Fast HdBNM for prediction of thermal properties of CNT-reinforced composites

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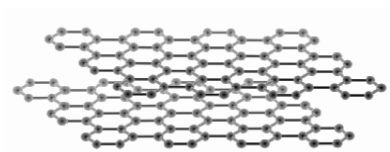
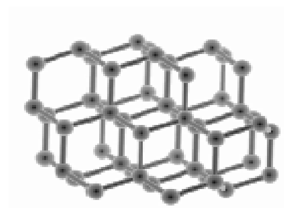
Background

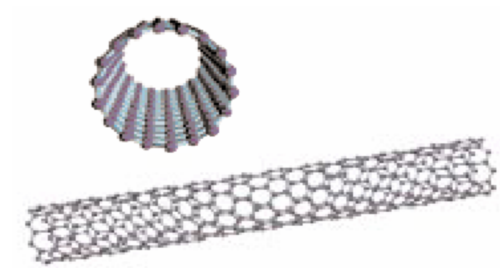
- Thermal conductivity of CNT (W/m·K)



Graphite
50~100



Diamond
3320



Nanotube
3000~6000

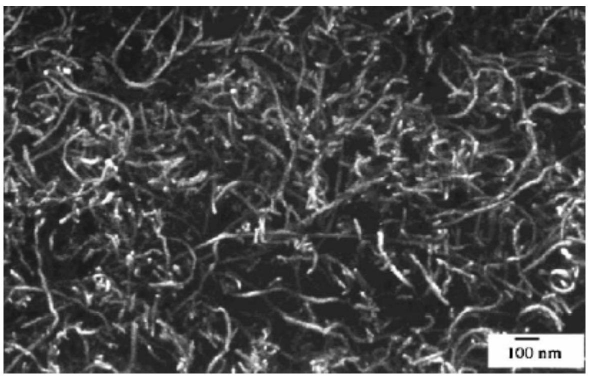
Resins: 0~1 W/m·K

Metals:

Fe	72	W/m·K
Cu	390	W/m·K

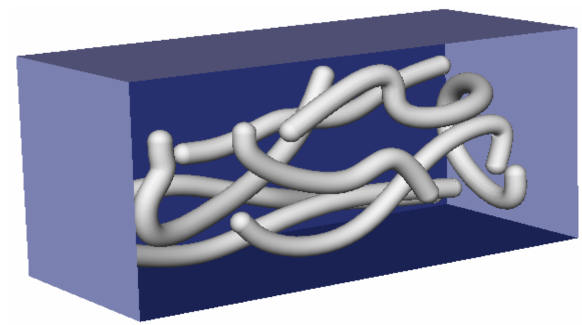
Background (2)

- Promising applications



Nanotube-reinforced polymers

- Numerical simulation model



RVE including curved CNTs

Background (3)

Two main difficulties in performing the numerical analysis using element based methods (e.g. FEM)

- Mesh generation
- Large computational scale

➢ To overcome the first difficulty

Hybrid Boundary Node Method (HdBNM)

➢ To overcome the second difficulty

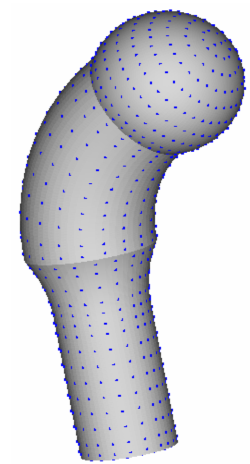
Simplified mathematic model

Fast Multipole Techniques (FMM)

Hybrid BNM

➢Main features:

- Combines a modified functional with the *Moving Least Squares* (MLS) approximation
- Three independent variables
  - internal temperature
  - boundary temperature
  - boundary normal flux



Example of meshless discretization

➢Variables approximation

- internal temperature

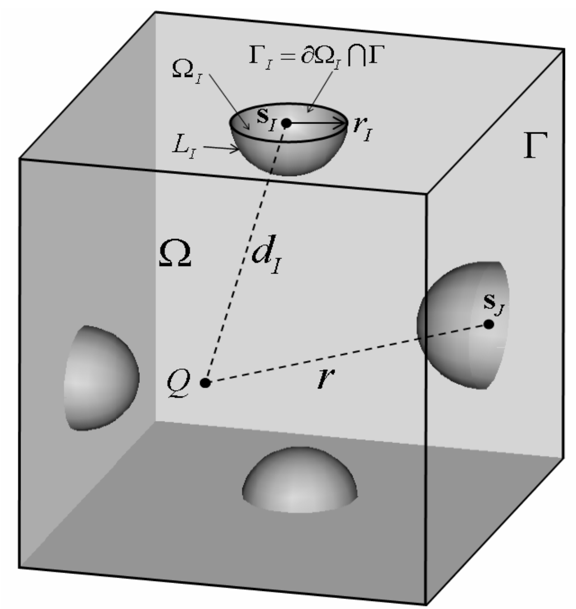
$$\phi = \sum_{I=1}^{N} \phi_I^s x_I \qquad \phi_I^s = \frac{1}{\kappa} \frac{1}{4\pi r(Q, \mathbf{s}_I)}$$

- Boundary variables

$$\tilde{\phi}(\mathbf{s}) = \sum_{I=1}^{N} \Phi_I(\mathbf{s}) \hat{\phi}_I \qquad \tilde{q}(\mathbf{s}) = \sum_{I=1}^{N} \Phi_I(\mathbf{s}) \hat{q}_I$$

Hybrid BNM (2)

➢ **System of equations**



$$\boxed{\mathbf{Ux} = \mathbf{H}\hat{\mathbf{q}}}$$

$$\boxed{\mathbf{Vx} = \mathbf{H}\hat{\phi}}$$

$$U_{IJ} = \int_{\Gamma_s^J} \phi_I^s v_J(Q)\, d\Gamma$$

$$V_{IJ} = \int_{\Gamma_s^J} q_I^s v_J(Q)\, d\Gamma$$

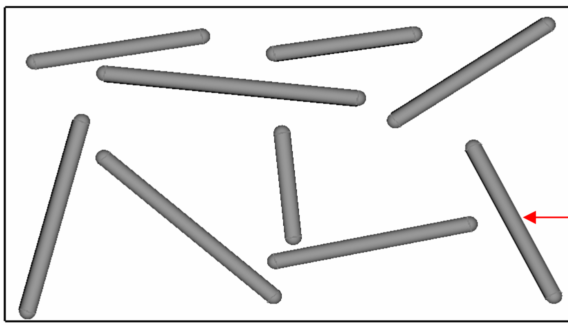
$$H_{IJ} = \int_{\Gamma_s^J} \Phi_I(\mathbf{s}) v_J(Q)\, d\Gamma$$

Elements in BEM are used to

- **interpolate Boundary variables**
- **facilitate boundary integration**
- **approximate the geometry**

