THERMAL CONDUCTIVITY EFFECTIVE TENSOR OF COMPOSITE MATERIALS DETERMINATION OF THE REPRESENTATIVE VOLUME ELEMENT (RVE)

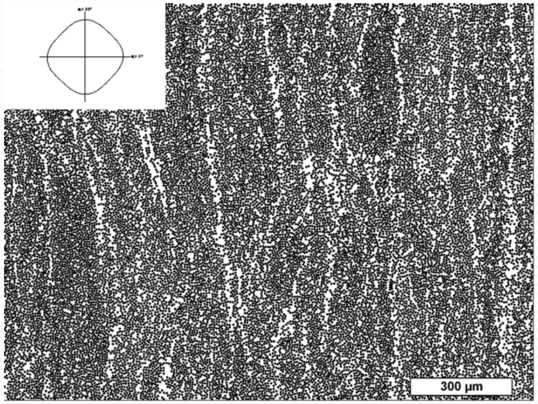
A Matine(1), N Boyard(1), Y Jarny(1),
G Legrain(2), P Cartraud(2),
M Thomas (3)
(1)LTN, Université de Nantes / CNRS UMR6607
(2)GeM, École Centrale de Nantes/CNRS UMR 6183
(3) Airbus, Toulouse

Outline

- **INTRODUCTION**
- **PROBLEM STATEMENT FOR A PERIODIC MEDIUM**
- **NUMERICAL RESULTS - PERIODIC MEDIUM**
- **NON PERIODIC MEDIUM: DETERMINATION OF THE RVE SIZE**
- **CONCLUSIONS**

1. INTRODUCTION

• Composite : heterogeneous material, structures at different scales



UD laminate
AS4/8552 (carbon fibres / epoxy matrix) prepreg (supplier: Hexcel Composite®).

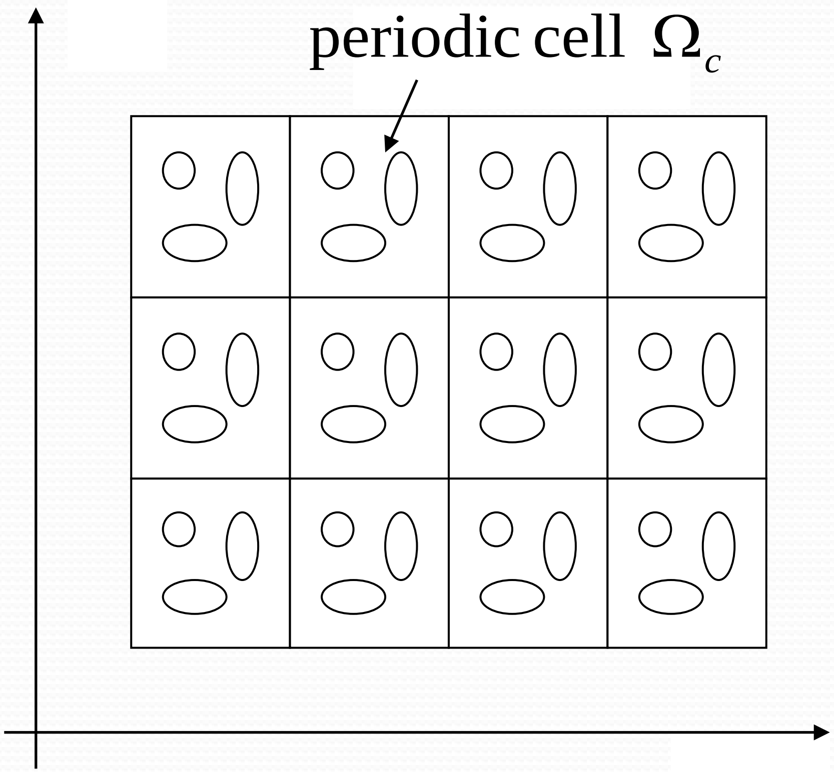
•To compute temperature fields : need of ***effective thermal properties***

• Interests in aeronautics : - system integration,
- temperature cartography,
- change of mechanical properties

• How to get these effective properties ?

- experiments
- numerical calculations, e.g. using ***homogenization*** theories

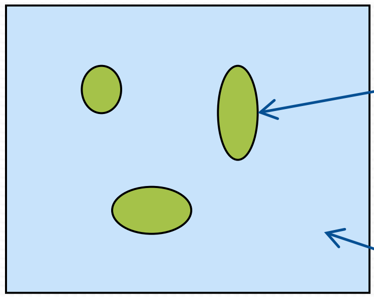
Periodic homogenization approach



$$\Omega_c \equiv R.V.E.$$

Example of 2-D periodic composite medium

2. PROBLEM STATEMENT FOR A PERIODIC MEDIUM



$$\Omega_c = \Omega_m \bigcup \Omega_f$$

Definitions :

$$\Gamma_{m-f} = \text{interface}$$

$$k(z) = \begin{cases} k_m, \text{in} \quad \Omega_m \\ k_f \text{in} \quad \Omega_f \end{cases}, z \in \Omega$$

$$\tau_f = \left|\Omega_f\right| / \left|\Omega_c\right| < 1$$

The periodic cell is assumed to be composed of

- a continuous phase, the polymer matrix (m),
- a dispersed phase, the fibres (f)

- Each phase is isotropic with constant thermal conductivity,

- The volume fraction of the dispersed phase.

THERMOCINÉTIQUE Nantes

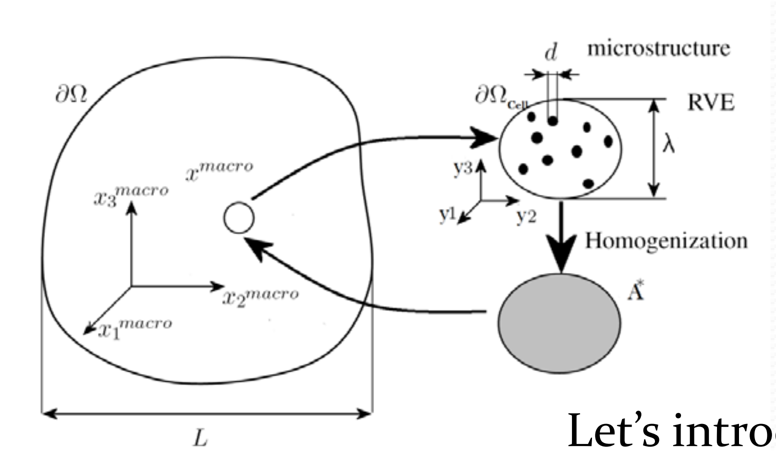
GeM Institut de Recherche en Génie Civil et Mécanique

