Advanced Simulation of CNT Composites by a Fast Multipole Hybrid Boundary Node Method

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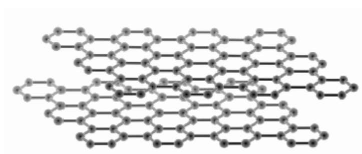
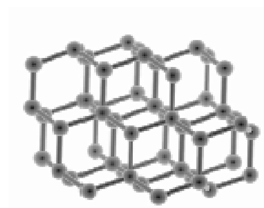
Background

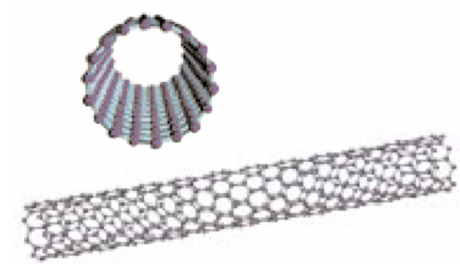
➢ Thermal conductivity of CNT (W/m·K)



Graphite
50~100



Diamond
3320



Nanotube
3000~6000

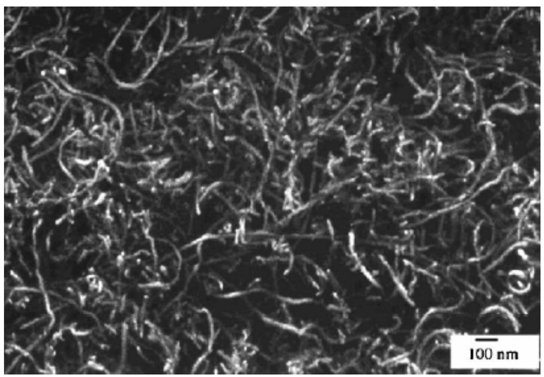
Resins: 0~1 W/m·K

Metals:

Fe	72	W/m·K
Cu	390	W/m·K

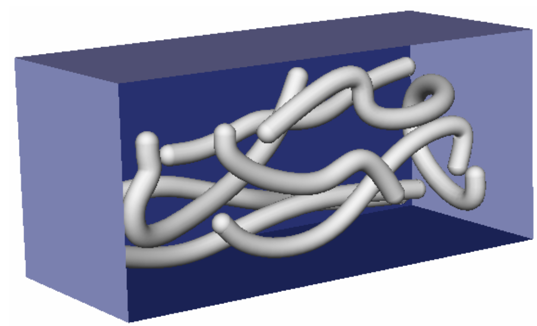
Background (2)

- **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

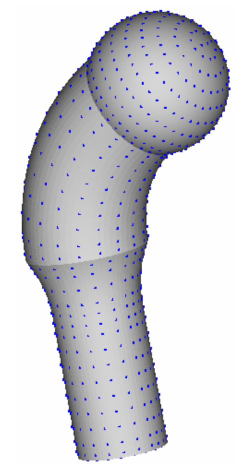
Simplified mathematic model

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

- 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**

$$\mathbf{U}\mathbf{x} = \mathbf{H}\hat{\mathbf{q}}$$

$$\mathbf{V}\mathbf{x} = \mathbf{H}\hat{\boldsymbol{\phi}}$$

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

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

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

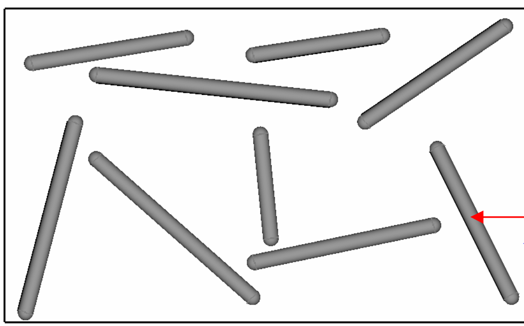
Remarks:

- **All integrations are performed in a local region without using any elements, the method is truely meshless.**