Simplified model

- **Hybrid BNM equations for polymer matrix**



An RVE including n CNTs

$$\begin{bmatrix} \boldsymbol{U}_{00}^{p} & \boldsymbol{U}_{01}^{p} & \cdots & \boldsymbol{U}_{0n}^{p} \\ \boldsymbol{U}_{10}^{p} & \boldsymbol{U}_{11}^{p} & \cdots & \boldsymbol{U}_{1n}^{p} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{U}_{n0}^{p} & \boldsymbol{U}_{n1}^{p} & \cdots & \boldsymbol{U}_{nn}^{p} \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}_0^p \\ \boldsymbol{x}_1^p \\ \vdots \\ \boldsymbol{x}_n^p \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}_0^p \hat{\boldsymbol{\phi}}_0^p \\ \boldsymbol{H}_1^p \hat{\boldsymbol{\phi}}_1^p \\ \vdots \\ \boldsymbol{H}_n^p \hat{\boldsymbol{\phi}}_n^p \end{Bmatrix}$$

$$\begin{bmatrix} \boxed{\boldsymbol{V}_{00}^{p}} & \boxed{\boldsymbol{V}_{01}^{p}} & \cdots & \boldsymbol{V}_{0n}^{p} \\ \boldsymbol{V}_{10}^{p} & \boldsymbol{V}_{11}^{p} & \cdots & \boldsymbol{V}_{1n}^{p} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{V}_{n0}^{p} & \boldsymbol{V}_{n1}^{p} & \cdots & \boldsymbol{V}_{nn}^{p} \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}_0^p \\ \boldsymbol{x}_1^p \\ \vdots \\ \boldsymbol{x}_n^p \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}_0^p \hat{\boldsymbol{q}}_0^p \\ \boldsymbol{H}_1^p \hat{\boldsymbol{q}}_1^p \\ \vdots \\ \boldsymbol{H}_n^p \hat{\boldsymbol{q}}_n^p \end{Bmatrix}$$

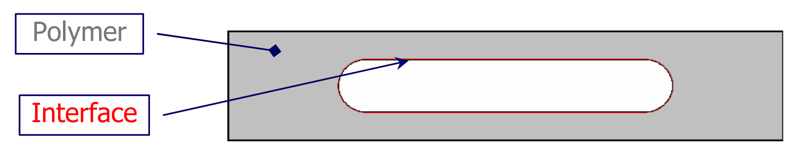
Simplified model (2)

- **Assembled equation for polymer domain**

$$\begin{bmatrix} \boldsymbol{U}_{00}^p & \boldsymbol{U}_{01}^p & \cdots & \boldsymbol{U}_{0n}^p \\ \boldsymbol{U}_{10}^p & \boldsymbol{U}_{11}^p & \cdots & \boldsymbol{U}_{1n}^p \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{U}_{n0}^p & \boldsymbol{U}_{n1}^p & \cdots & \boldsymbol{U}_{nn}^p \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}_0^p \\ \boldsymbol{x}_1^p \\ \vdots \\ \boldsymbol{x}_n^p \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}_0^p \hat{\boldsymbol{\phi}}_0^p \\ \boldsymbol{H}_1^p \hat{\boldsymbol{\phi}}_1^p \\ \vdots \\ \boldsymbol{H}_n^p \hat{\boldsymbol{\phi}}_n^p \end{Bmatrix}$$

$$\begin{bmatrix} \boldsymbol{V}_{00}^p & \boldsymbol{V}_{01}^p & \cdots & \boldsymbol{V}_{0n}^p \\ \boldsymbol{V}_{10}^p & \boldsymbol{V}_{11}^p & \cdots & \boldsymbol{V}_{1n}^p \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{V}_{n0}^p & \boldsymbol{V}_{n1}^p & \cdots & \boldsymbol{V}_{nn}^p \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}_0^p \\ \boldsymbol{x}_1^p \\ \vdots \\ \boldsymbol{x}_n^p \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}_0^p \hat{\boldsymbol{q}}_0^p \\ \boldsymbol{H}_1^p \hat{\boldsymbol{q}}_1^p \\ \vdots \\ \boldsymbol{H}_n^p \hat{\boldsymbol{q}}_n^p \end{Bmatrix}$$

$$\Rightarrow \begin{bmatrix} \boldsymbol{A}_{00} & \boldsymbol{A}_{01} & \cdots & \boldsymbol{A}_{0n} \\ \boldsymbol{U}_{10} & \boldsymbol{U}_{11} & \cdots & \boldsymbol{U}_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{U}_{n0} & \boldsymbol{U}_{n1} & \cdots & \boldsymbol{U}_{nn} \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}_0 \\ \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_n \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}_0 \boldsymbol{d}_0 \\ \boldsymbol{H}_1 \hat{\boldsymbol{\phi}}_1 \\ \vdots \\ \boldsymbol{H}_n \hat{\boldsymbol{\phi}}_n \end{Bmatrix}$$



- **Constant temperature at interfaces**

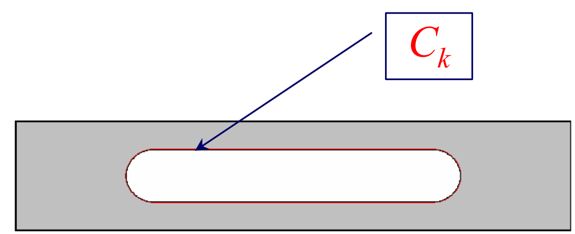
$$\{\phi_k\} = \{\mathbf{1}\}_k \, \phi_c^k$$

Simplified model (3)

- **Equation with constraint**

$$
\begin{bmatrix}
\boldsymbol{A}_{00} & \boldsymbol{A}_{01} & \cdots & \boldsymbol{A}_{0n} & \mathbf{0} & \cdots & \mathbf{0} \\
\boldsymbol{U}_{10} & \boldsymbol{U}_{11} & \cdots & \boldsymbol{U}_{1n} & \boldsymbol{H}_1\{\mathbf{1}\}_1 & \cdots & \mathbf{0} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\boldsymbol{U}_{n0} & \boldsymbol{U}_{n1} & \cdots & \boldsymbol{U}_{nn} & \mathbf{0} & \cdots & \boldsymbol{H}_n\{\mathbf{1}\}_n
\end{bmatrix}
\begin{Bmatrix} \boldsymbol{x}_0 \\ \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_n \\ \phi_c^1 \\ \vdots \\ \phi_c^n \end{Bmatrix}
=
\begin{Bmatrix} \boldsymbol{H}_0\boldsymbol{d}_0 \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{Bmatrix}
$$