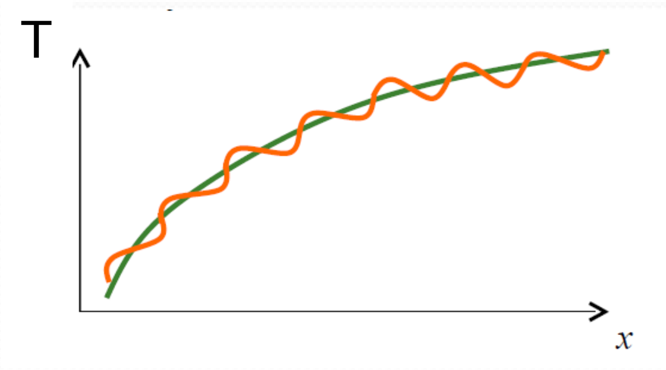
Steady-state Heat conduction equation and interface conditions

$$
\begin{cases}
div_z(k_m \nabla_z u_m(z)) = 0,\ in\ \Omega_m \\
div_z(k_f \nabla_z u_f(z)) = 0,\ in\ \Omega_f \\
-k_m \nabla_z u_m.\vec{n} = h\lfloor u_m - u_f \rfloor on\ \Gamma_{m-f} \\
-k_m \nabla_z u_m.\vec{n} = -k_f \nabla_z u_f.\vec{n}\ on\ \Gamma_{m-f} \\
u_\varepsilon\ periodic\ on\ \partial\Omega_c
\end{cases}
$$

$h = 1/Rtc$ The inverse of the thermal contact resistance between the matrix and the fibres is supposed to be uniform

Multi-scale approach and asymptotic expansion: Principle





Let's introduce ***dimensionless variables*** :

x : macroscopic scale (composite)
y : microscopic scale (fibres)

$$y = z / l_c \quad \text{and} \quad x = z / L = \varepsilon y$$

→ Scaling ratio: $\varepsilon = \lambda / L << 1$

The temperature field ***u(z)*** is searched under the form of a multi-scale asymptotic expansion

$$u_\varepsilon(z) = u_0(x,y) + \varepsilon u_1(x,y) + \varepsilon^2 u_2(x,y) + O(\varepsilon^2)$$

Variational formulation

Find $u \in V$, such that, $\forall \mathbf{v} \in \mathbf{V} \left(V = H^1_{per}(\Omega_c) \right)$

$$\int_{\Omega_c} \nabla_y v . \tilde{k} \nabla_y u d\Omega + \int_{\Gamma_{m-f}} Bi(u_m - u_f)(v_m - v_f) d\Gamma = 0$$

$$\tilde{k}(y) = \begin{cases} 1, \text{in} \quad \Omega_m \\ \alpha \ \text{ in} \quad \Omega_f \end{cases}, y \in \Omega_c$$

Dimensionless conductivity function

$$Bi = \frac{hl_c}{k_m} \geq 0$$

Dimensionless Biot number (l_c =cell size)

$$\alpha = k_f / k_m$$

Thermal contrast

Multi-scale approach and asymptotic expansion (1)

- Combining heat conduction equations and asymptotic expansion
- Identifying the terms which have equal powers of ε

$$\epsilon^0 \Longrightarrow \begin{cases} u_0 \; est \; continue \\ u_0\,(x,y) = u_0\,(x) \end{cases}$$

$$\epsilon^1 \Longrightarrow pas\, d'information$$

$$\epsilon^2 \Longrightarrow \begin{cases} 1: \int_\Omega \nabla_x v_0 . \tilde{k} . (\nabla_x u_0 + \nabla_y u_1) = 0 \\ 2: \int_\Omega (\nabla_y v_1 . \tilde{k} . (\nabla_x u_0 + \nabla_y u_1))\, d\Omega + \int_{\partial\Omega_{f-m}} \lambda h \left(u_1^m - u_1^f\right)\left(v_1^m - v_1^f\right) = 0 \end{cases}$$

To separate variables, we write: $u_1(x,y) = -[\nabla_x u_0(x)]^t \cdot w(y)$

Equation 1:

$$\sum_{i=1}^{3} \int_\Omega \nabla_x v_0 . \tilde{k} (e_i - \nabla_y w_i) \frac{\partial u_0(x)}{\partial x_i} = 0$$

Equation 2:

$$\int_\Omega \left(\nabla_y v_1 . \tilde{k} \frac{\partial u_0(x)}{\partial x_i} (e_i - \nabla_y w_i)\right) d\Omega + \int_{\partial\Omega_{f-m}} \lambda h \left(w_i^m - w_i^f\right)\left(v_1^m - v_1^f\right) \frac{\partial u_0(x)}{\partial x_i} = 0$$

The homogenized problem is obtained when ε → 0 :

Equation 1 → Macroscopic equation

$$\nabla_x.(\tilde{k}^*\nabla_x u^0(x)) = 0, \; in \; \Omega$$

Equation 2 → Microscopic equation

$$\int_{\Omega_c}(\nabla_y v_1.\tilde{k}(e_i - \nabla_y w_i))dy + \int_{\partial\Omega_c}\lambda h(w_i^m - w_i^f)(v_1^m - v_1^f)ds = 0$$

w_i is computed from the microscopic equation

$$\tilde{k}^*_{i,j} = \frac{1}{meas(\Omega_c)}\int_{\Omega_c}\tilde{k}(y)(e_j - \nabla_y w_i)d\Omega$$

$\tilde{k}^*$ **: *effective thermal conductivity tensor* of the homogenized medium.**

