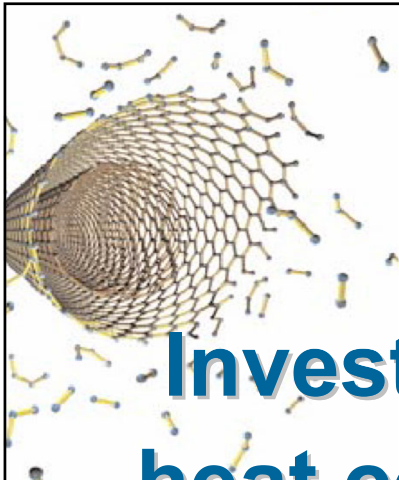

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Investigation of the equivalent heat conductivity of CNT-based composites using a simplified approach

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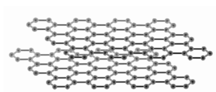
Outline

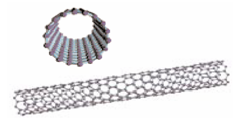
- Introduction
- Computational models for CNT materials
- Hybrid boundary node method
- Formulations of multi-domain model and simplified approach
- Numerical results
- Conclusions

Introduction

➢ Thermal conductivity of CNT (W/m·K)


Graphite
50~100


Diamond
3320


Nanotube
3000~6000

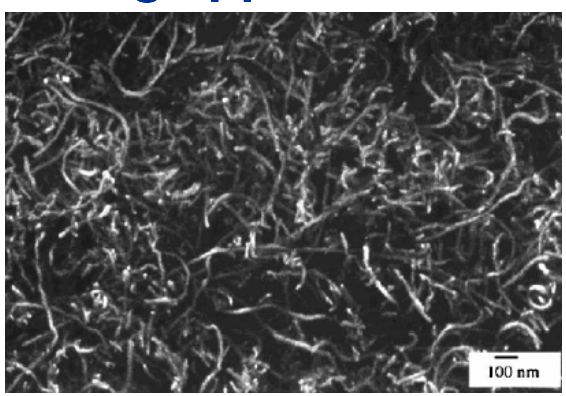
Resins:

0~1 W/m·K

Metals:

Fe	72	W/m·K
Al	240	W/m·K
Cu	390	W/m·K

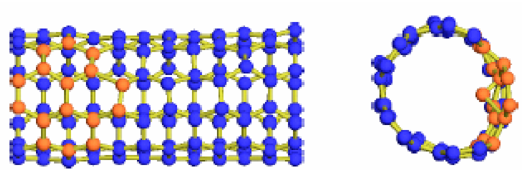
➢ Promising applications



Nanotube-reinforced polymers

Computational Models

◆Molecular dynamics

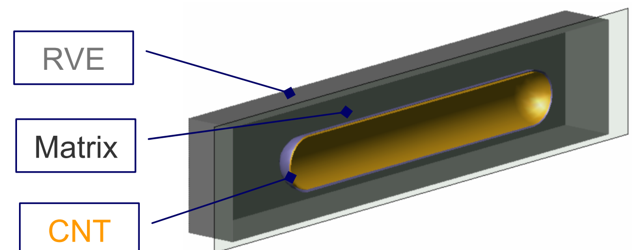


Motion of molecules and atoms, governed by Hamilton's equation

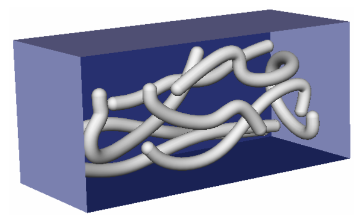
Remarks:

- Accurate but limited to very small length and time scales;
- Suitable for only individual or isolated nanotubes, and cannot deal with CNT-based composites.