- **Additional equations**



$$\int_{C_k} q\, d\Gamma = 0$$

$$q = \sum_{I=1}^{N} \frac{\partial \phi_I^s}{\partial n} x_I$$

$$\sum_{I=1}^{N} \int_{C_k} \frac{\partial \phi_I^s}{\partial n} d\Gamma x_I = 0$$

$$\int_{C_k} \frac{\partial \phi_I^s}{\partial n} d\Gamma = \begin{cases} 1, & \forall \mathbf{s}_I \in C_k \\ 0, & \forall \mathbf{s}_I \notin C_k \end{cases}$$

$$\{\mathbf{1}\}^{\mathrm{T}} \{\boldsymbol{x}_k\} = 0$$

Simplified model (4)

- **Final system of equations**

$$
\begin{bmatrix}
\boldsymbol{A}_{00}^0 & \boldsymbol{A}_{01}^0 & \cdots & \boldsymbol{A}_{0n}^0 & \mathbf{0} & \cdots & \mathbf{0} \\
\boldsymbol{U}_{10}^0 & \boldsymbol{U}_{11}^0 & \cdots & \boldsymbol{U}_{1n}^0 & \boldsymbol{H}_1\{\mathbf{1}\}_1 & \cdots & \mathbf{0} \\
\mathbf{0} & \{\mathbf{1}\}_1^{\mathrm{T}} & \cdots & \mathbf{0} & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\boldsymbol{U}_{n0}^0 & \boldsymbol{U}_{n1}^0 & \cdots & \boldsymbol{U}_{nn}^0 & \mathbf{0} & \cdots & \boldsymbol{H}_n\{\mathbf{1}\}_n \\
\mathbf{0} & \mathbf{0} & \cdots & \{\mathbf{1}\}_n^{\mathrm{T}} & 0 & \cdots & 0
\end{bmatrix}
\begin{Bmatrix} \boldsymbol{x}_0 \\ \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_n \\ \phi_c^1 \\ \vdots \\ \phi_c^n \end{Bmatrix}
=
\begin{Bmatrix} \boldsymbol{H}_0\boldsymbol{d}_0 \\ \mathbf{0} \\ 0 \\ \vdots \\ \mathbf{0} \\ 0 \end{Bmatrix}
$$

Complexity of an iterative solver:
Memory: *O*(N^2)
CPU time: *O*(N^2)

Remarks: The product of a row of the matrix and a guess vector can be expressed by one of the following four sums:

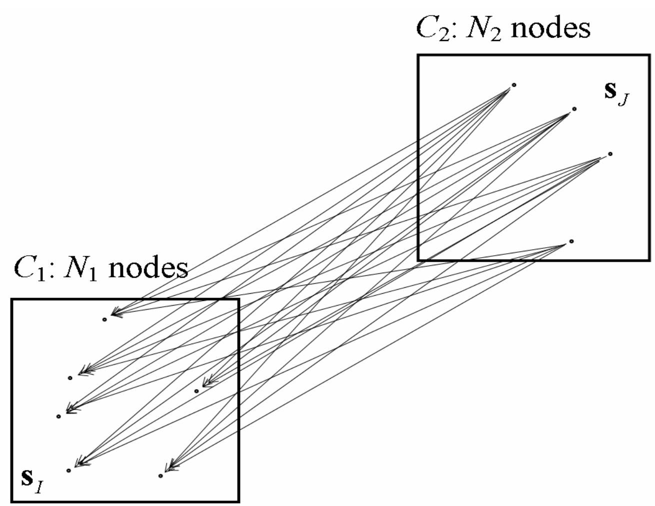
$$\sum_{J=1}^{N} \int_{\Gamma_I} \phi_J^s v_I(Q) x_J \, d\Gamma \qquad \sum_{J=1}^{N} \int_{\Gamma_I} \phi_J^s v_I(Q) x_J \, d\Gamma + \phi_c^k \sum_{J}^{m_k} H_{IJ}$$

$$\sum_{J=1}^{N} \int_{\Gamma_I} -\kappa \frac{\partial \phi_J^s}{\partial n} v_I(Q) x_J \, d\Gamma \qquad \sum_{J}^{m_k} x_J^k$$

Fast multipole

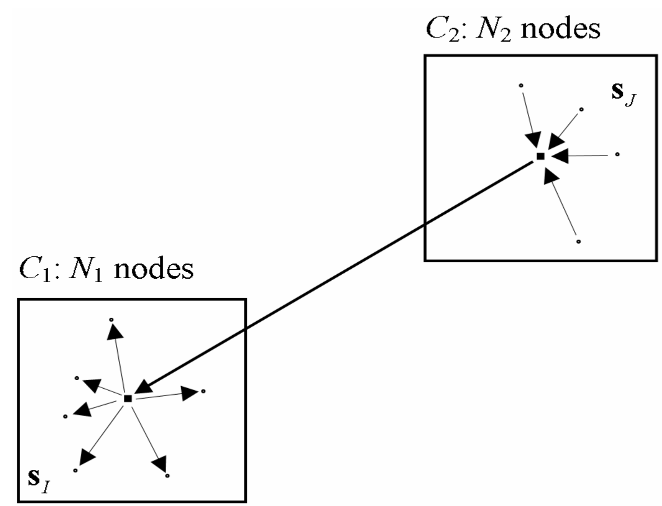
- **Ideas of FMM**

Node-node interactions



Complexity $O(N_1 N_2)$

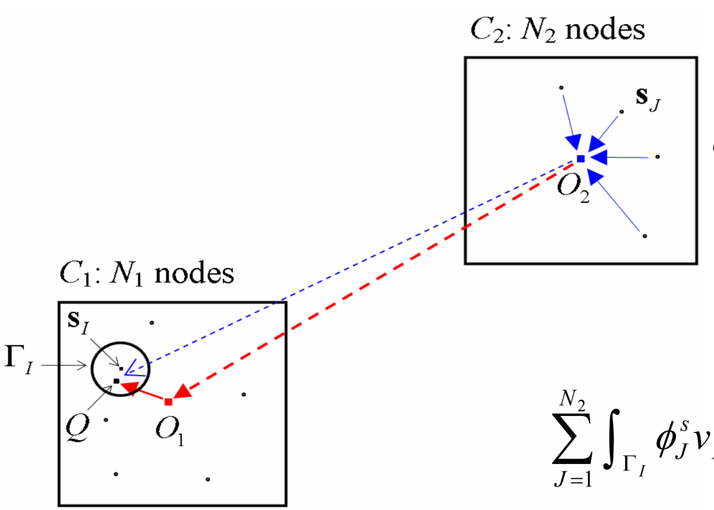
Cell-cell interactions



Complexity $O(N_1 + N_2)$

Fast multipole (2)

