SHAPE OPTIMIZATION OF CNT FOR ENHANCING THERMAL CONDUCTANCE OF CNT-BASED COMPOSITES

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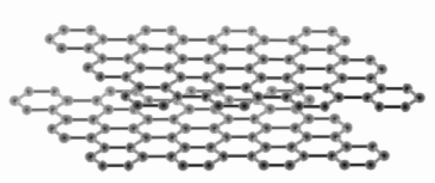
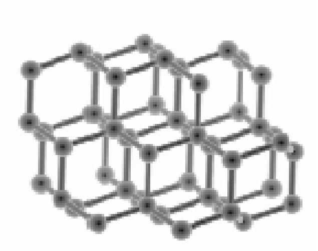
Background

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



Graphite
50~100



Diamond
3320

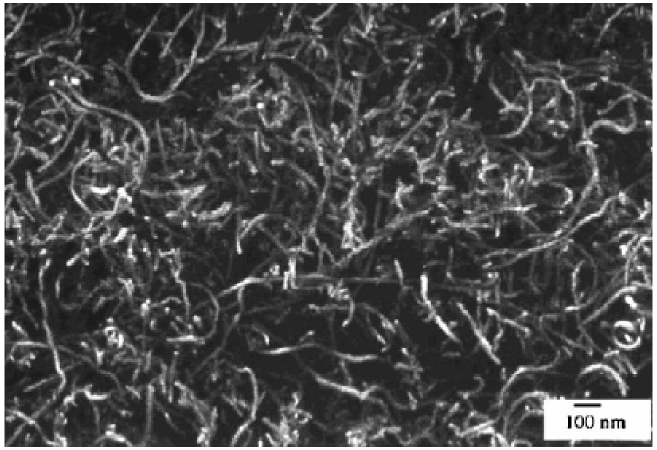
Nanotube
3000~6000

Resins: 0~1 W/m·K

Metals:
Fe 72 W/m·K
Cu 390 W/m·K

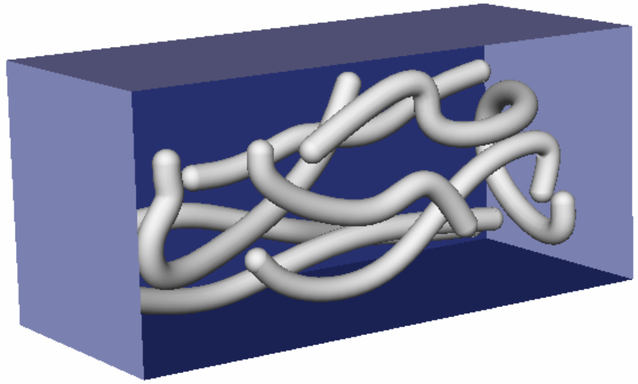
Background (2)

- 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)

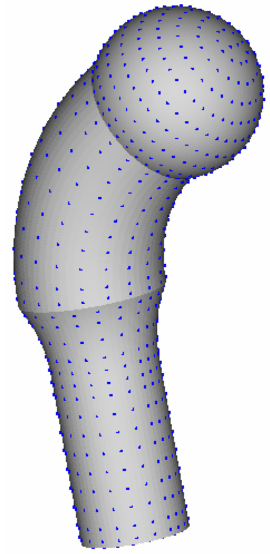
- To overcome the second difficulty

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

- Domain variables

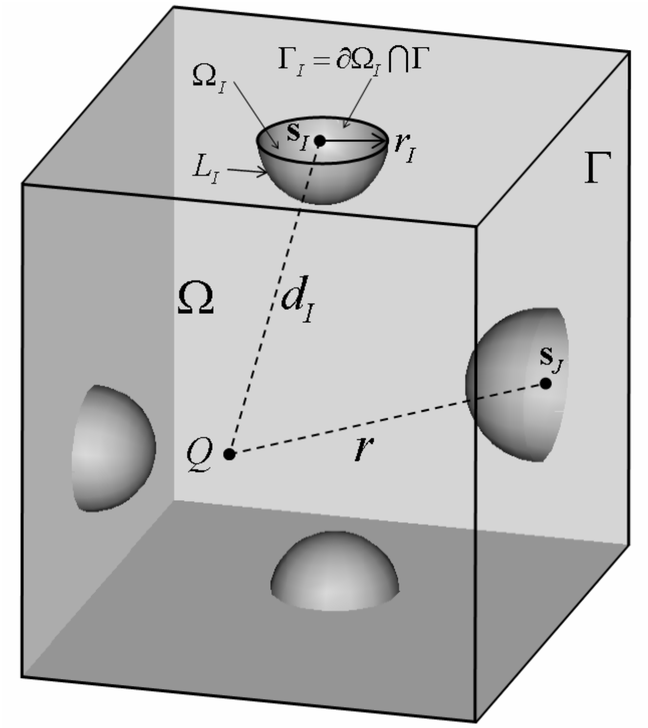
$$\phi = \sum_{I=1}^{N} \phi_I^s x_I \qquad \phi_I^s = \frac{1}{\kappa} \frac{1}{4\pi r(Q, \mathbf{s}_I)}$$