◆Continuum approach



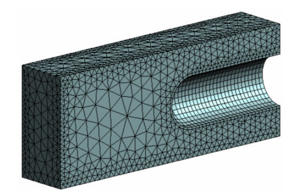
Physical behavior is governed by continuum mechanics equations



An RVE including many curved CNTs

Two difficulties:

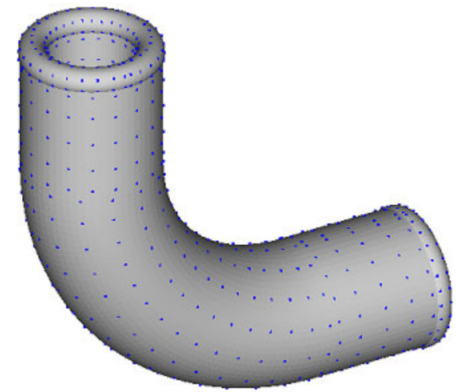
- Discretization.
- Computational scale.



Hybrid BNM

➢ Main features:

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



Example of meshless discretization

➢ Variables approximation

- Domain variables

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

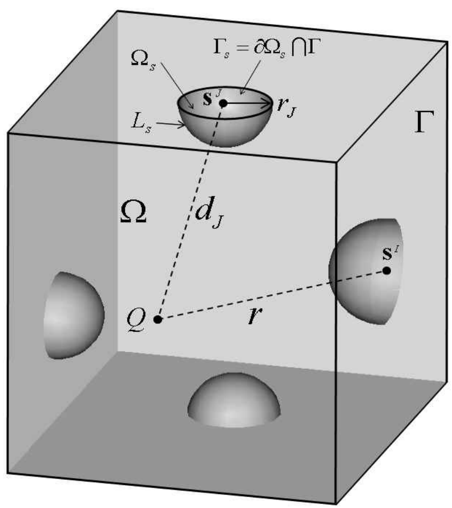
- Boundary variables

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

Hybrid BNM (2)

- **Local weak form**

$$\int_{\Gamma}(q-\tilde{q})\delta\phi d\Gamma-\int_{\Omega}\phi_{,ii}\delta\phi d\Omega+\int_{\Gamma_q}(\tilde{q}-\bar{q})\delta\tilde{\phi} d\Gamma-\int_{\Gamma}(\phi-\tilde{\phi})\delta\tilde{q} d\Gamma=0$$



$$\sum_{I=1}^{n}\int_{\Gamma_s}\frac{\partial\phi_I^s}{\partial n}v_J(Q)x_I d\Gamma=\sum_{I=1}^{n}\int_{\Gamma_s}\Phi_I(\mathbf{s})v_J(Q)\hat{q}_I d\Gamma$$

$$\sum_{I=1}^{n}\int_{\Gamma_s}\phi_I^s v_J(Q)x_I d\Gamma=\sum_{I=1}^{n}\int_{\Gamma_s}\Phi_I(\mathbf{s})v_J(Q)\hat{\phi}_I d\Gamma$$

- **System of equations – final form**

$$\mathbf{Ux}=\mathbf{H}\hat{\mathbf{q}} \qquad \mathbf{Vx}=\mathbf{H}\hat{\phi}$$

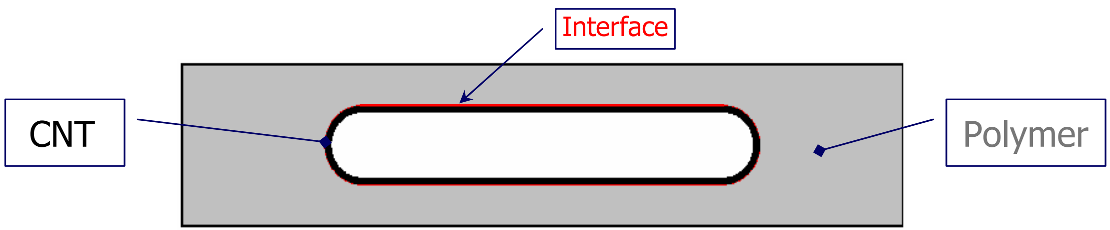
Simplified approach

- **HBNM equations for CNT**

$$\begin{bmatrix} U_{00}^{p} & U_{01}^{p} \\ U_{10}^{p} & U_{11}^{p} \end{bmatrix} \begin{Bmatrix} x_0^p \\ x_1^p \end{Bmatrix} = \begin{Bmatrix} H_0^p \hat{\phi}_0^p \\ H_1^p \hat{\phi}_1^p \end{Bmatrix}$$