Simplified model

- **Hybrid BNM equations for Polymer matrix**

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



An RVE including n CNTs

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

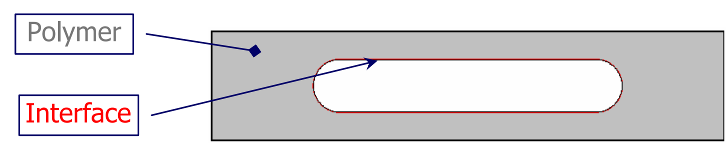
Simplified model (2)

- **Assembled equation for polymer domain**

$$\begin{bmatrix} \boldsymbol{U}^p_{00} & \boldsymbol{U}^p_{01} & \cdots & \boldsymbol{U}^p_{0n} \\ \boldsymbol{U}^p_{10} & \boldsymbol{U}^p_{11} & \cdots & \boldsymbol{U}^p_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{U}^p_{n0} & \boldsymbol{U}^p_{n1} & \cdots & \boldsymbol{U}^p_{nn} \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}^p_0 \\ \boldsymbol{x}^p_1 \\ \vdots \\ \boldsymbol{x}^p_n \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}^p_0 \hat{\boldsymbol{\phi}}^p_0 \\ \boldsymbol{H}^p_1 \hat{\boldsymbol{\phi}}^p_1 \\ \vdots \\ \boldsymbol{H}^p_n \hat{\boldsymbol{\phi}}^p_n \end{Bmatrix}$$

$$\begin{bmatrix} \boldsymbol{V}^p_{00} & \boldsymbol{V}^p_{01} & \cdots & \boldsymbol{V}^p_{0n} \\ \boldsymbol{V}^p_{10} & \boldsymbol{V}^p_{11} & \cdots & \boldsymbol{V}^p_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{V}^p_{n0} & \boldsymbol{V}^p_{n1} & \cdots & \boldsymbol{V}^p_{nn} \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}^p_0 \\ \boldsymbol{x}^p_1 \\ \vdots \\ \boldsymbol{x}^p_n \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}^p_0 \hat{\boldsymbol{q}}^p_0 \\ \boldsymbol{H}^p_1 \hat{\boldsymbol{q}}^p_1 \\ \vdots \\ \boldsymbol{H}^p_n \hat{\boldsymbol{q}}^p_n \end{Bmatrix}$$

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



- **Constant temperature at interfaces**

$$\{\phi_k\} = \{\mathbf{1}\}_k \phi^k_c$$

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**

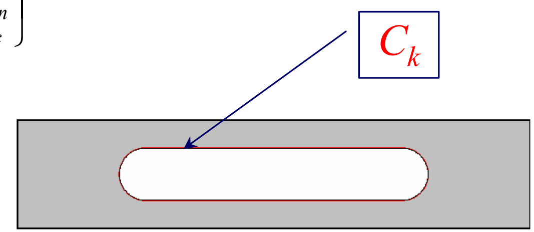
$$\int_{C_k} q \, d\Gamma = 0$$

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

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

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

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



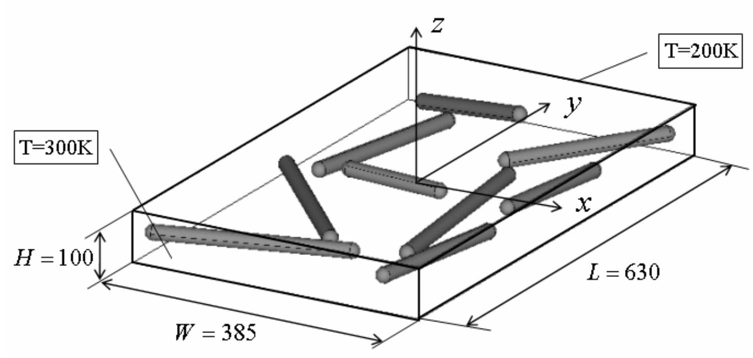
Simplified model (4)