$\{e_i \in R^2, i = 1,2\}$ = standard set of basis vectors

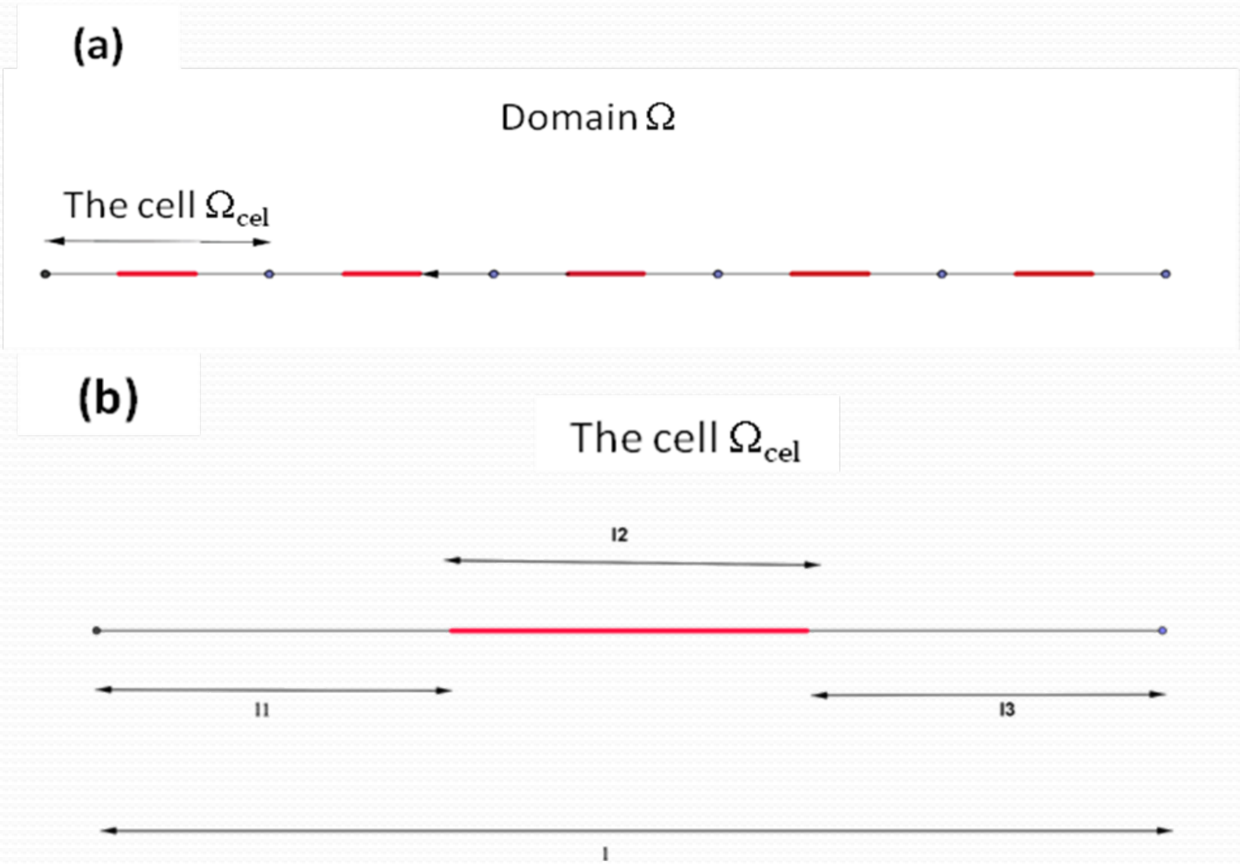
Multi-scale approach and asymptotic expansion (3)

- The periodic homogenization method is valid in a more general 3-D anisotropic cell,
- Computations can be performed by taking the thermal conductivity of each phase as a symmetrical tensor, instead of the diagonal form considered here for simplicity.

$$k_p = \begin{bmatrix} k_{11,p} & k_{12,p} & k_{13,p} \\ & k_{22,p} & k_{23,p} \\ & & k_{33,p} \end{bmatrix}, \; p = m, f$$

3. NUMERICAL RESULTS- PERIODIC MEDIUM

1-D example



THERMOCINÉTIQUE

Institut de Recherche en Génie Civil et Mécanique

The exact value of the effective thermal conductivity of the homogenized medium is

$$k^*_{exact} = \frac{k_m}{(1-\tau_f) + \tau_f/\alpha + 2/Bi} \quad \text{with} \quad Bi = \frac{hl_c}{k_m} \geq 0$$

Application:

$$\tau_f = \frac{l_2}{l_1 + l_2 + l_3} = \frac{l_2}{l_c} = 0.2$$

$$\alpha = \frac{k_f}{k_m} = \frac{50}{1}$$

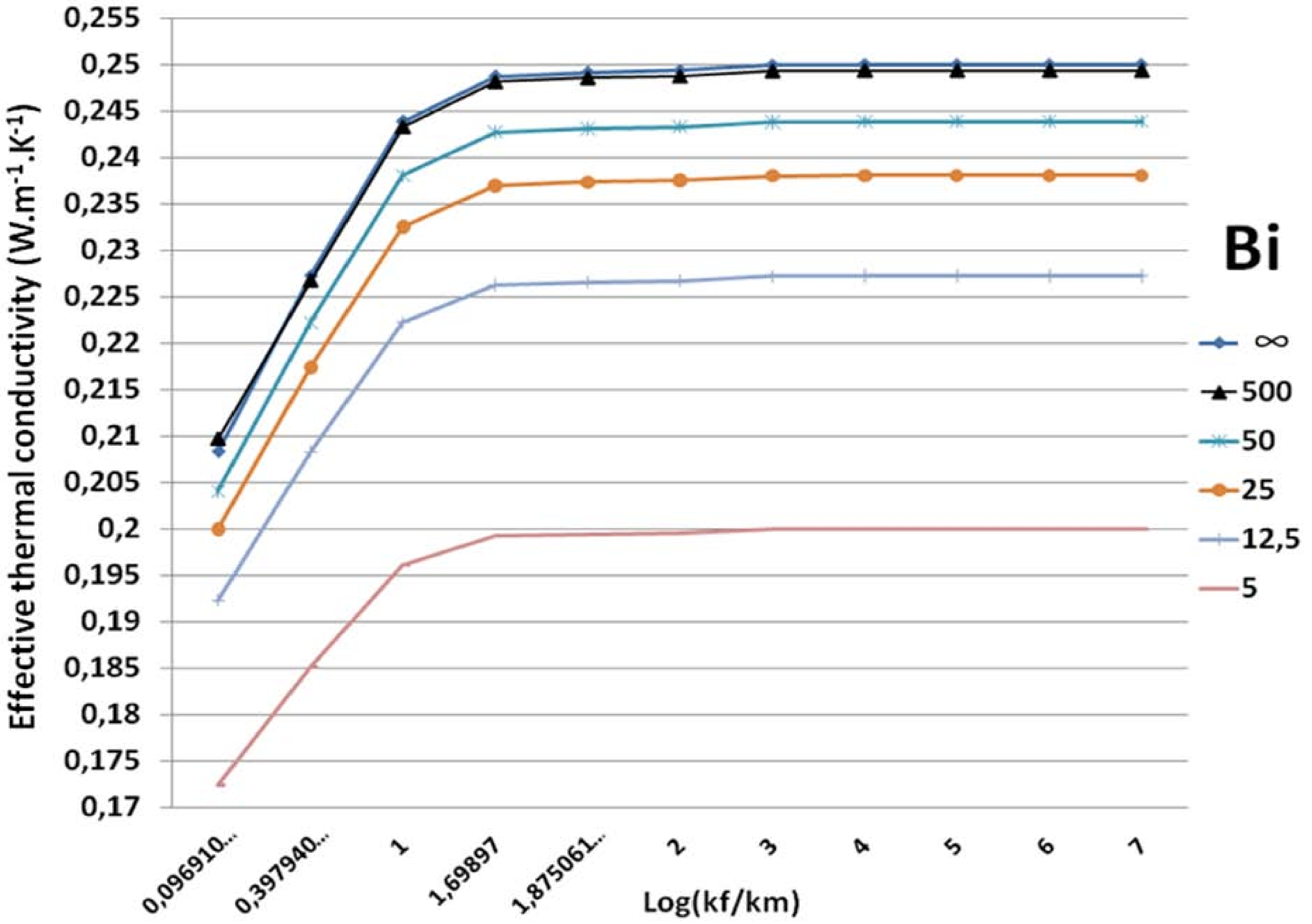
Bi	k^*	*exact value*
10^4	1.243	1.242
10	1.213	1.220
10^{-3}	10^{-4}	10^{-4}