- 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



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

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

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

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

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

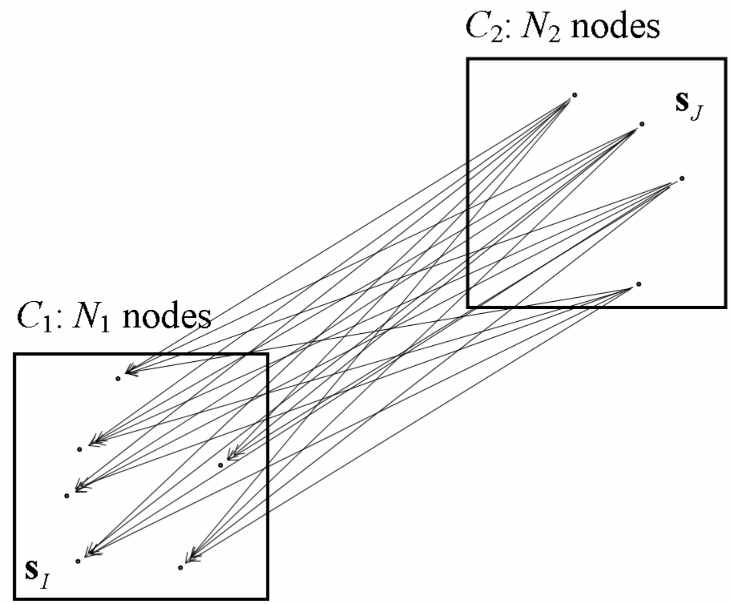
Three purposes of elements in BEM:

- ➢ **To interpolate Boundary variables;**
- ➢ **To facilitate boundary integration;**
- ➢ **To approximate the geometry.**

Fast multipole

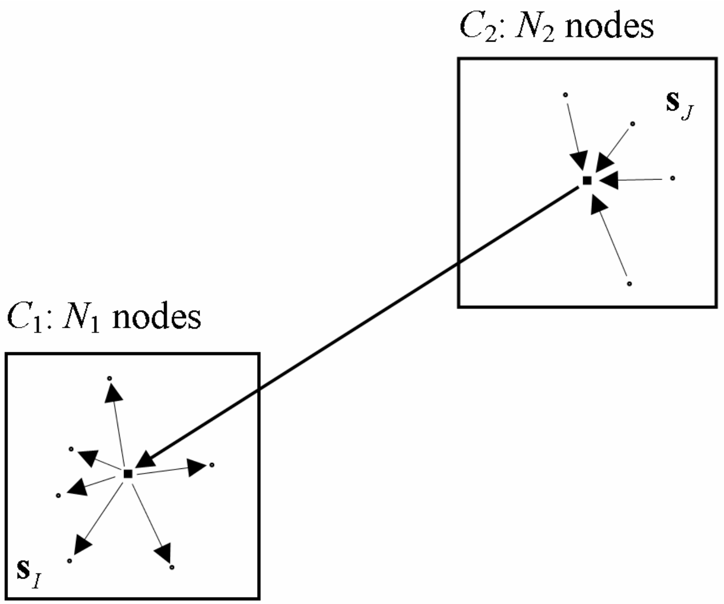
- **Ideas of FMM**

Node-node interactions



Complexity $O(N_1 N_2)$

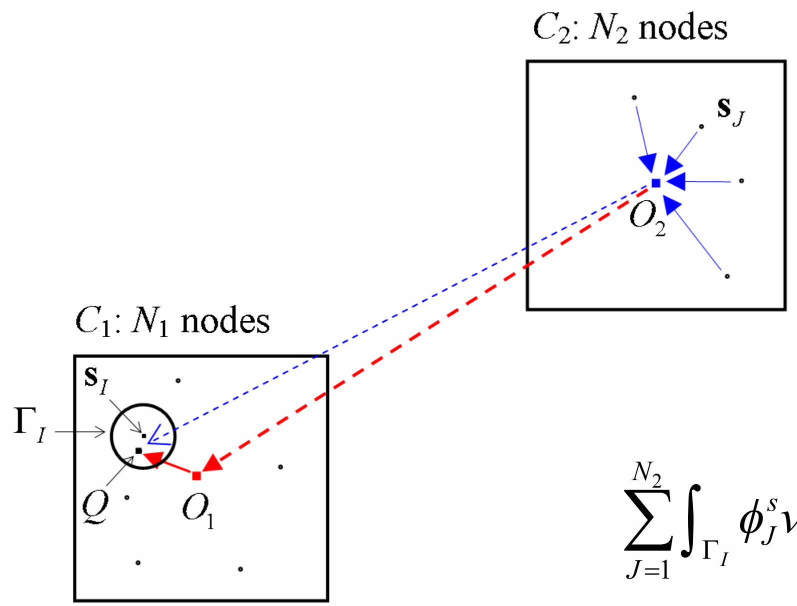
Cell-cell interactions



Complexity $O(N_1+N_2)$

Fast multipole (2)