$$\begin{bmatrix} V_{00}^{p} & V_{01}^{p} \\ V_{10}^{p} & V_{11}^{p} \end{bmatrix} \begin{Bmatrix} x_0^p \\ x_1^p \end{Bmatrix} = \begin{Bmatrix} H_0^p \hat{q}_0^p \\ H_1^p \hat{q}_1^p \end{Bmatrix}$$

$$\begin{bmatrix} A_{00}^{p} & A_{01}^{p} \\ U_{10}^{p} & U_{11}^{p} \\ V_{10}^{p} & V_{11}^{p} \end{bmatrix} \begin{Bmatrix} x_0^p \\ x_1^p \end{Bmatrix} = \begin{Bmatrix} H_0^p d_0^p \\ H_1^p \hat{\phi}_1^p \\ H_1^p \hat{q}_1^p \end{Bmatrix}$$



- **HBNM equations for Polymer**

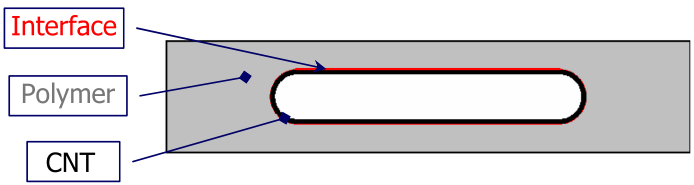
$$\begin{bmatrix} U_{00}^{c} & U_{01}^{c} \\ U_{10}^{c} & U_{11}^{c} \end{bmatrix} \begin{Bmatrix} x_0^c \\ x_1^c \end{Bmatrix} = \begin{Bmatrix} H_0^c \hat{\phi}_0^c \\ H_1^c \hat{\phi}_1^c \end{Bmatrix}$$

$$\begin{bmatrix} V_{00}^{c} & V_{01}^{c} \\ V_{10}^{c} & V_{11}^{c} \end{bmatrix} \begin{Bmatrix} x_0^c \\ x_1^c \end{Bmatrix} = \begin{Bmatrix} H_0^c \hat{q}_0^c \\ H_1^c \hat{q}_1^c \end{Bmatrix}$$

$$\begin{bmatrix} A_{00}^{c} & A_{01}^{c} \\ U_{10}^{c} & U_{11}^{c} \\ V_{10}^{c} & V_{11}^{c} \end{bmatrix} \begin{Bmatrix} x_0^c \\ x_1^c \end{Bmatrix} = \begin{Bmatrix} H_0^c d_0^c \\ H_1^c \hat{\phi}_1^c \\ H_1^c \hat{q}_1^c \end{Bmatrix}$$

Simplified approach (2)

◆Multi-domain model



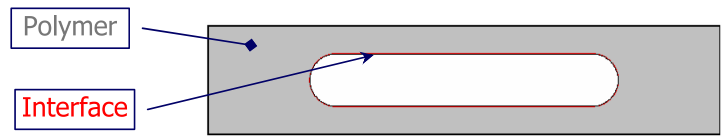
▪**Continuity and equilibrium at interface**

$$\{\phi_1^p\} = \{\phi_1^c\} \qquad \{q_1^p\} = -\{q_1^c\}$$

▪**Assembled system of equation**

$$\begin{bmatrix} A_{00}^p & A_{01}^p & 0 & 0 \\ U_{10}^p & U_{11}^p & -U_{10}^c & -U_{11}^c \\ V_{10}^p & V_{11}^p & V_{10}^c & V_{11}^c \\ 0 & 0 & A_{00}^c & A_{01}^c \end{bmatrix} \begin{Bmatrix} x_0^p \\ x_1^p \\ x_0^c \\ x_1^c \end{Bmatrix} = \begin{Bmatrix} H_0^p d_0^p \\ 0 \\ 0 \\ H_0^c d_0^c \end{Bmatrix}$$