- **Final system of equations**

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

Advanced simulation

- **RVE containing a number of CNTs**



Dimensions (nm) *and Boundary condition of RVE*

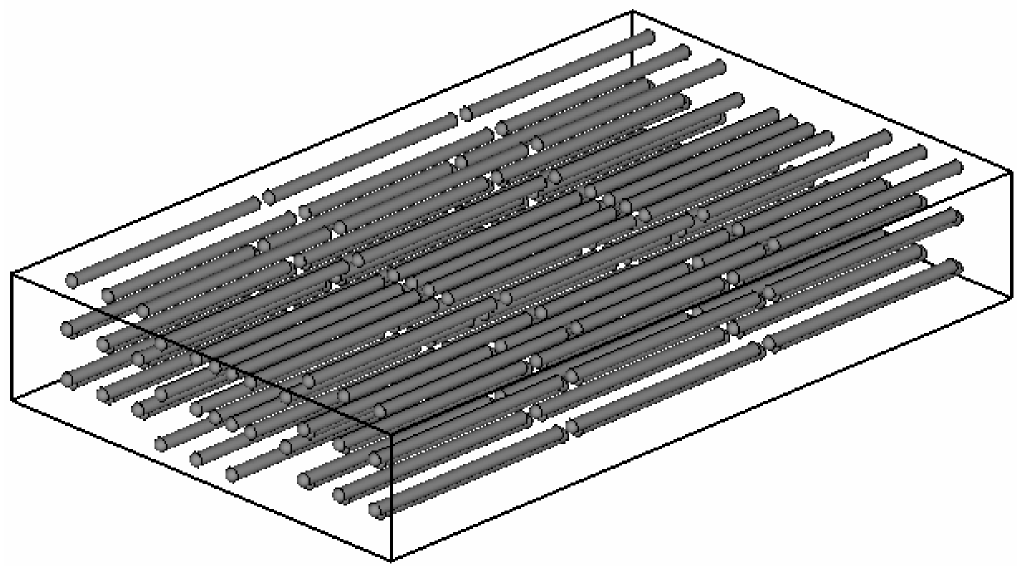
Heat conductivity used for polymer: 0.37 W/m·K

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

Equivalent heat conductivity

Advanced simulation (2)

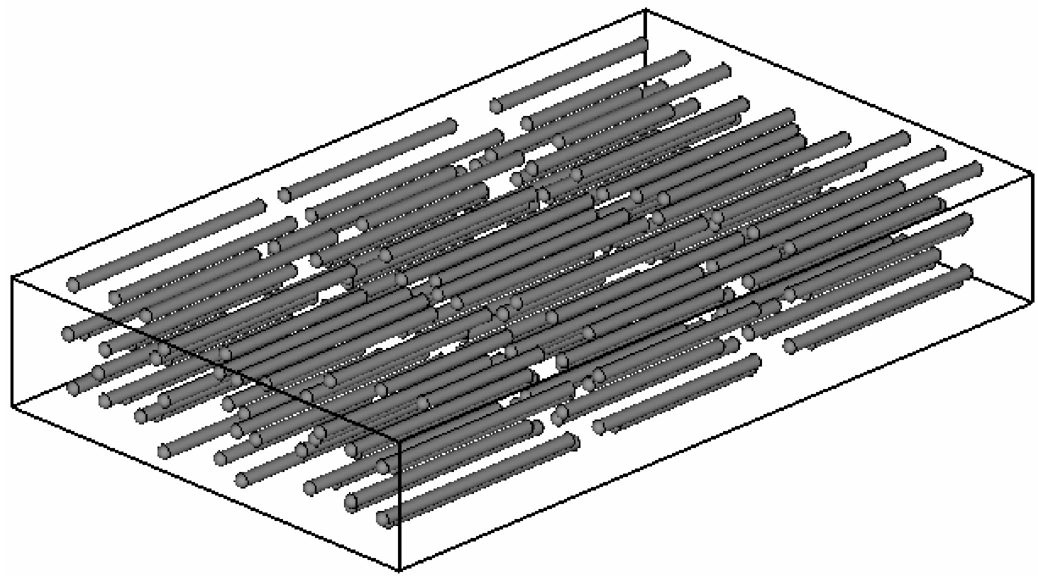
- Uniformly located CNTs



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
135	8.4%	3.746 W/m·K	115,335	164 hours

Advanced simulation (3)