- **Multipole expansion**



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

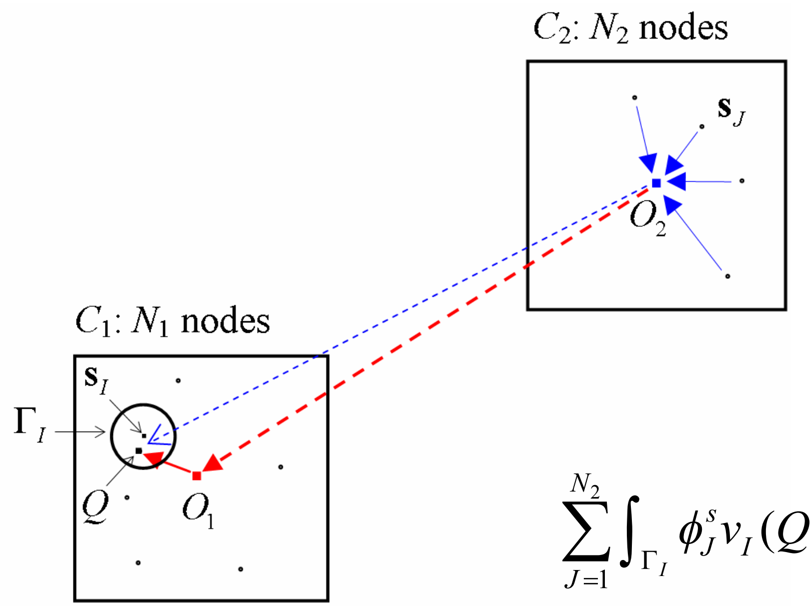
for $\left|\overrightarrow{O_2Q}\right| > \left|\overrightarrow{O_2\mathbf{s}_J}\right|$

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

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

Fast multipole (3)

- **Local expansion**



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

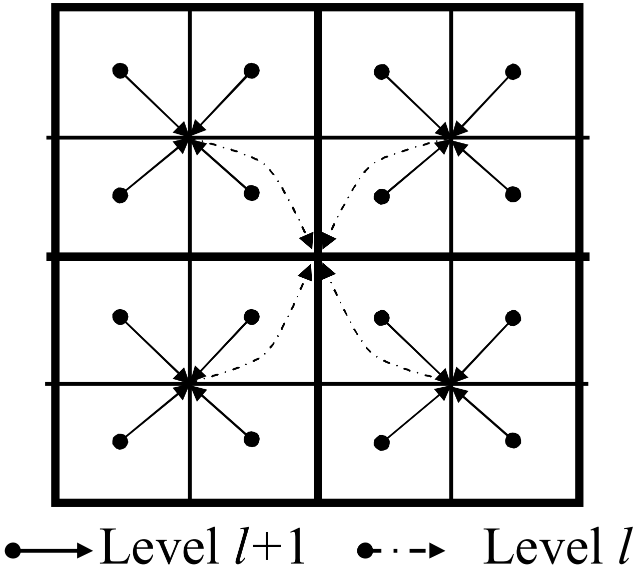
for $\left|\overrightarrow{O_1O_2}\right| > 2\left|\overrightarrow{O_1Q}\right|$

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

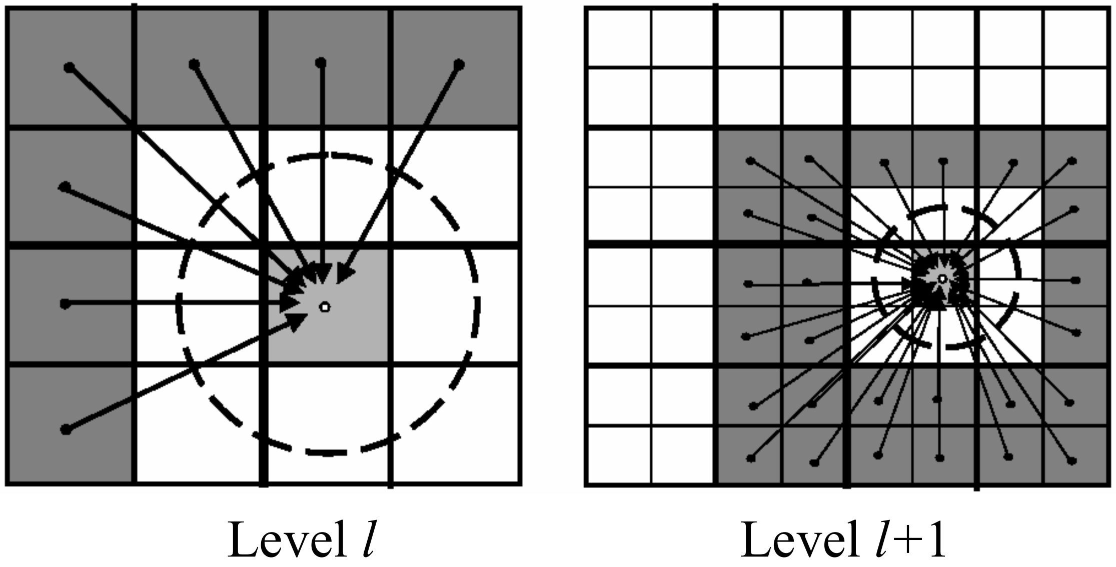
where $\boxed{L_{n',m'}(O_1) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}(-1)^{n'}\overline{S_{n+n',m+m'}}(\overrightarrow{O_1O_2})M_{n,m}(Q_2)}$

