\Omega}; \ \Omega$ denotes the RVE

$$n = \frac{k_1 e_1 + k_2 e_2}{\sqrt{k_1^2 + k_2^2}} = \frac{k}{\bar{k}}$$

Let us remind that $k_1$ and $k_2$ are coprime.