➢ **Multipole expansion**



$$\phi_J^s = \frac{1}{4\pi\kappa}\frac{1}{r(Q,\mathbf{s}_J)} = \frac{1}{4\pi\kappa}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\overline{S_{n,m}}(\overrightarrow{O_2Q})\,\boxed{R_{n,m}(\overrightarrow{O_2\mathbf{s}_J})}$$

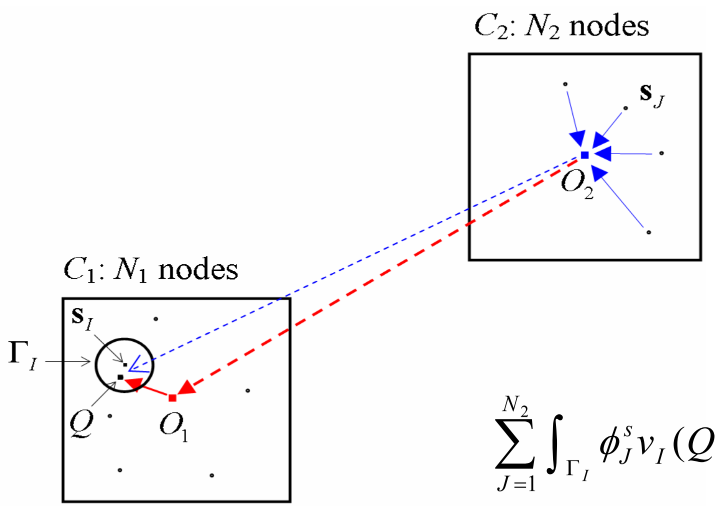
for $\quad |\overrightarrow{O_2Q}| > |\overrightarrow{O_2\mathbf{s}_J}|$

$$\sum_{J=1}^{N_2}\int_{\Gamma_I}\phi_J^s v_I(Q)x'_J\,d\Gamma = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\int_{\Gamma_I}\frac{1}{4\pi\kappa}\overline{S_{n,m}}(\overrightarrow{O_2Q})v_I(Q)\,d\Gamma\,\boxed{M_{n,m}(O_2)}$$

where $\quad \boxed{M_{n,m}(O_2) = \sum_{J=1}^{N_2} R_{n,m}(\overrightarrow{O_2\mathbf{s}_J})x'_J}$

Fast multipole (3)

- **Local expansion**



$$\boxed{\overline{S_{n,m}}(\overrightarrow{O_2Q})} = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} (-1)^{n'} \boxed{R_{n',m'}(\overrightarrow{O_1Q})}\, \boxed{\overline{S_{n+n',m+m'}}(\overrightarrow{O_1O_2})}$$

$$\text{for} \quad \left|\overrightarrow{O_1O_2}\right| > 2\left|\overrightarrow{O_1Q}\right|$$

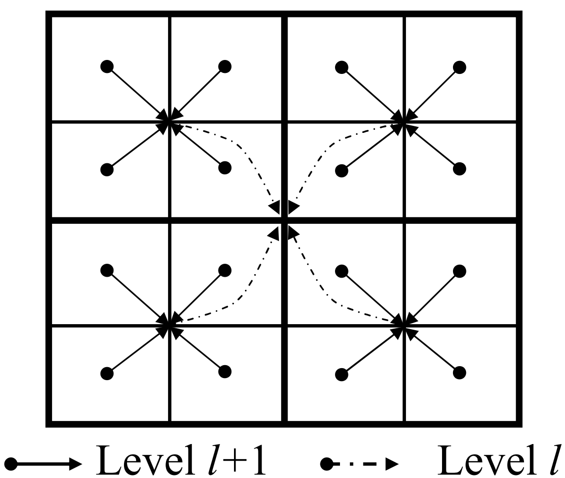
$$\sum_{J=1}^{N_2} \int_{\Gamma_I} \phi_J^s v_I(Q) x'_J \, d\Gamma = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \boxed{\int_{\Gamma_I} \frac{1}{4\pi\kappa} R_{n',m'}(\overrightarrow{O_1Q}) v_I(Q)\, d\Gamma}\, \boxed{L_{n',m'}(O_1)}$$

where
$$\boxed{L_{n',m'}(O_1) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (-1)^{n'} \overline{S_{n+n',m+m'}}(\overrightarrow{O_1O_2}) M_{n,m}(Q_2)}$$

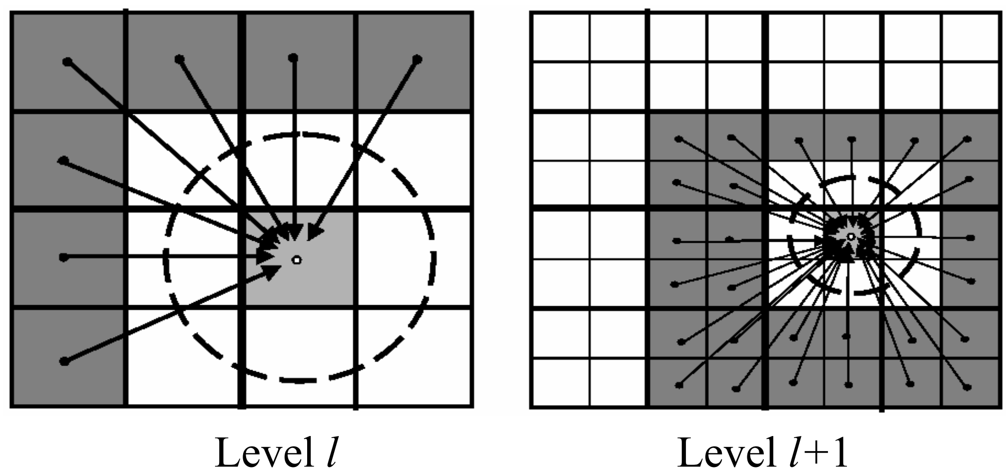
Fast multipole (4)

➢ **Recursive algorithm**

Upward pass



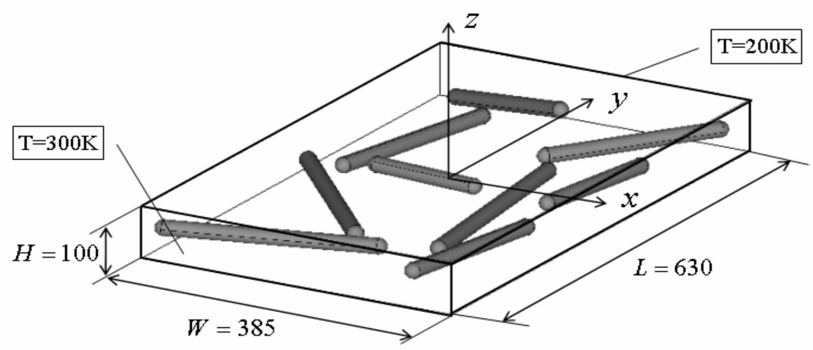
Downward pass



Multipole moments are accumulated from leaves to the root (***Upward pass***); and local moments are distributed from the root to the leaves (***Downward pass***). This is accomplished at a linear complexity.