Fast multipole (4)

- **Recursive algorithm**



Upward pass

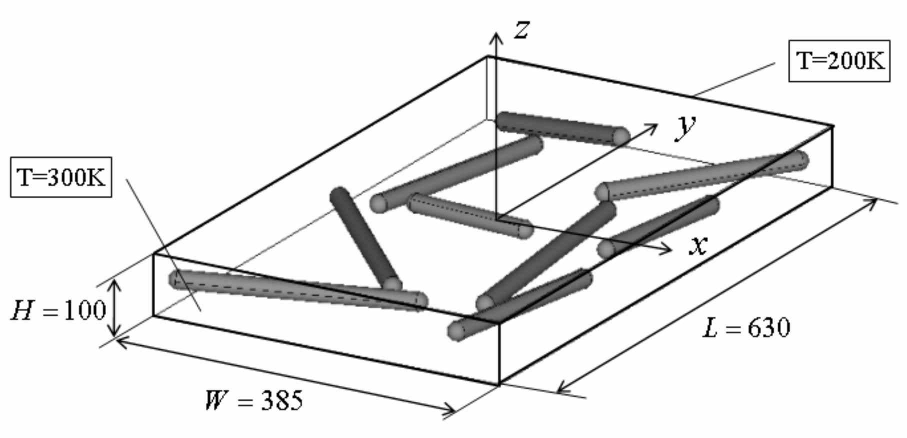


Downward pass

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**



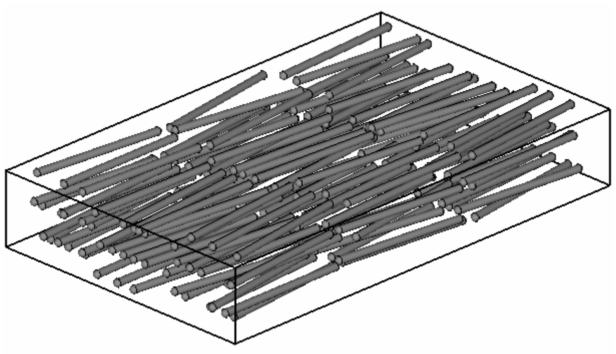
Dimensions (nm) *and Boundary condition of RVE*

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

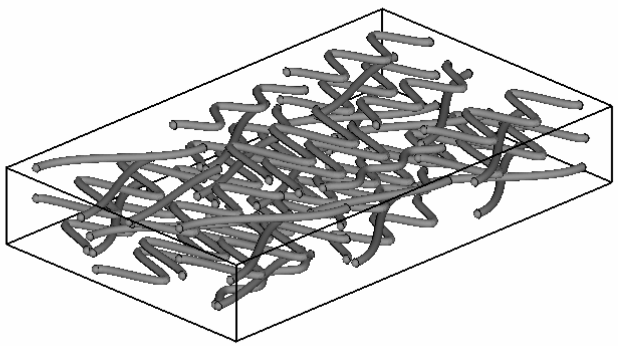
$$\boxed{\kappa = -\frac{qL}{\Delta T}}$$

Equivalent heat conductivity

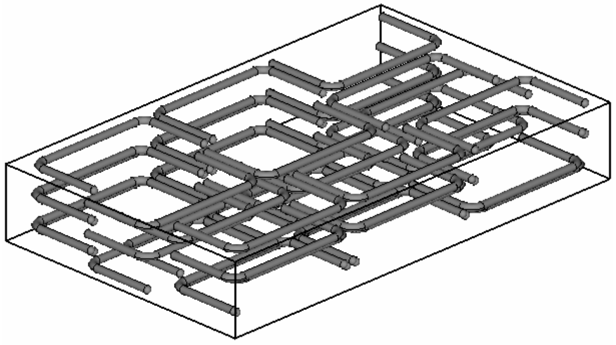
Advanced simulations (2)