k^* is calculated from the expression presented previously

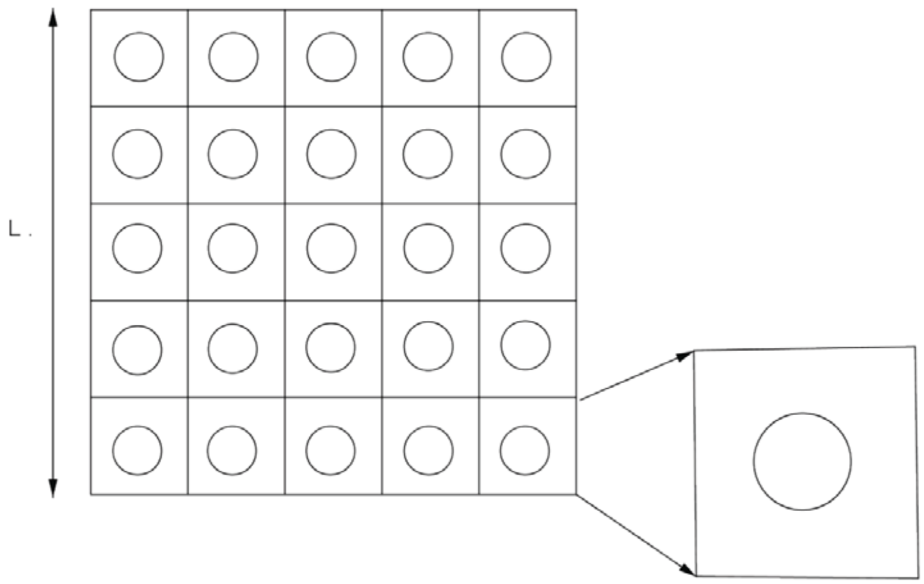
Influences of *Bi* and the contrast α

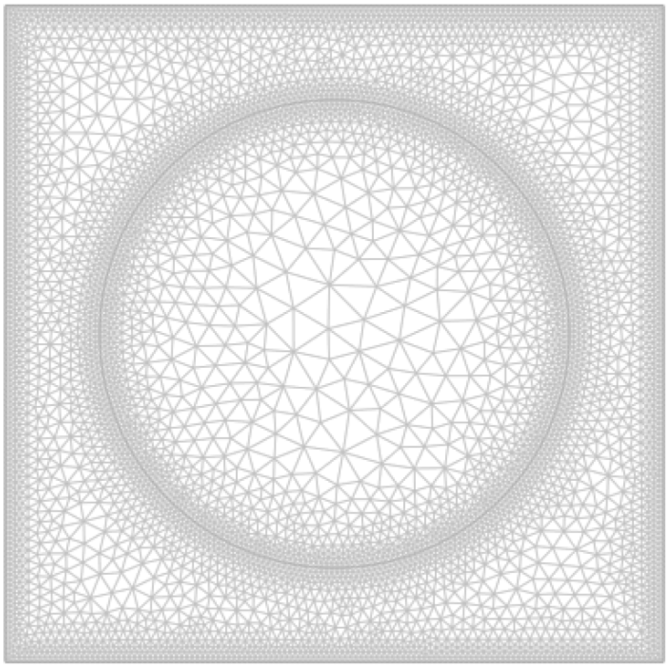
$$Bi = \frac{hl_c}{k_m} \geq 0$$

$$\tau_f = \frac{l_2}{l_c} = 0.2$$



2-D example : Centered fibre





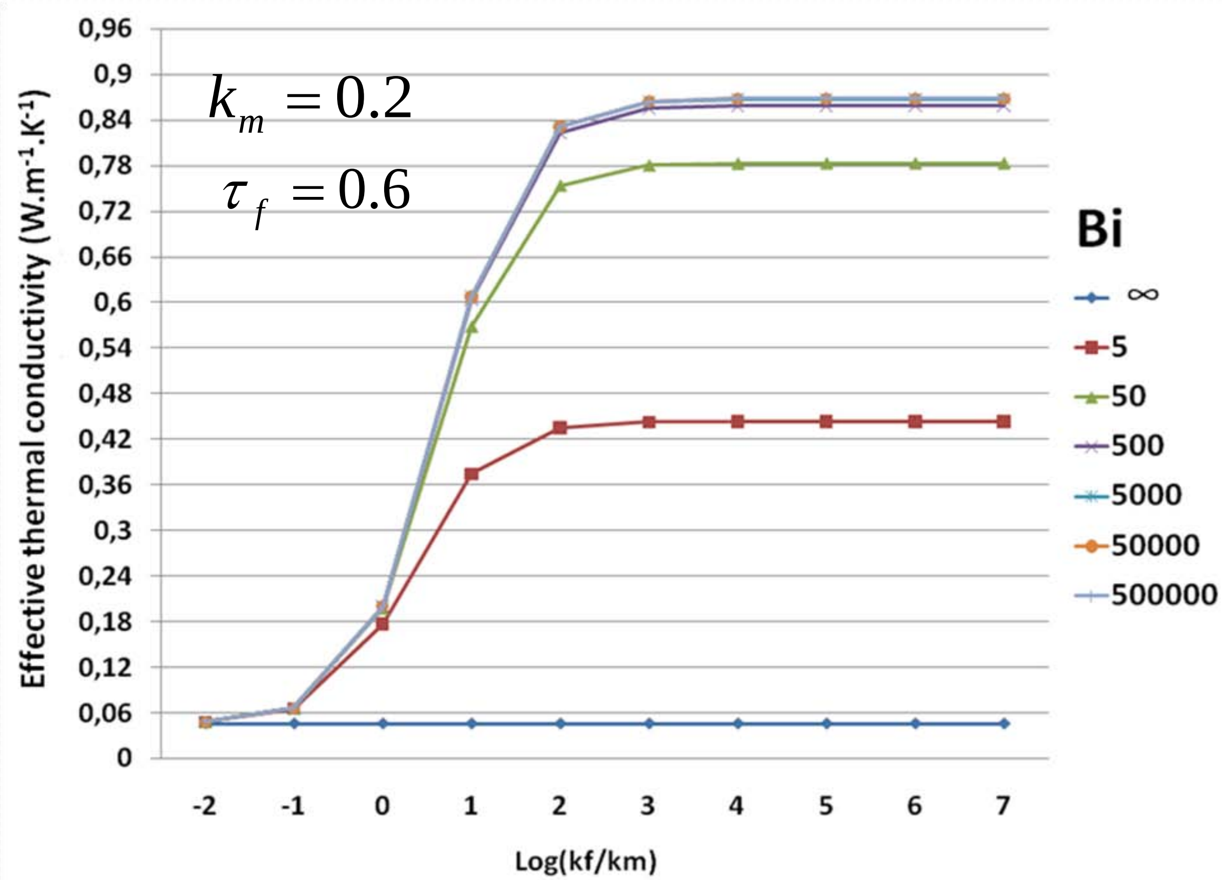
$$\tau_f = \frac{|\Omega_f|}{|\Omega_c|} = 0.3 \qquad \alpha = \frac{k_f}{k_m} = \frac{2}{1} = 2$$