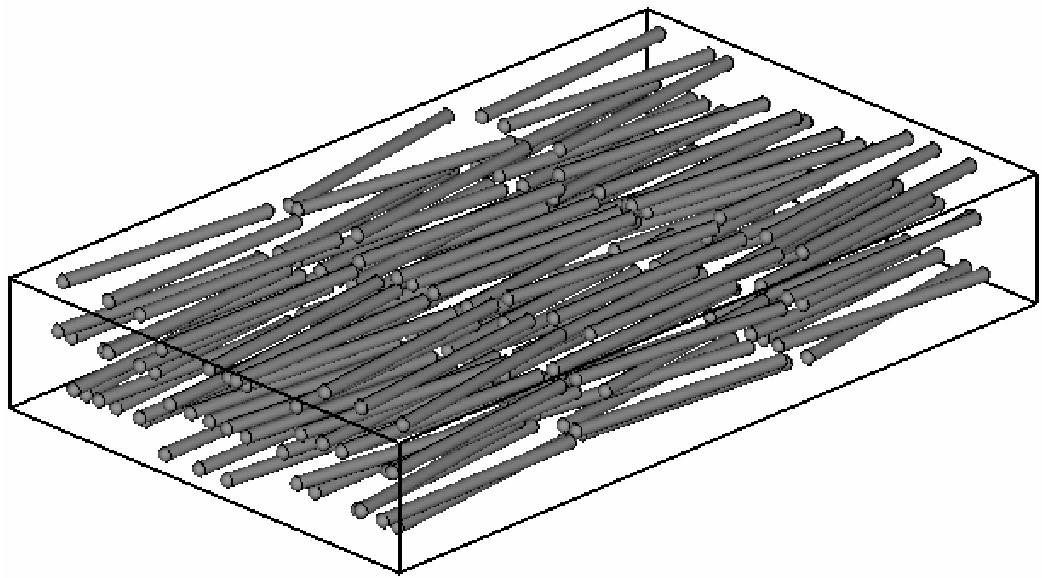
- "Randomly" located CNTs



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
135	7.7%	2.668 W/m·K	113,880	163 hours

Advanced simulation (4)

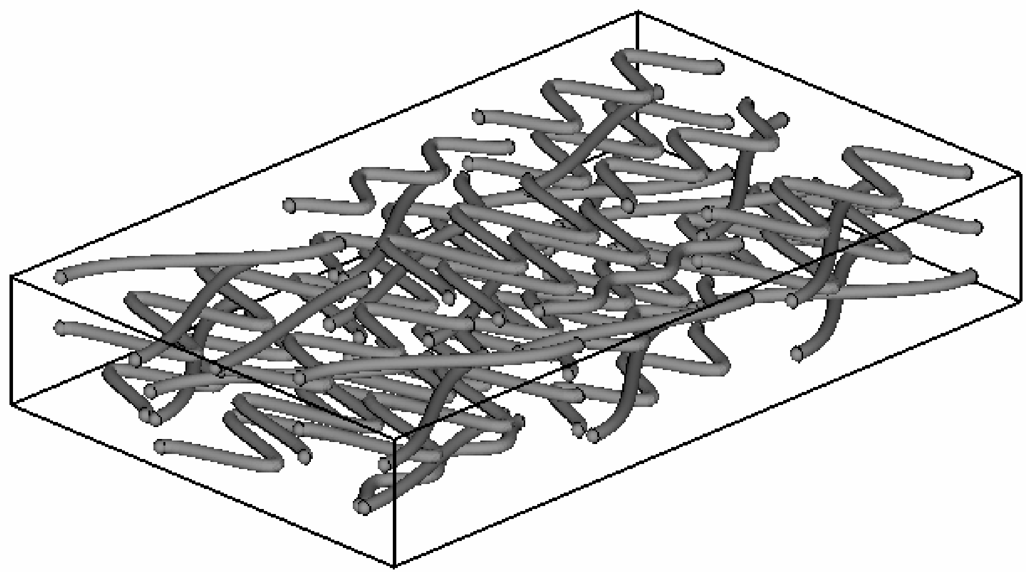
- "Randomly" oriented CNTs



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
135	8.4%	3.470 W/m·K	115,200	156 hours

Advanced simulation (5)