(a) “Randomly” oriented CNTs



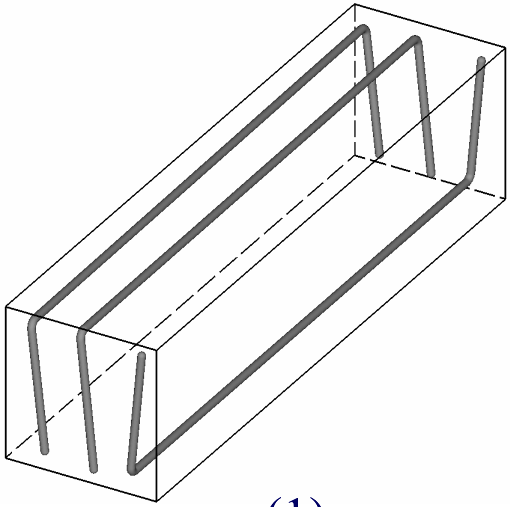
(b)“Randomly” located CNTs



(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)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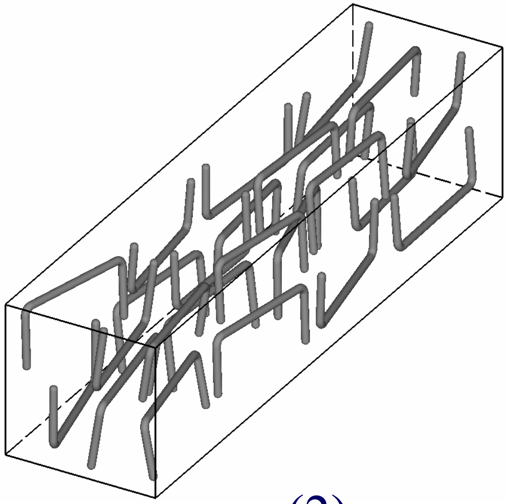
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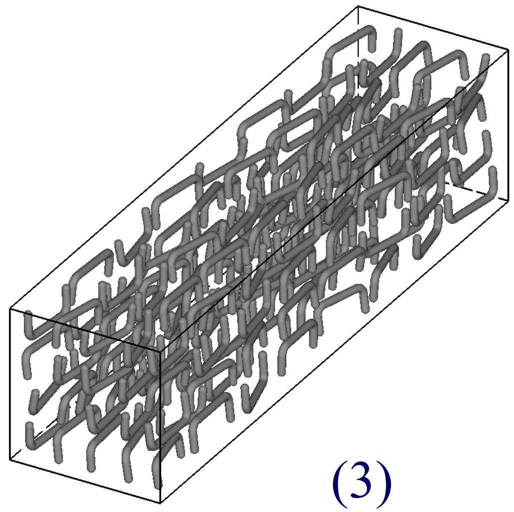
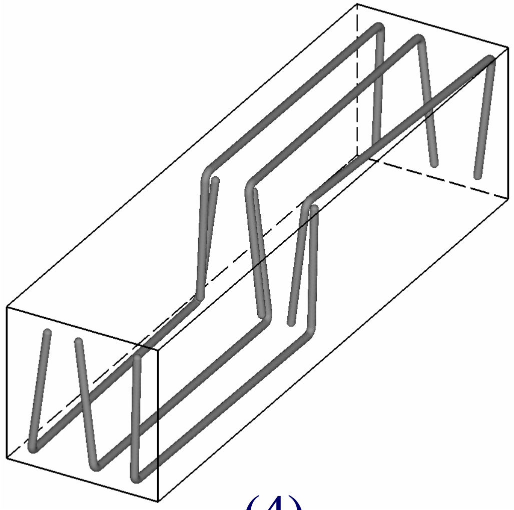

(3)

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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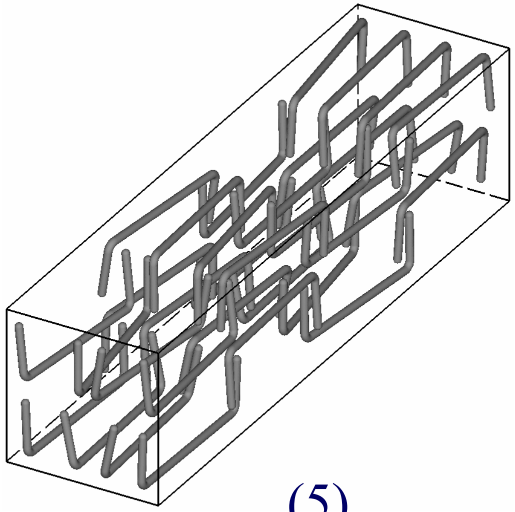
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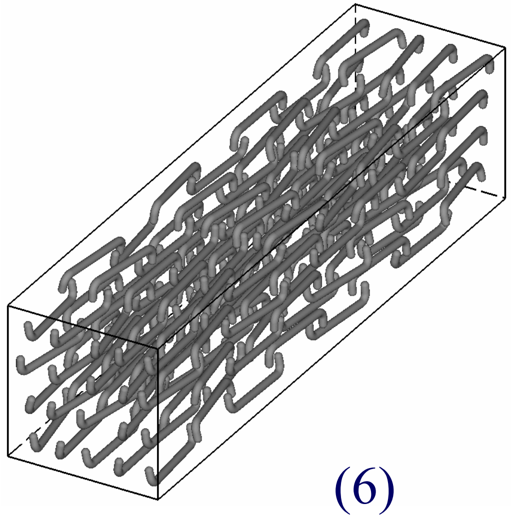
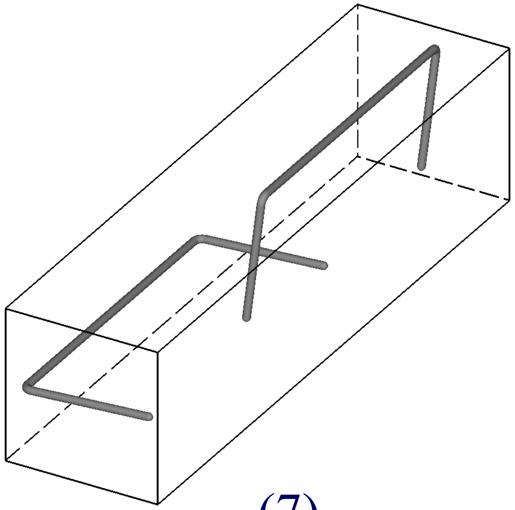