Influences of *Bi* and α

$$\alpha = \frac{k_f}{k_m} = 50$$

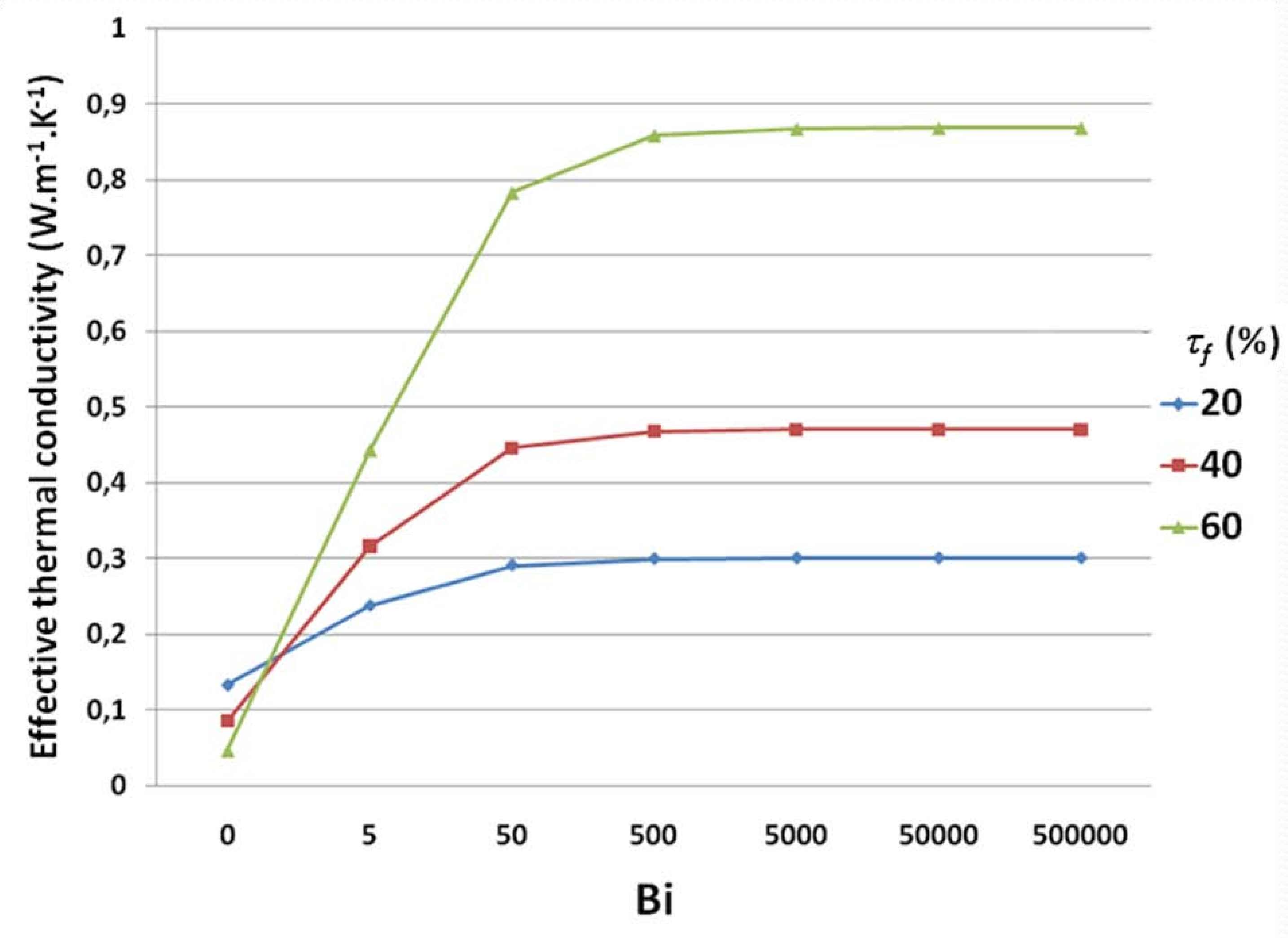
$$\tau_f = 0.3$$

Bi	Effective conductivity (W.m^{-1}.K^{-1})	
	k^*	Literature (1)
10^{-3}	0.538	0.538
10^{-1}	0.578	0.572
1	0.825	0.815
10	1.490	1.474
10^2	1.776	1.768
10^5	1.813	1.812