◆Simplified model



▪**Constant temperature constraint at interface**

$$\{\boldsymbol{\phi}_1^p\} = \{\mathbf{1}\}\phi^c$$

▪**Flux relationship at interface**

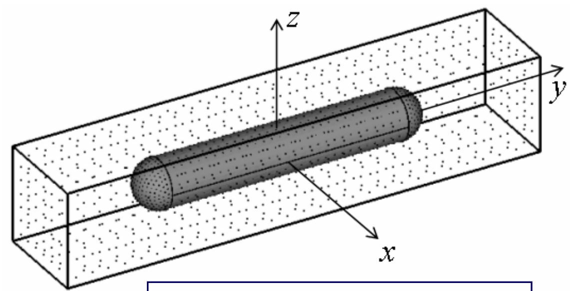
$$\int_C q\,d\Gamma = 0 \quad \xrightarrow{q = \sum_{I=1}^{N} \frac{\partial \phi_I^s}{\partial n} x_I} \quad \{\mathbf{1}\}^{\mathrm{T}} \{\boldsymbol{x}_1^p\} = 0$$

▪**Assembled system of equation**

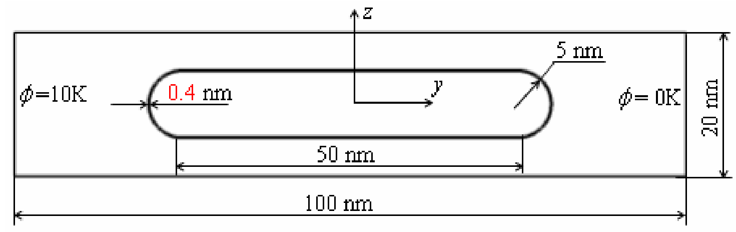
$$\begin{bmatrix} \boldsymbol{A}_{00}^p & \boldsymbol{A}_{01}^p & \mathbf{0} \\ \boldsymbol{U}_{10}^p & \boldsymbol{U}_{11}^p & \boldsymbol{H}_1^p\{\mathbf{1}\} \\ 0 & \{\mathbf{1}\}^{\mathrm{T}} & 0 \end{bmatrix} \begin{Bmatrix} \boldsymbol{x}_0^p \\ \boldsymbol{x}_1^p \\ \phi^c \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{H}_0^p \boldsymbol{d}_0^p \\ \mathbf{0} \\ 0 \end{Bmatrix}$$

Numerical results

- **RVE containing single CNT**



Discretization of RVE



Dimensions (nm) *and Boundary condition*

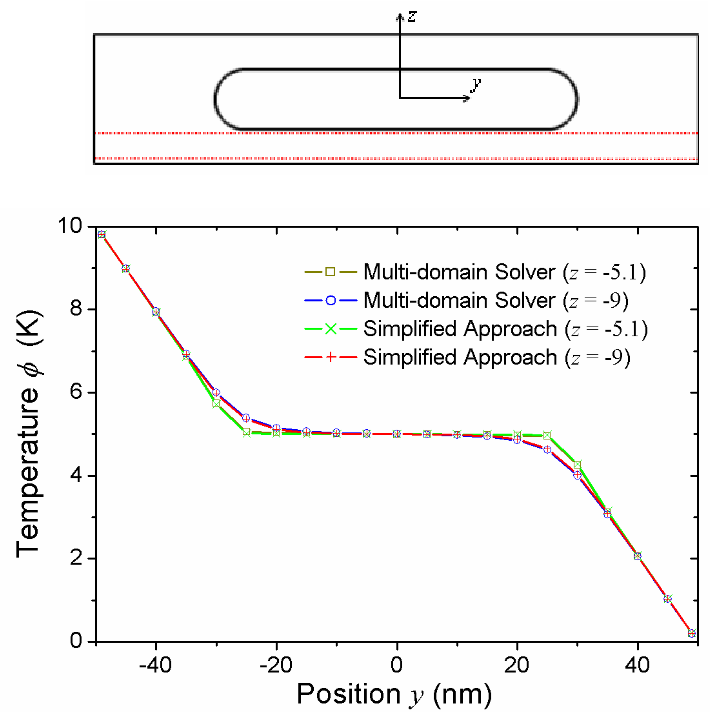
Equivalent heat conductivity $\kappa = -\dfrac{qL}{\Delta\phi}$