(6)

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)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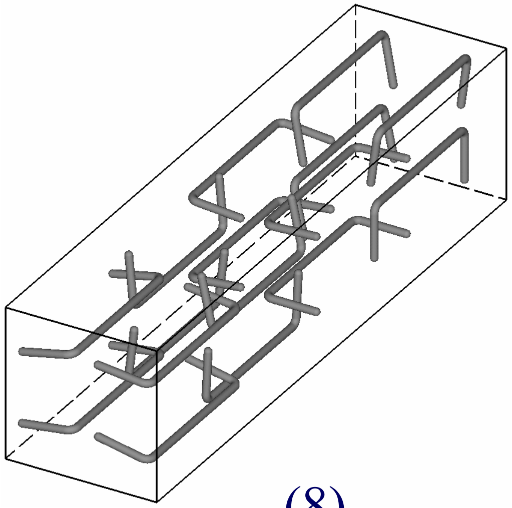
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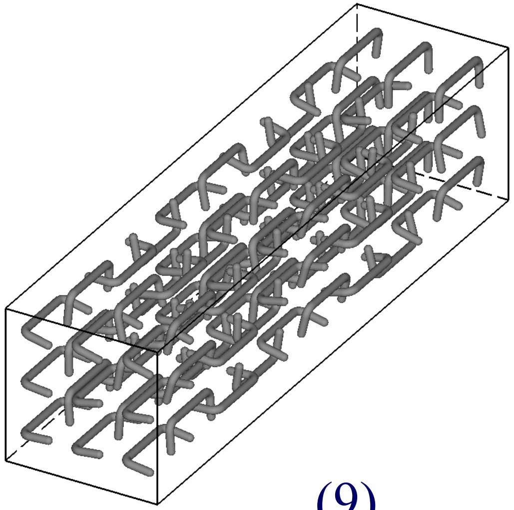
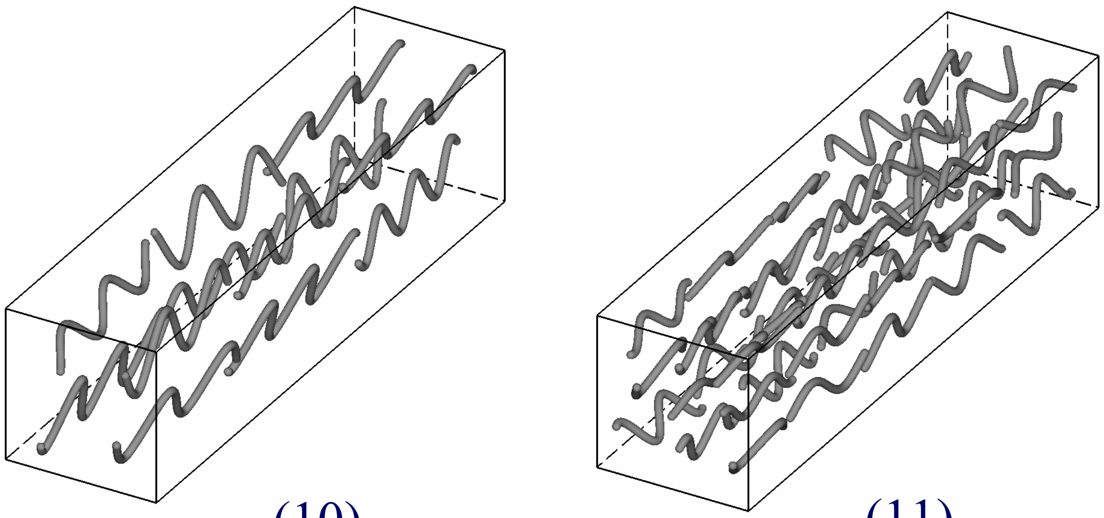
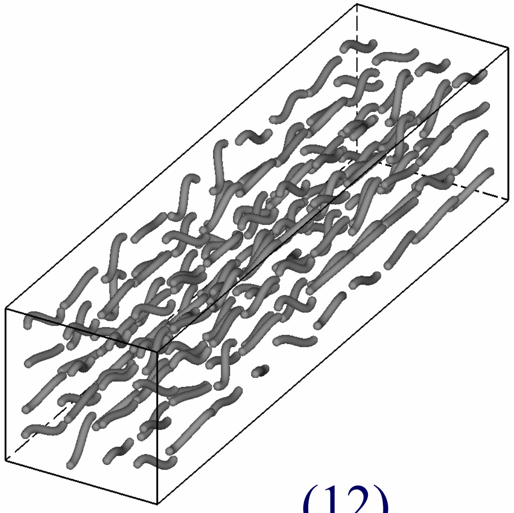