(1) R.P.A. Rocha, M.E. Cruz, Numerical Heat Transfer A, vol.39, pp 179-203, 2001

Influences of *Bi* and τ_f

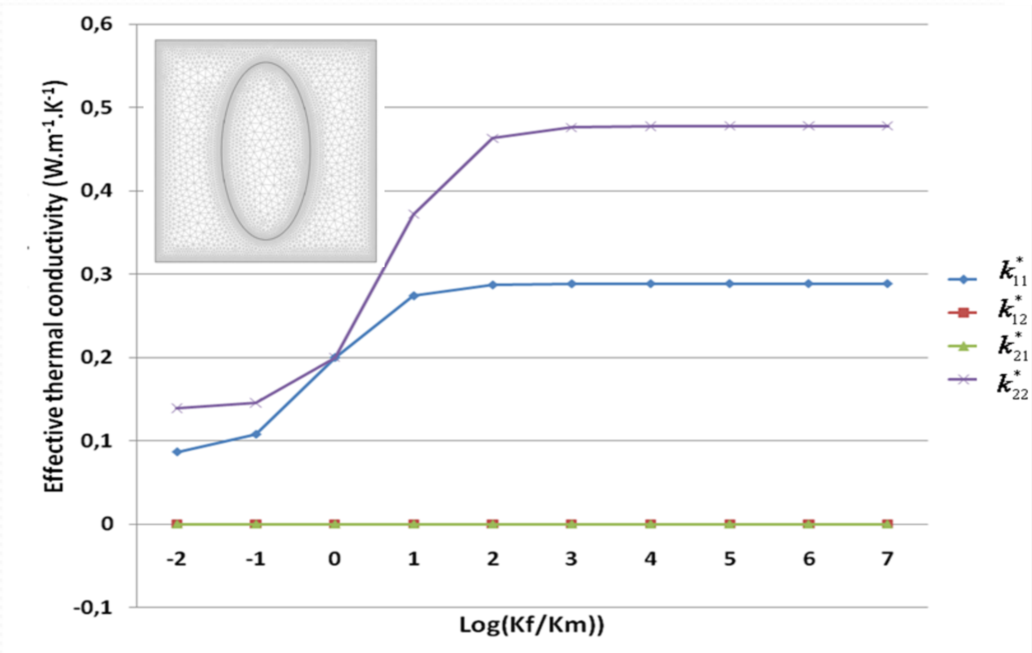


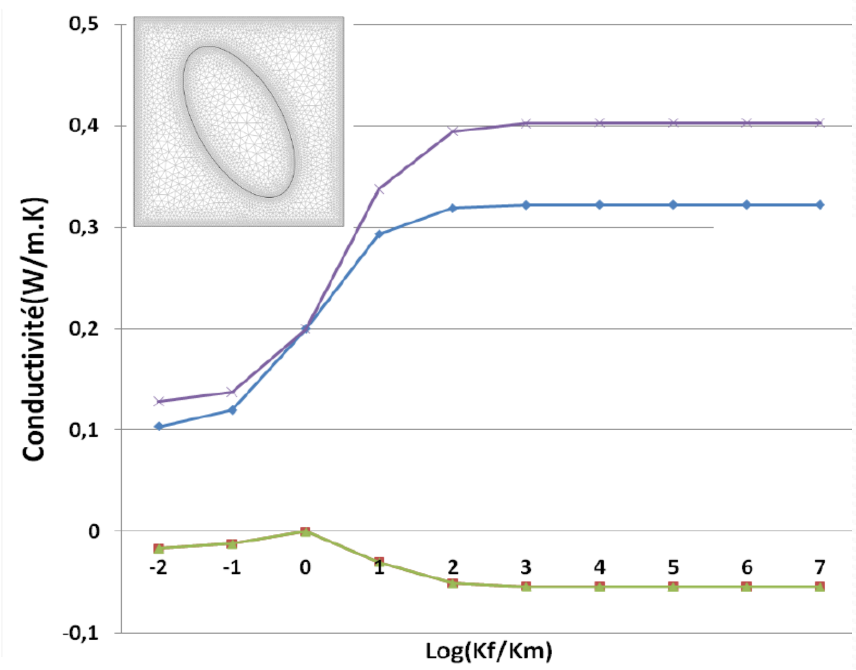
$$k_m = 0.2$$
$$k_f = 100$$

$$Bi = \frac{hl_c}{k_m} \geq 0$$

2-D example : Elliptic inclusion

Orthotropic homogenized medium



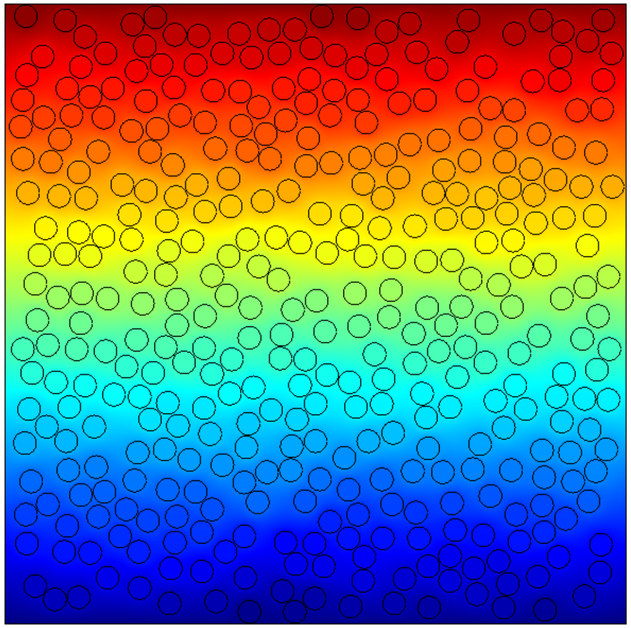


$$k_m = 0.2 \quad \tau_f = 0.3 \quad Bi = 5000$$

4. NON-PERIODIC MEDIUM: random structures

DETERMINATION OF THE RVE SIZE

In a first step, square images of 2-D random structures are generated numerically . Their sizes are assumed to be large enough to apply the homogenization method.



Example: image size=167 x 167 µm²
(600 x 600 pixels²).

The mains parameters are

- the volume fraction (τ_f = 0.4)
- the mean value of the diameter <*d*> = 7µm

The probability density of the random distribution is supposed to be uniform.

STATISTICAL DETERMINATION OF THE RVE SIZE (1)

The **convergence analysis** consists in

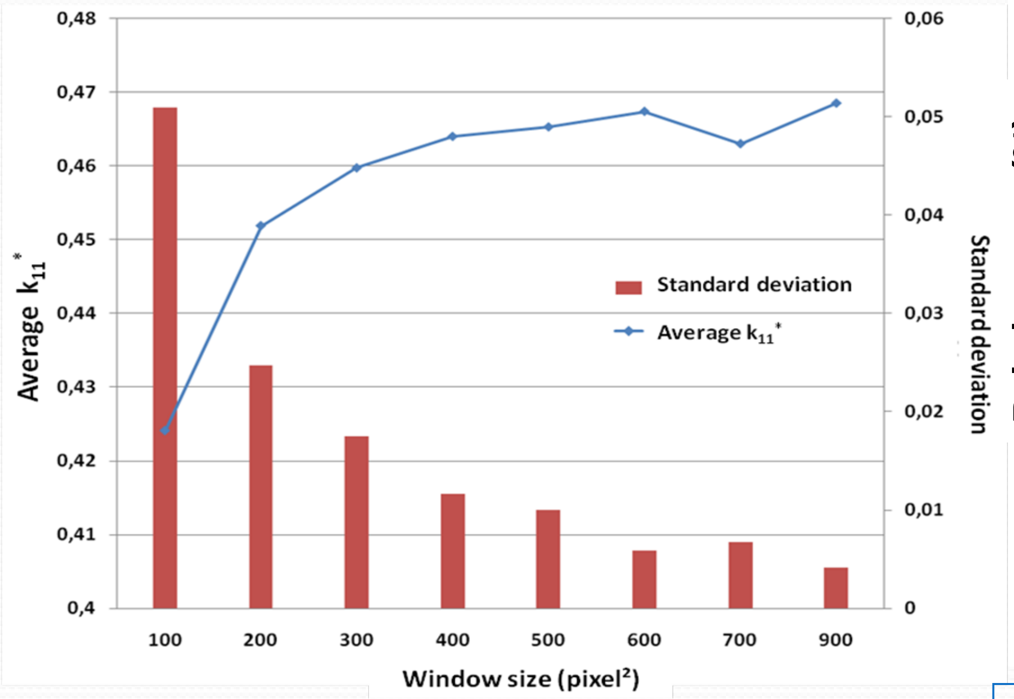
- *dividing* the area s_{max} of an original image in a set of N sub-windows with same size s_N : $N \times s_N = s_{max}$,
- *computing* the effective thermal conductivity tensor $k^*_{ij}(s_p)$ (p = 1,2,…,N)