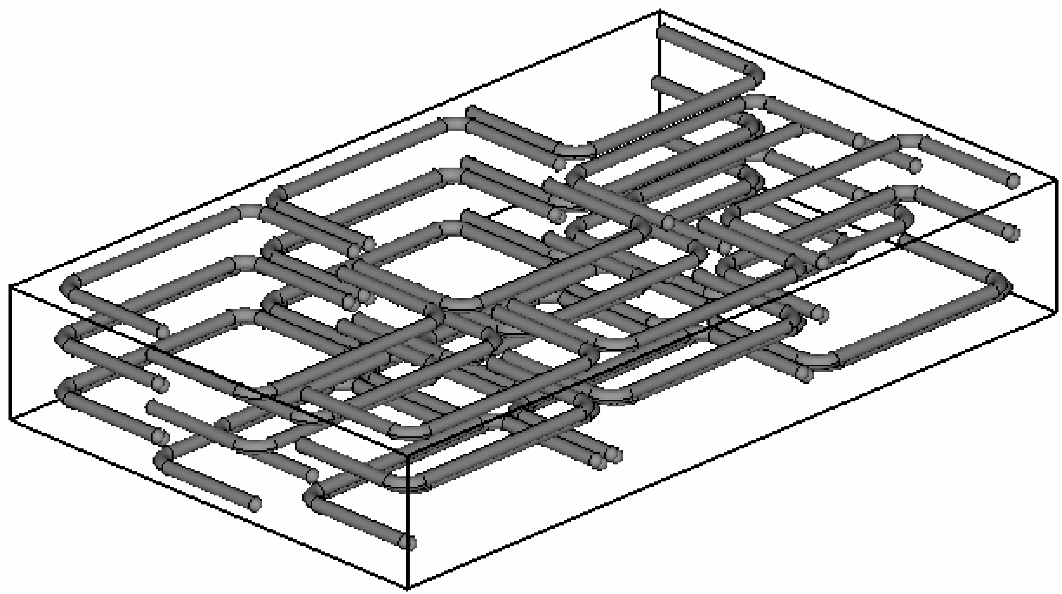
- "Randomly" located curved CNTs



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
45	4.8%	1.717 W/m·K	66,245	108 hours

Advanced simulation (6)

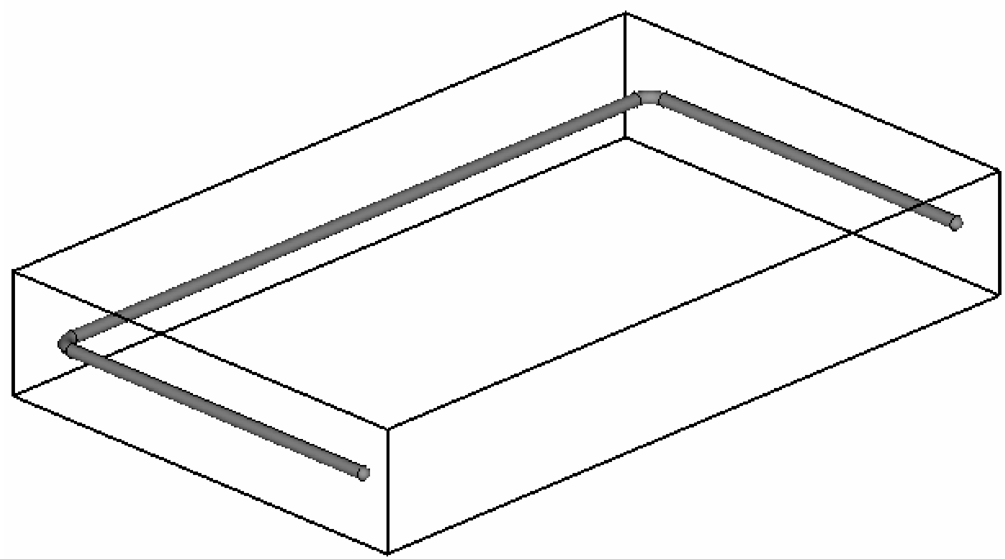
- **Forty-five CNTs of "C" shape**



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
45	5.5%	6.319 W/m·K	150,435	78 hours