(9)

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

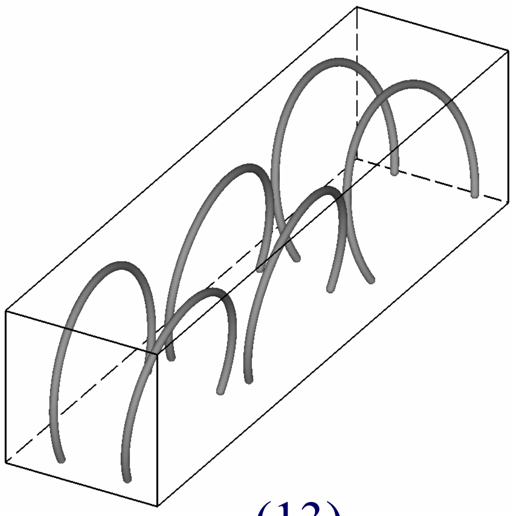
Advanced simulations (6)


(10) (11)


(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)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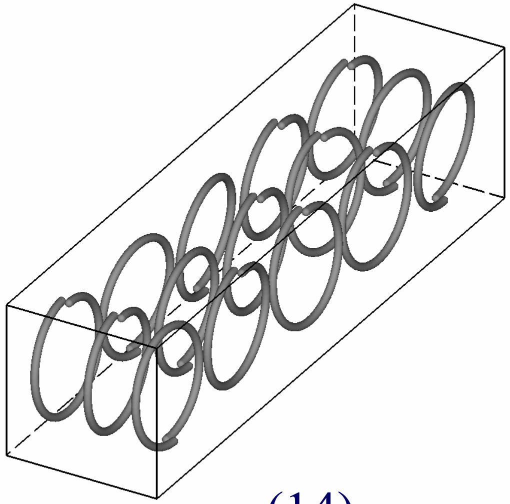
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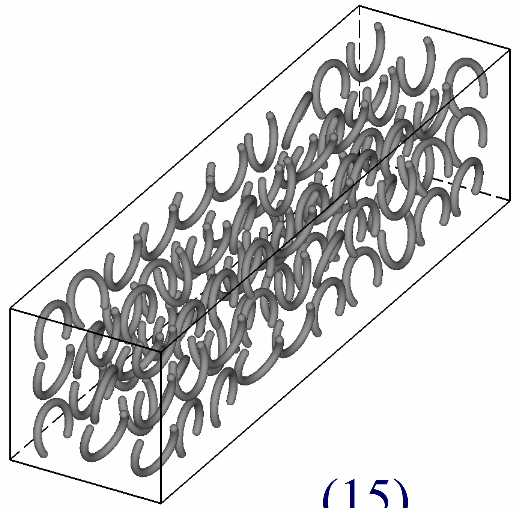
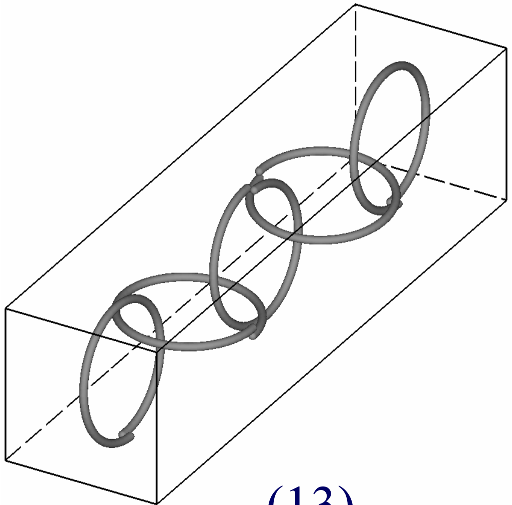

(15)

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)



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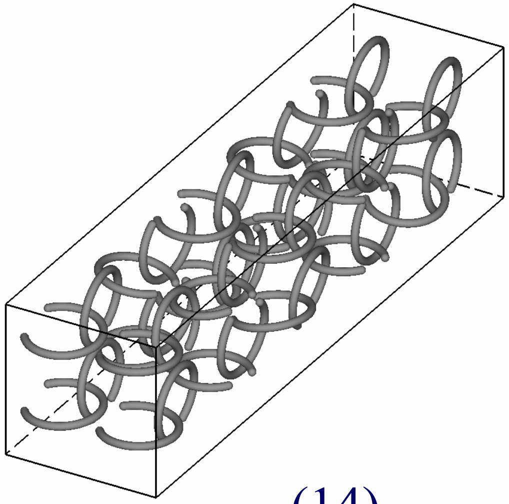