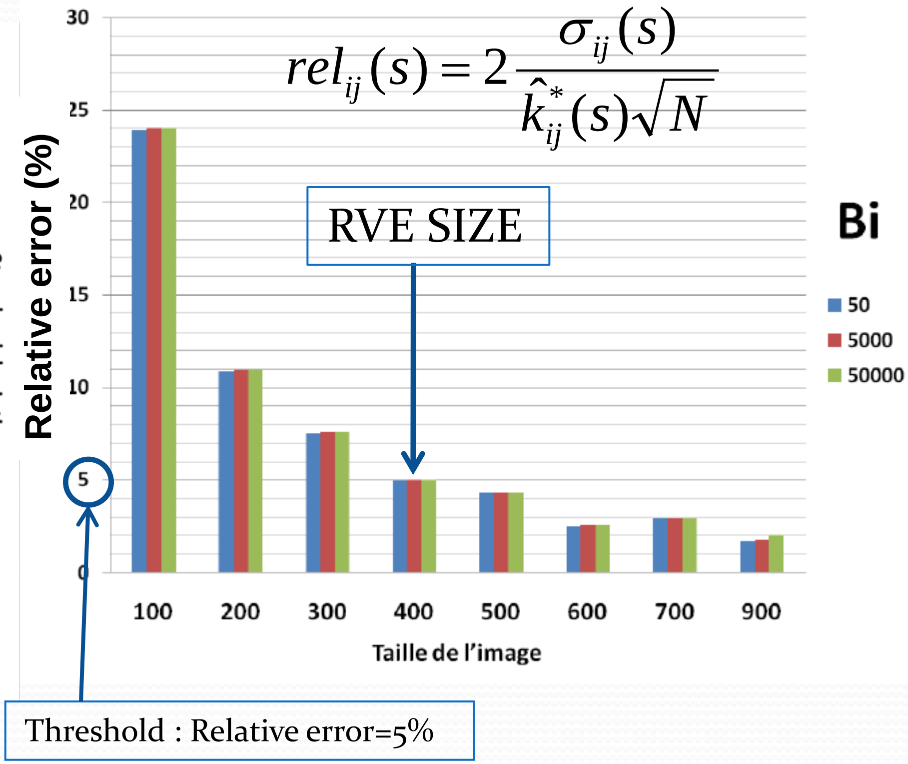
  for each of these set of sub-windows, assuming periodic conditions ,
- performing statistical analysis on each set of windows, to get
  - the mean value $\hat{k}^*_{ij}(s_N)$
  - and the standard deviation $\sigma_{ij}(s_N)$ and the associated relative error

  for each component of the effective tensor, as a function of the size s_N ,
- *repeating* the computations for different values of N.

STATISTICAL DETERMINATION OF THE RVE SIZE (2)

k_f = 10 W/m.K, k_m = 0.2 W/m.K, τ_f = 0.4, Bi=5

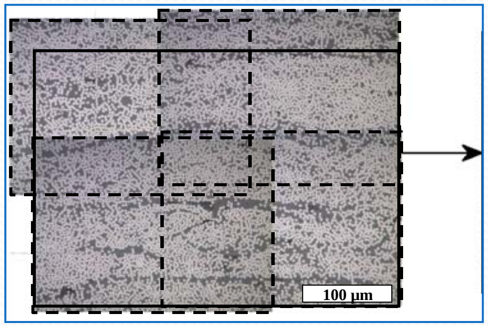


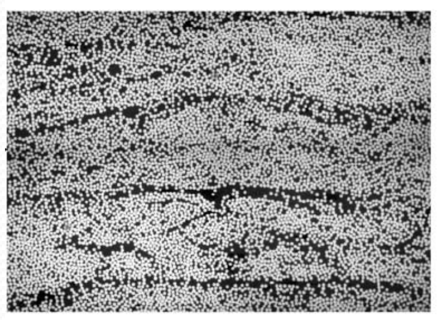


$$rel_{ij}(s) = 2\frac{\sigma_{ij}(s)}{\hat{k}_{ij}^*(s)\sqrt{N}}$$

The RVE size associated to k^* for the random structure is **110 x 110 μm²** (400 x 400 pixels²) for <u>a threshold relative error = 5%</u>

5. NON-PERIODIC MEDIUM: Real unidirectional (UD) composite sample



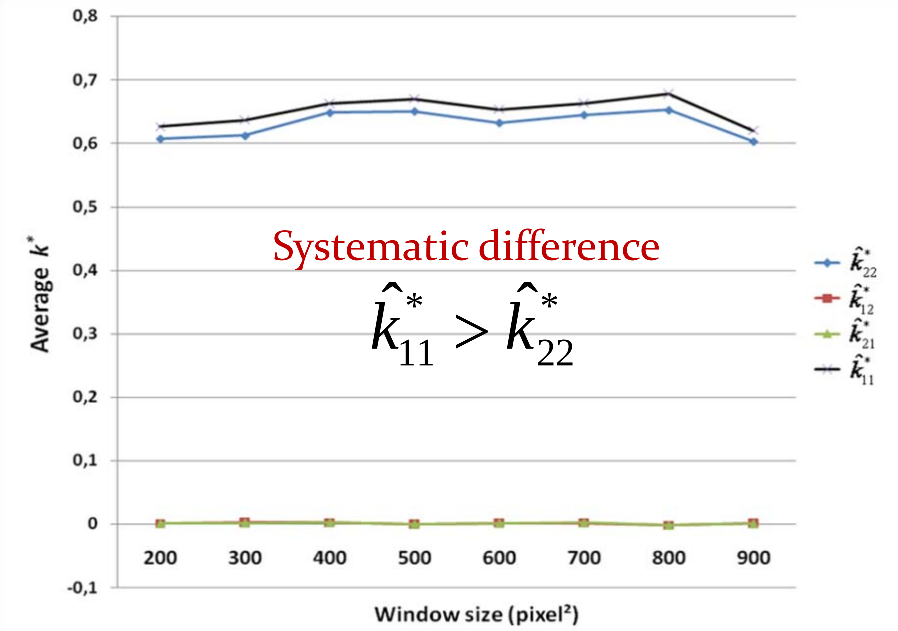


$\tau_f = 0.514$

The RVE size associated to τ_f for a real UD composite is 195 x 195 µm² (700 x 700 pixels²) for a threshold relative error = 5%