Heat conductivity:
Nanotube: 6000 W/m·K
Polymer: 0.37 W/m·K

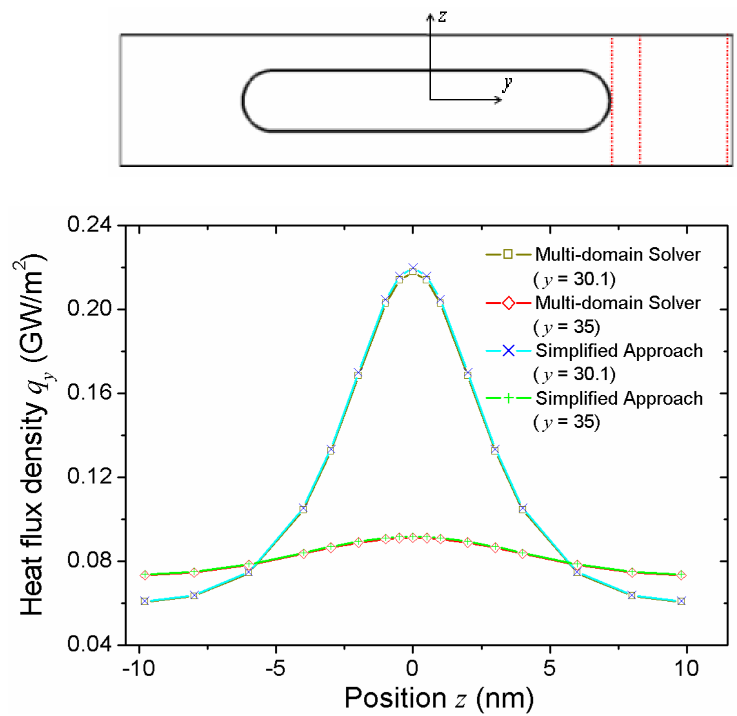
	Degrees of freedom	CPU seconds for		Equivalent heat conductivity
		integration	solving equation	
Multi-domain Solver	4402	294	477	0.7719
Simplified Approach	2193	144	62	0.7771

Comparison between the two methods

Numerical results (2)