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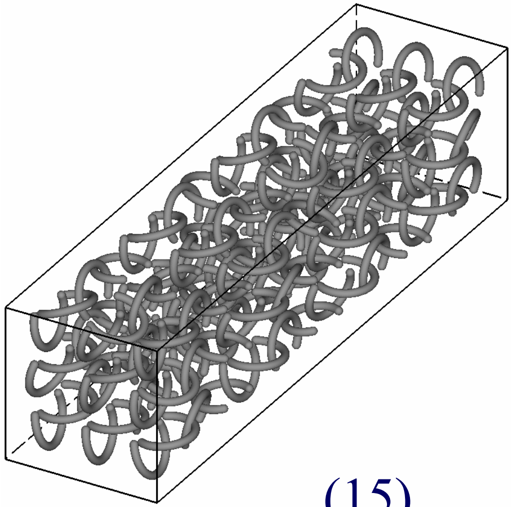
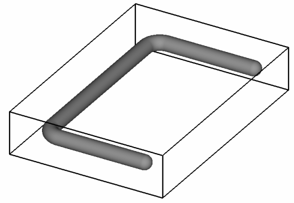


(15)

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

Optimization by case study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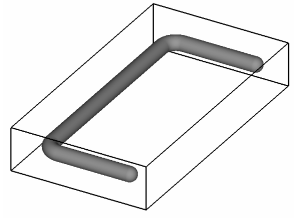
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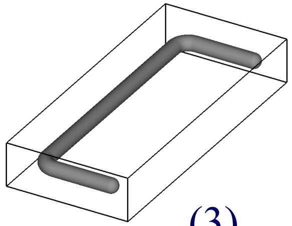
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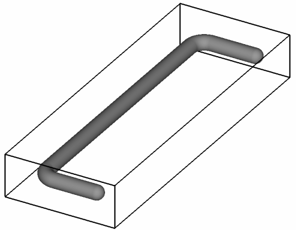
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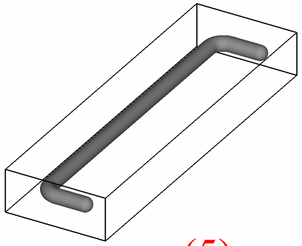
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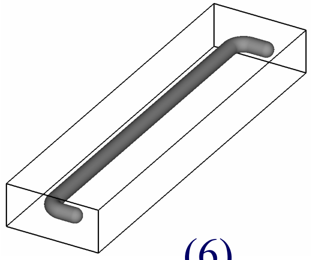
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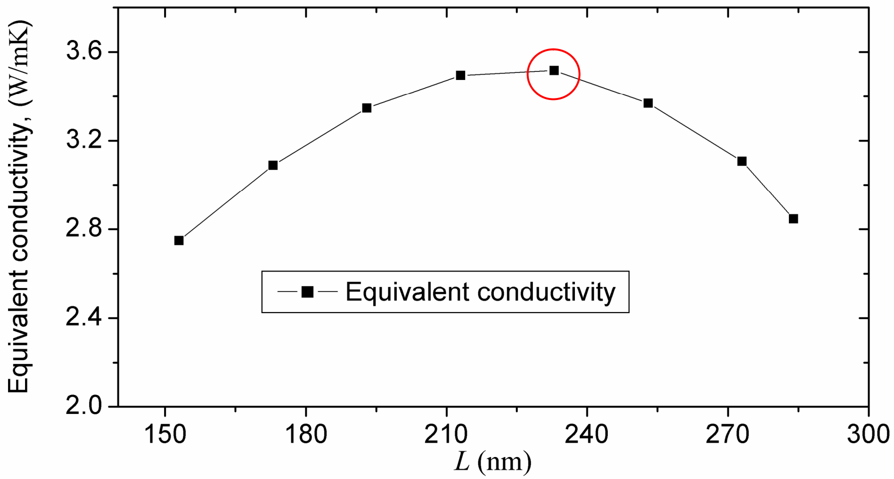

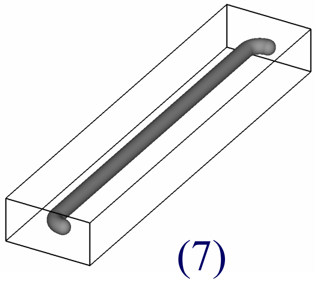
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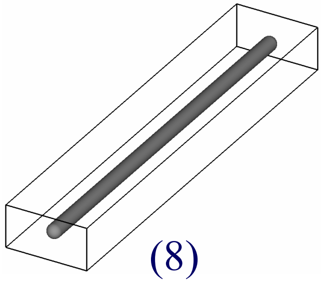
(8)

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.

- Various RVEs have been analyzed. The length of CNT is found to be 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.