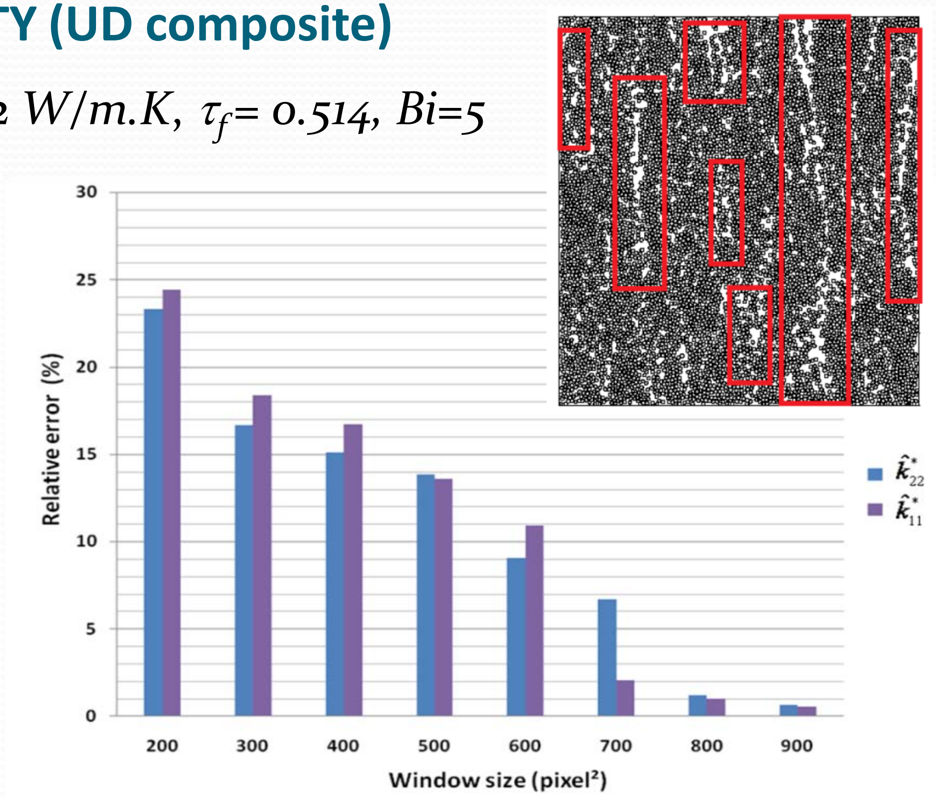
RVE SIZE FOR THERMAL CONDUCTIVITY (UD composite)

$k_f = 10$ W/m.K, $k_m = 0.2$ W/m.K, $\tau_f = 0.514$, $Bi=5$



Systematic difference

$$\hat{k}^*_{11} > \hat{k}^*_{22}$$

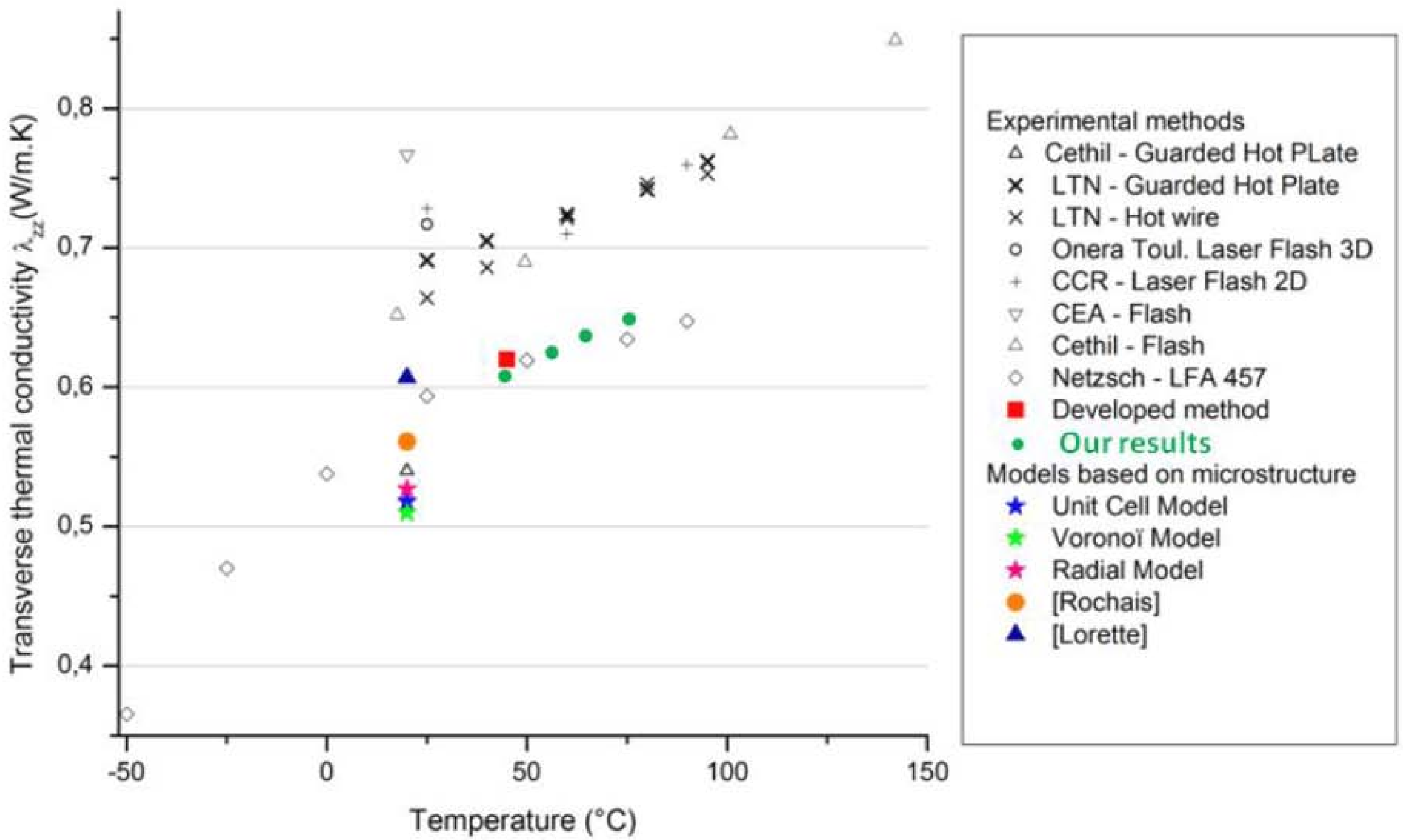


RVE = max (RVE(k^*_{11}), RVE(k^*_{22}))

The RVE size associated to k^* for the real UD composite =<u>220 x 220 µm²</u> (800 x 800 pixels²) for a <u>threshold relative error = 5%</u>

6. CONCLUSIONS

- The periodic homogenization theory is well suited for the determination of the effective thermal conductivity tensor of composite materials, like UD carbon-epoxy
- The method is easily implemented by using a finite element software (2-D structures)
- The influences of the volume fraction of the dispersed phase, of the thermal contrast and of the thermal contact are readily analyzed
- The numerical algorithm was extended to random structures and statistical analysis leads to the estimation of the RVE size.
- For real UD composite micrographs, a weak orthotropic behavior was observed. The values of effective conductivity are close to those calculated from a random structure (same α, τ_f).



Cross-bench SFT, Toulouse 2005