Advanced simulations

➢ **RVE containing a number of CNTs**



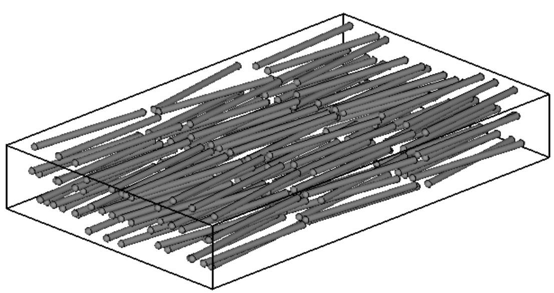
Dimensions (nm) *and Boundary condition of RVE*

Heat conductivity used for polymer: 0.37 W/m·K

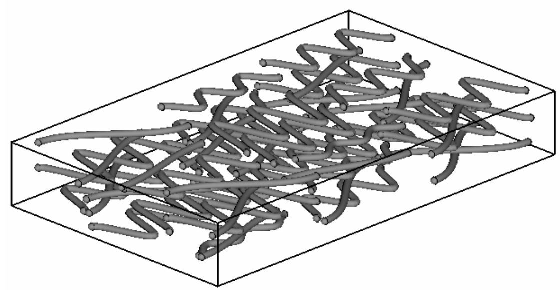
$$\boxed{\kappa = -\frac{qL}{\Delta T}}$$

Equivalent heat conductivity

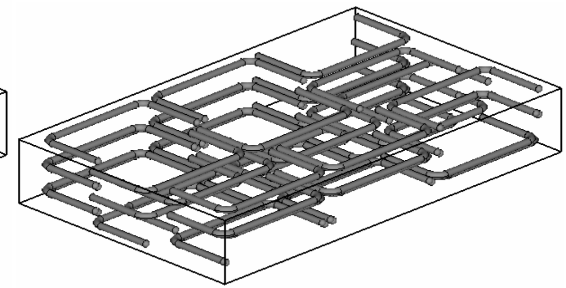
Advanced simulations (2)



(a) "Randomly" oriented CNTs



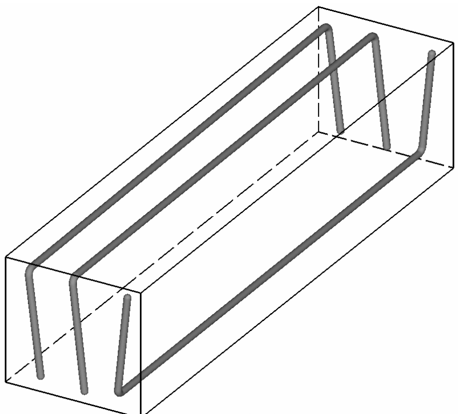
(b)"Randomly" located CNTs

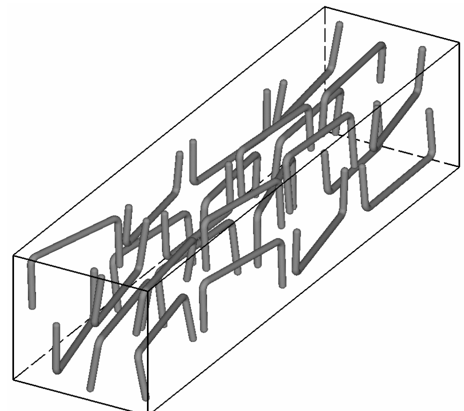


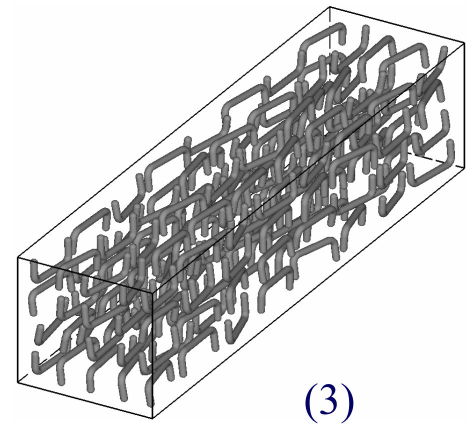
(c) Forty-five CNTs of "C" shape

RVE	(a)	(b)	(c)
Conductivity(κ)	3.470	1.717	6.319
Percentage(r)	8.4%	4.8%	5.5%
κ/r	41.41	36.00	114.5

Advanced simulations (3)

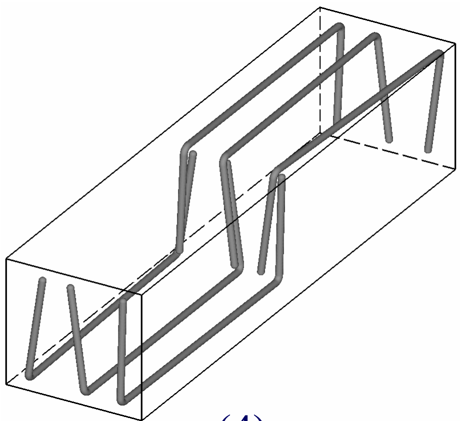

(1)


(2)


(3)

No.	*AVR Len*	*CNT Num*	*Fraction, v*	*k*	*k/v*
(1)	1117	3	0.59%	8.472	1436
(2)	312.3	24	1.09%	1.432	131.4
(3)	139.8	160	3.78%	1.356	35.87