Advanced simulation (7)

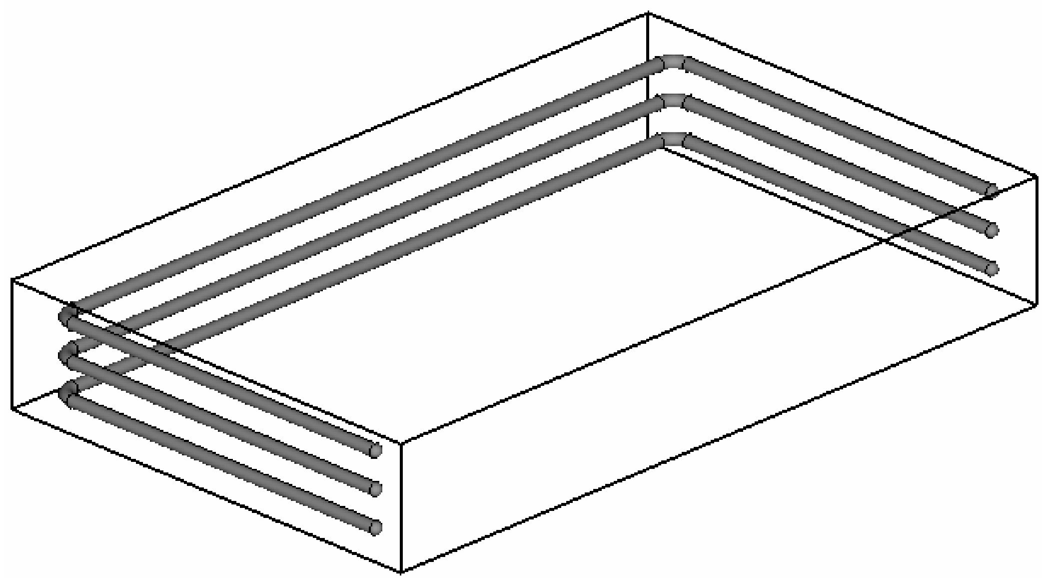
- Single CNT of "C" shape



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
1	0.4%	4.868 W/m·K	22,617	1.3 hours

Advanced simulation (8)

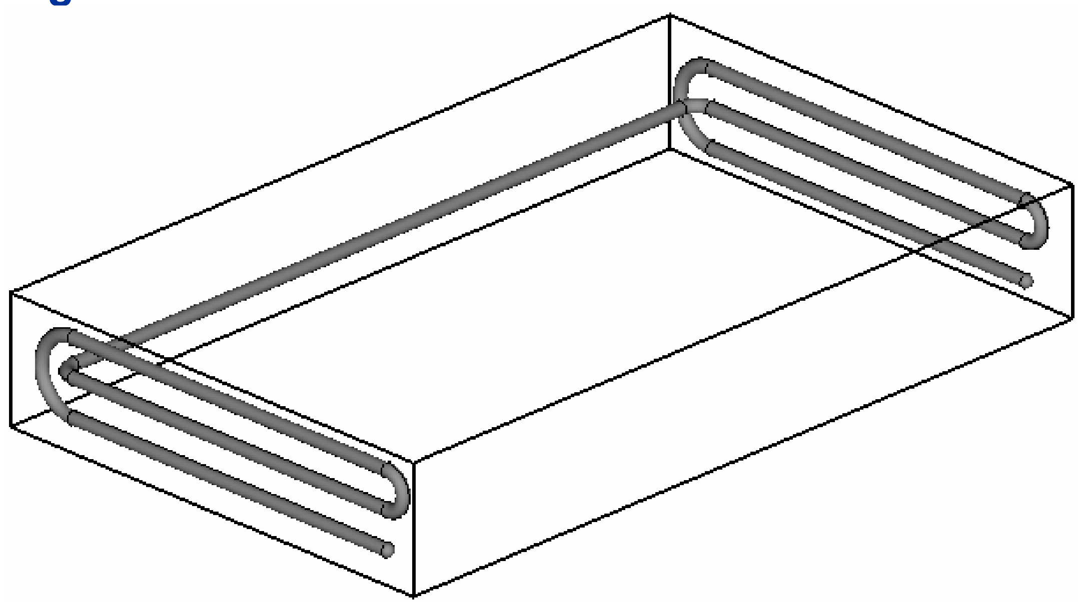
- Three CNTs of "C" shape



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
3	1.2%	11.15 W/m·K	37,251	4.4 hours