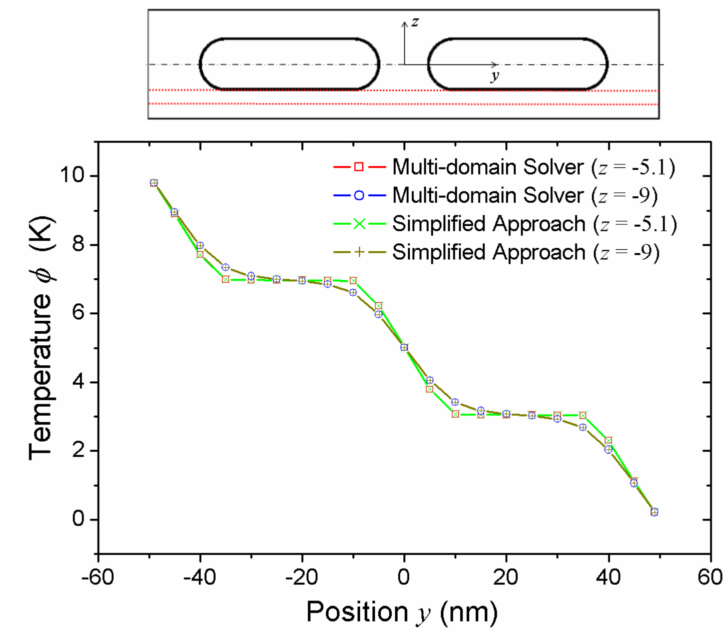
Temperature distribution



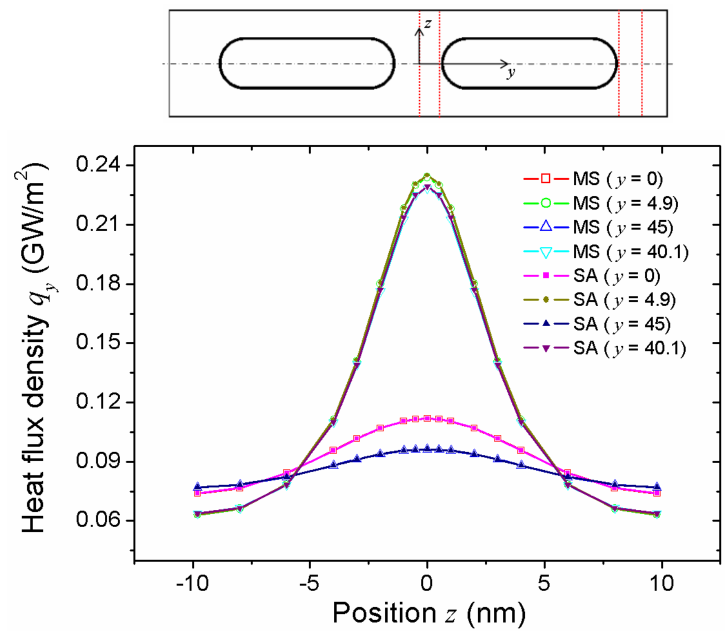
Flux distribution

Numerical results (3)

- **RVE containing two CNTs**



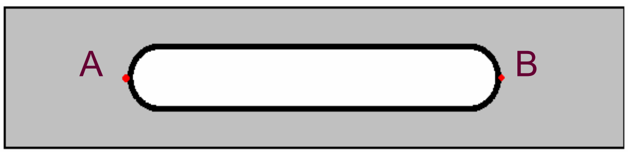
Temperature distribution



Flux distribution

Numerical results (4)

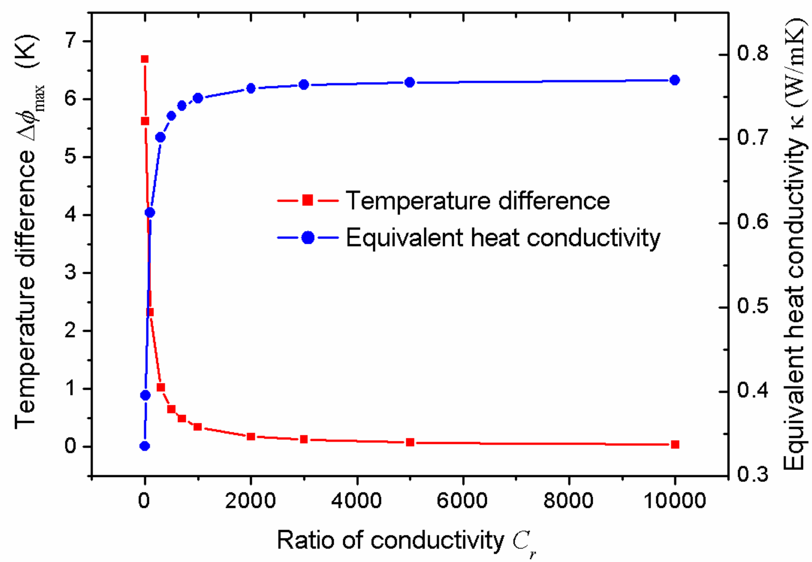
- **Maximum temperature difference within a CNT**



$$\Delta\phi_{\max} = \phi(A) - \phi(B)$$

$$C_r = \frac{\kappa_{CNT}}{\kappa_{polymer}}$$

$$\kappa_{polymer} = 0.37 \ \ \mathrm{W/m{\bullet}K}$$



Maximum temperature differences and equivalent heat conductivities for various C_r

Conclusions

- A simplified approach is proposed for simulation of thermal behavior of CNT-based composites. This method provides remarkable improvement in computational efficiency. Numerical results obtained via this method are found to be in excellent consistency with that by full model analysis (multi-domain solver)
- Influence of the ratio of phase heat conductivity on equivalent thermal properties is investigated. It is demonstrated that for the ratios above 2000, the simplified approach can give sufficient accuracy. Since the lowest value of the ratio between CNT and polymers ever reported in literature is much higher than 2000, the simplified approach can be readily used to analyze the CNT-based composites
- The simplified approach, combined with FMM to further reduce the computational scale, should be capable of solving an RVE containing many randomly distributed CNTs