Advanced simulations (4)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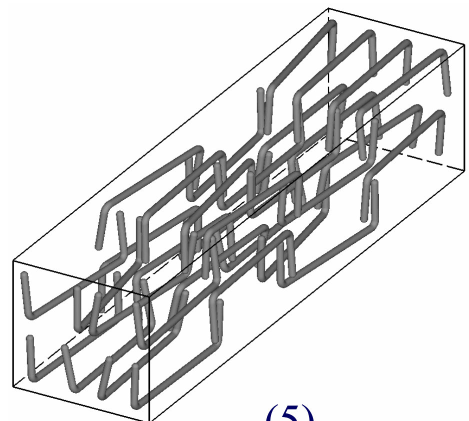
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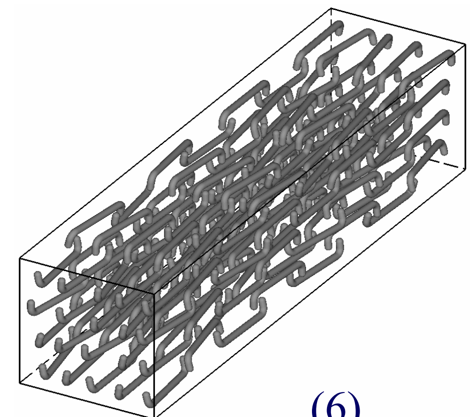
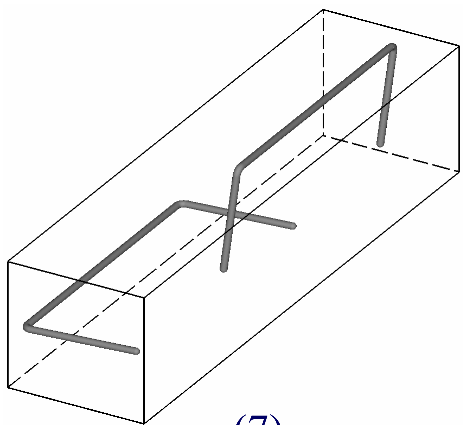
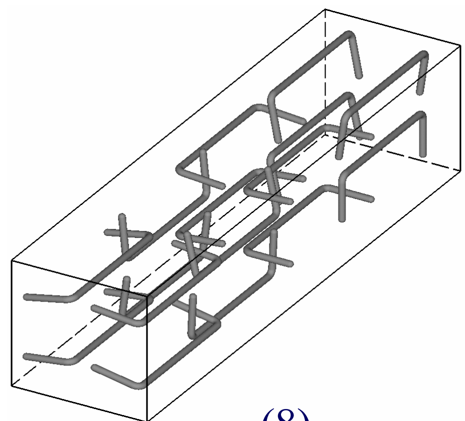

(6)

No.	AVR Len	CNT Num	Fraction, v	k	k/v
(4)	728.9	6	0.61%	5.010	821.4
(5)	342.7	32	1.77%	3.937	222.4
(6)	160	149.5	5.07%	2.833	55.87

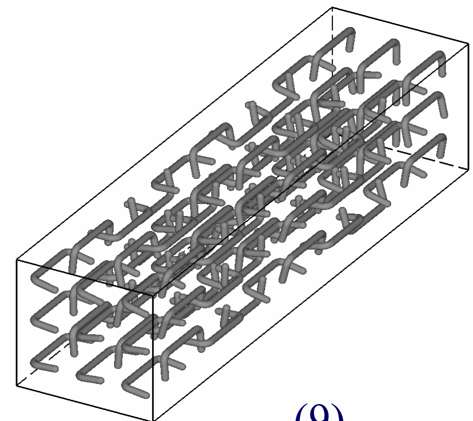
Advanced simulations (5)



(7)



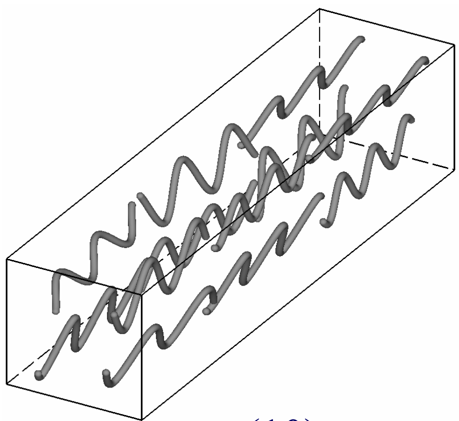
(8)



(9)

No.	*AVR Len*	*CNT Num*	*Fraction, v*	*k*	*k/v*
(7)	728.9	2	0.28%	1.773	633.1
(8)	342.7	16	1.11%	2.086	187.9
(9)	162.9	90	2.97%	1.745	58.75

Advanced simulations (6)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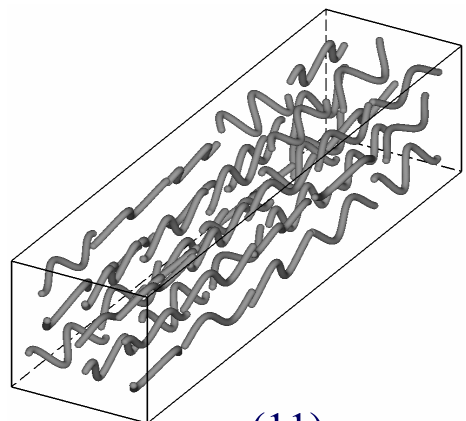
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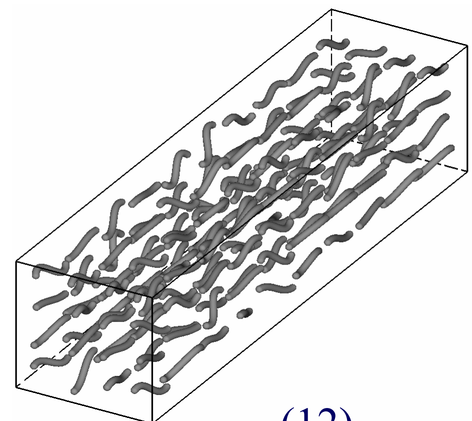
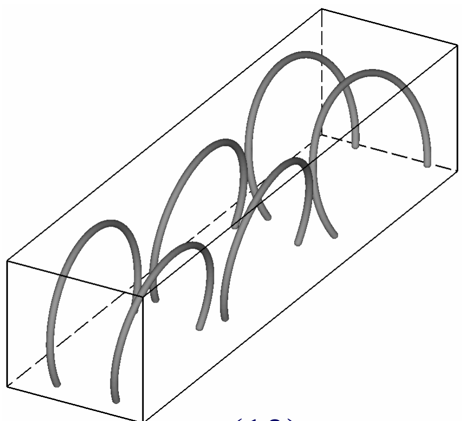
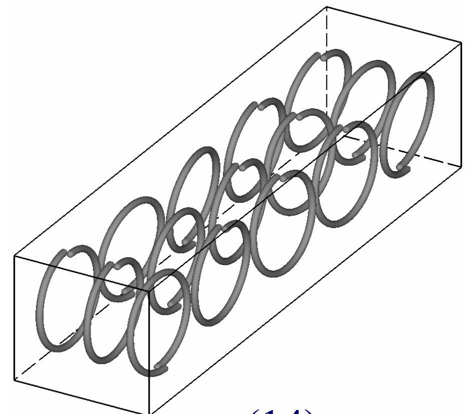

(12)

No.	*AVR Len*	*CNT Num*	*Fraction, v*	*k*	*k/v*
(10)	437.7	12	1.29%	1.186	91.91
(11)	205.1	45	2.23%	1.097	49.18
(12)	80.2	160	3.06%	0.760	24.83

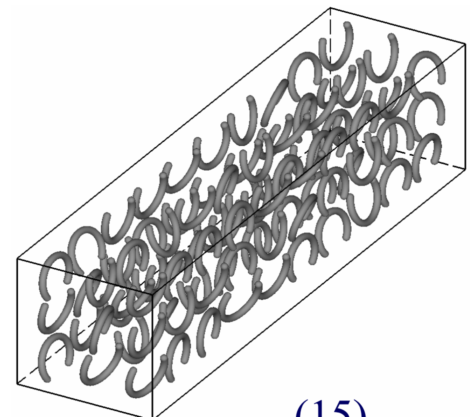
Advanced simulations (7)