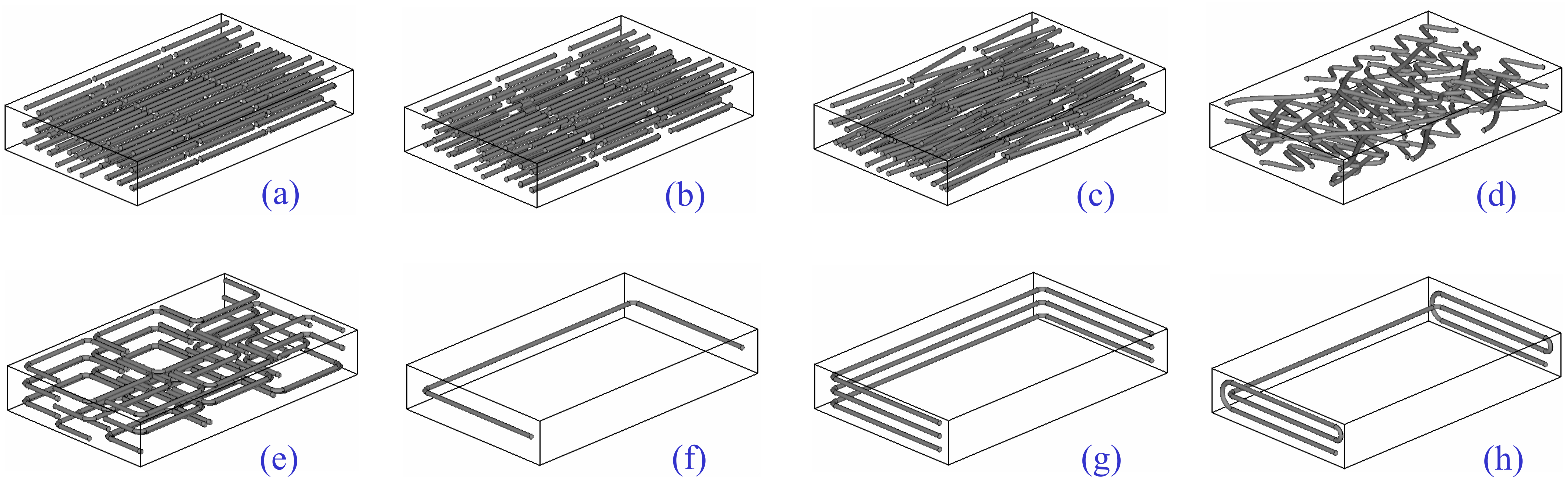
Advanced simulation (9)

- Single long and curved CNTs



Number of CNTs	Volume Percentage	Conductivity	Number of Nodes	CPU time
1	0.88%	11.76 W/m·K	21,909	1.0 hours

Advanced simulations (10)



RVE	(a)	(b)	(c)	(d)
Conductivity (κ)	3.746	2.668	3.470	1.717
Percentage (r)	8.4%	7.7%	8.4%	4.8%
κ/r	44.71	35.55	41.41	36.00

RVE	(e)	(f)	(g)	(h)
Conductivity (κ)	6.319	4.868	11.15	11.76
Percentage (r)	5.5%	0.40%	1.2%	0.88%
κ/r	114.5	1218	929.9	1337

Conclusions

- The CNT distribution, orientation and curvature have strong influence on the overall thermal properties of CNT composites.
- The length of CNT is of crucial importance in enhancing the thermal property of CNT-based composites. Increasing the lengths of CNTs is the most effective way to increase the heat conductivity of the composites.
- The best shape of CNTs for enhancing the composites is the “C” shape. Further studies will include optimization of the dimensions of the CNTs, which will be reported in subsequent conference.