(13)



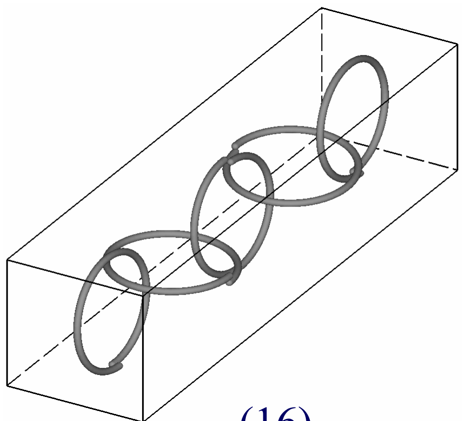
(14)



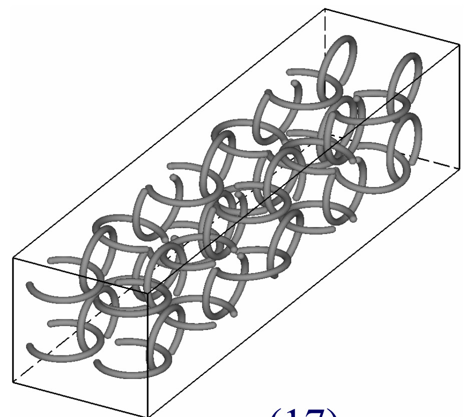
(15)

No.	*AVR Len*	*CNT Num*	*Fraction, v*	*k*	*k/v*
(13)	516.6	6	0.755%	1.551	205.5
(14)	462.5	15	1.69%	1.184	70.06
(15)	149.1	90	3.17%	0.917	28.92

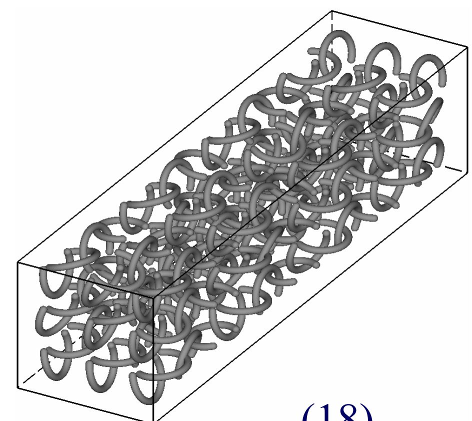
Advanced simulations (8)



(16)



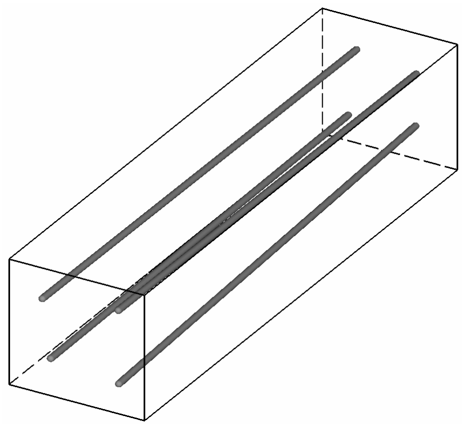
(17)



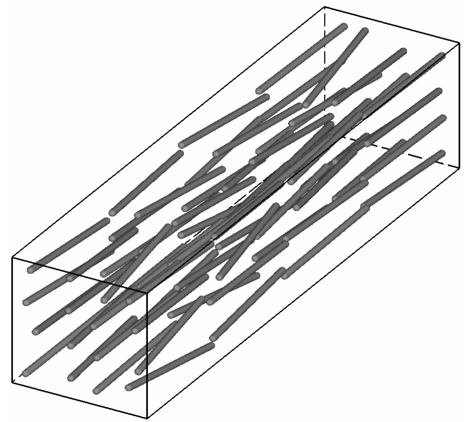
(18)

No.	*AVR Len*	*CNT Num*	*Fraction, v*	*k*	*k/v*
(16)	537.9	5	0.656%	0.796	121.3
(17)	239.2	40	2.31%	1.094	47.34
(18)	149.6	135	4.84%	1.709	35.31

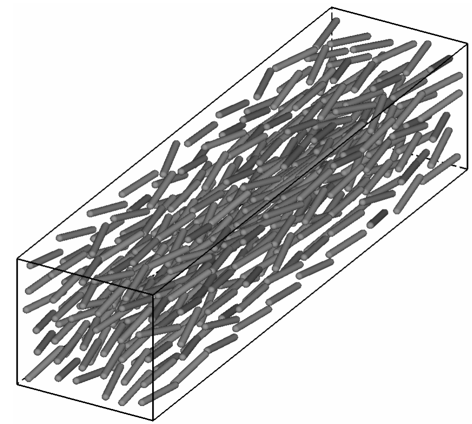
Advanced simulations (9)



(19)



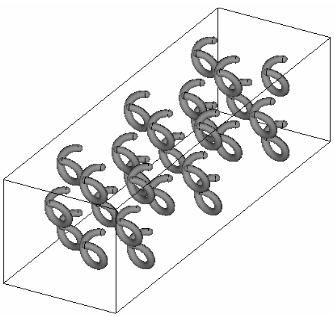
(20)



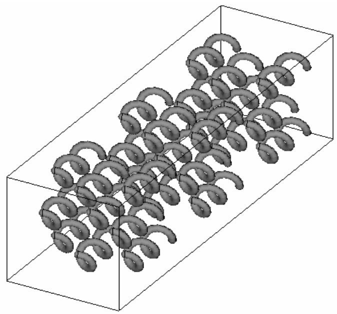
(21)

No.	*AVR Len*	*CNT Num*	*Fraction, v*	*k*	*k/v*
(19)	790.0	4	0.77%	2.990	387.4
(20)	194.7	64	2.99%	1.790	59.85
(21)	77.0	360	4.84%	1.204	19.02

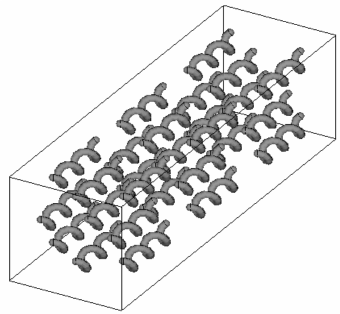
Sensitive studies



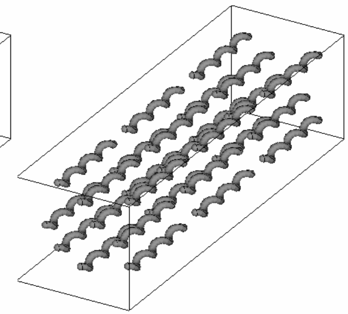
$\kappa = 0.4362$



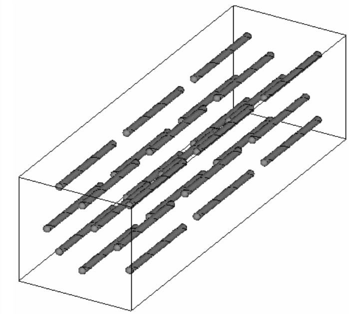
$\kappa = 0.6975$



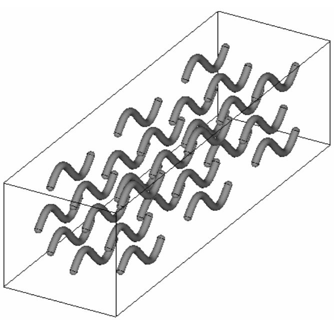
$\kappa = 0.8703$



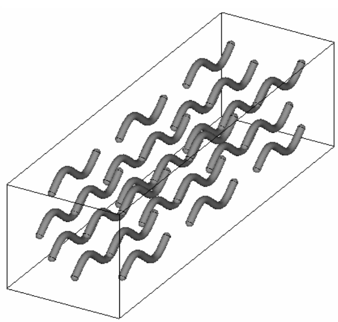
$\kappa = 0.9445$



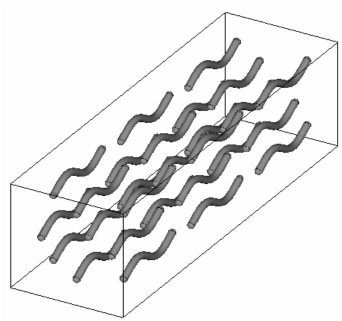
$\kappa = 0.9482$



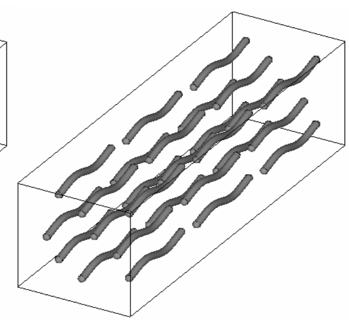
$\kappa = 0.6679$



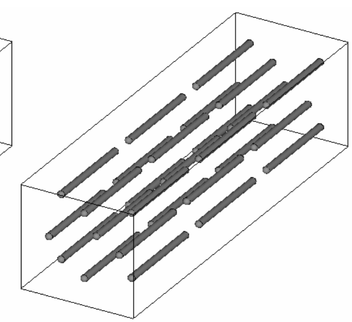
$\kappa = 0.7431$



$\kappa = 0.8257$

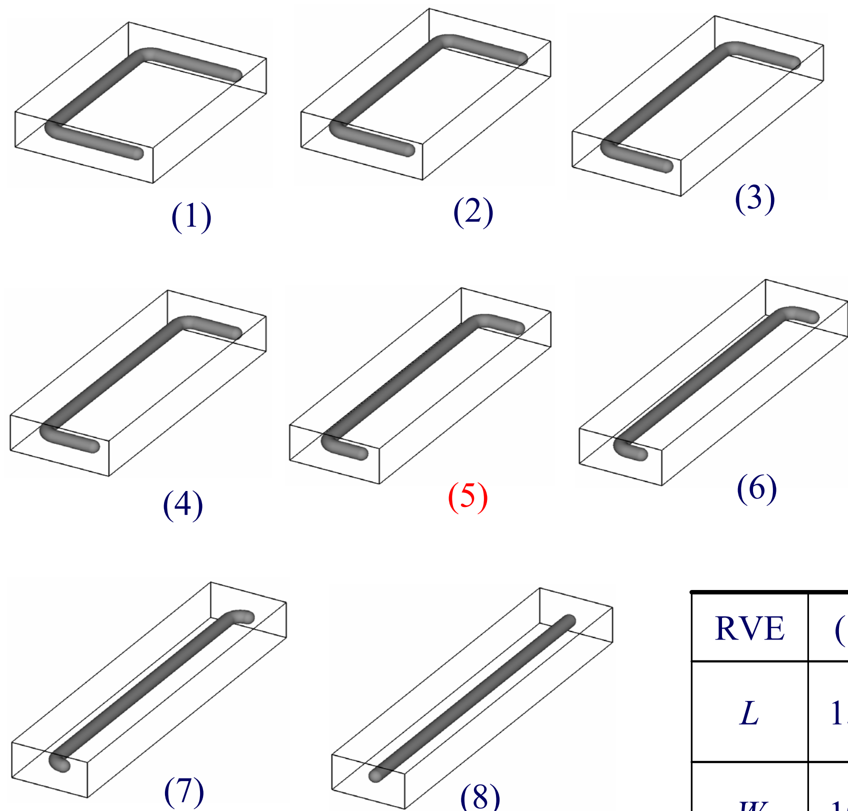


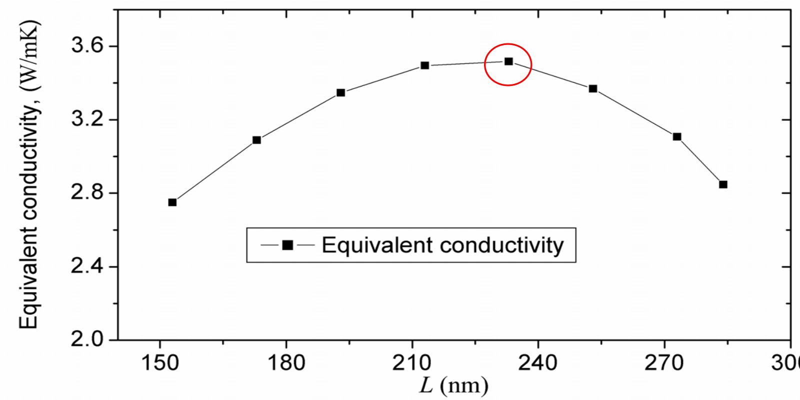
$\kappa = 0.9381$



$\kappa = 0.9482$

Optimization by case study





RVE	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
L	153	173	193	213	233	253	273	284
W	107	94.6	84.8	76.8	70.2	64.7	59.9	57.5

Conclusions

- The Fast multipole HdBNM is demonstrated to be very promising for large-scale analysis of CNT composites, especially concerning the complex geometries of the CNTs.
- The length, shape, orientation and curvature of the CNTs are found to have strong influence on the overall property of the composites.
- The length of CNT is of most crucial importance to enhance the thermal property of CNT-based composites.
- For a specific length, the “C” shape is the best shape for enhancing the composites. The optimal dimensions of the “C” shape CNT is obtained by case studies.