Multi-Scale Analysis of Graphene Carbon Nanotubes and Related Nanostructures

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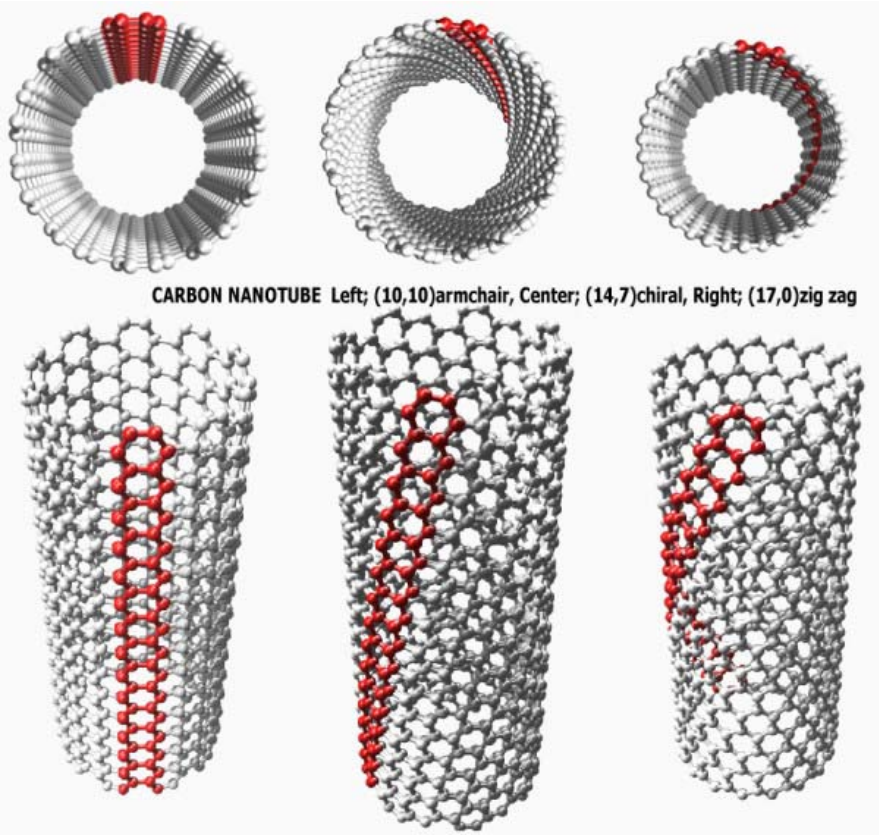
Objectives

- **Discuss Army Relevance of Work**
- **Provide Brief History of Nanomechanics to Date**
- **Develop Exact Graphene $\longrightarrow$ Nanotube Map**
- **Develop Higher-Order Born Rule**
- **Conclude with Remarks on Future Work**

Army Relevance

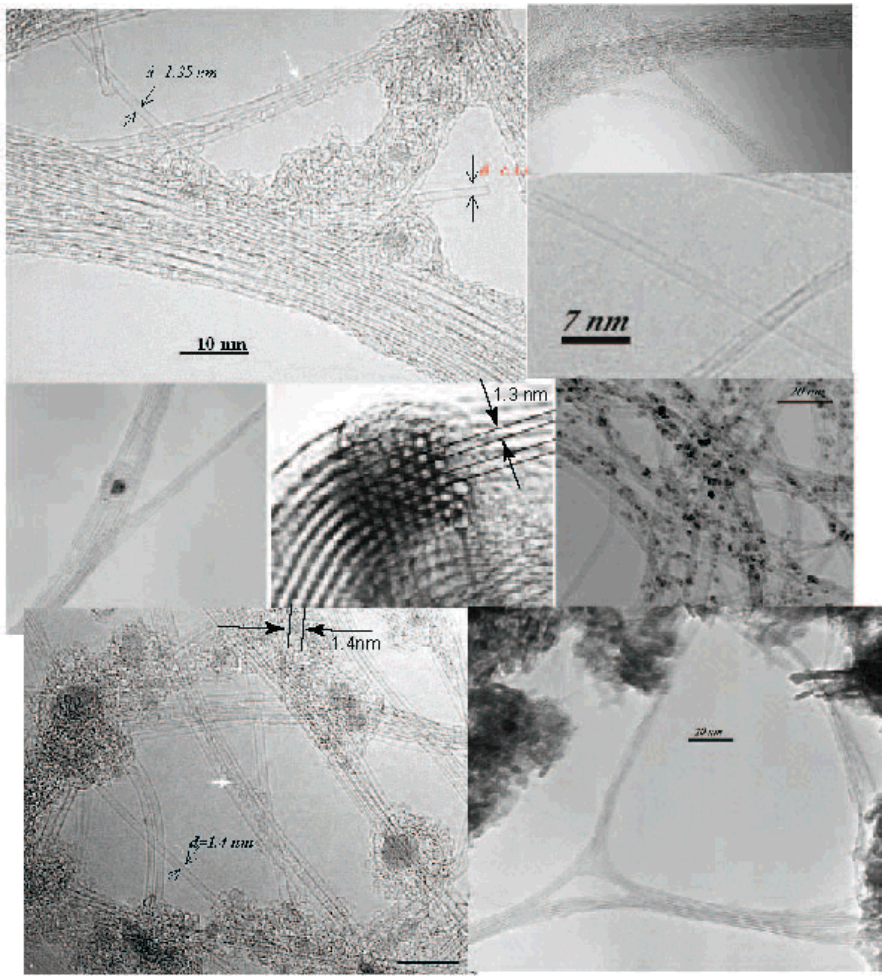
- **Impressive Electrical, Chemical, & Mechanical Properties**
  - **change with chirality**
  - **extremely strong (rolled-up graphite, perfect crystals)**
    100X Tensile Strength of Steel
  - **semiconductor or metal**
  - **absorb hydrogen**



$300 per gram

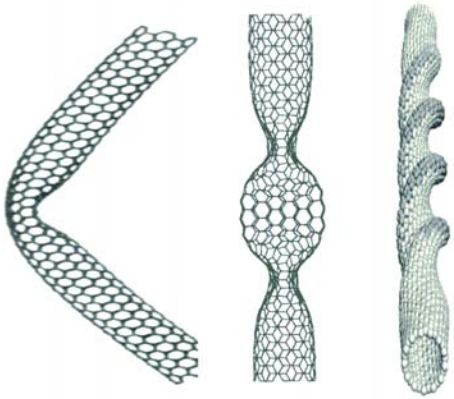
Army Relevance

- **Envisioned Applications**
  - **EMI/RFI shielding and radar absorbing materials**
  - **Highly durable electrodes and fuel cell components**
  - **Extremely light and strong vehicle and body armor**
  - **Composites with altered mechanical and electrical characteristics (nanotube doping)**
  - **Replacement for silicon chips**



Nanomechanics History

- **Discovery of Nanotubes**
  - **Sumio Iijima, NEC Corporation, 1991**
- **Experimental Characterization**
  - **Using AFM or mechanical resonance**
  - **Axial Rigidity, Bending and Torsional Rigidity, Strengths, Instabilities**
- **Molecular Dynamics**
  - **Simulations to Determine Above Quantities**
  - **Computationally Expensive**



• Reduced-Order Modeling

- Hybrid continuum-atomistic modeling

- Bulk-scale and atomistic kinematics linked through the Born Rule (Cauchy, 1828)

- Relatively recent: (Tadmor et al., 1996; Zhang et al., 2002; Arroyo and Belytschko, 2002; Sunyk and Steinmann, 2003)

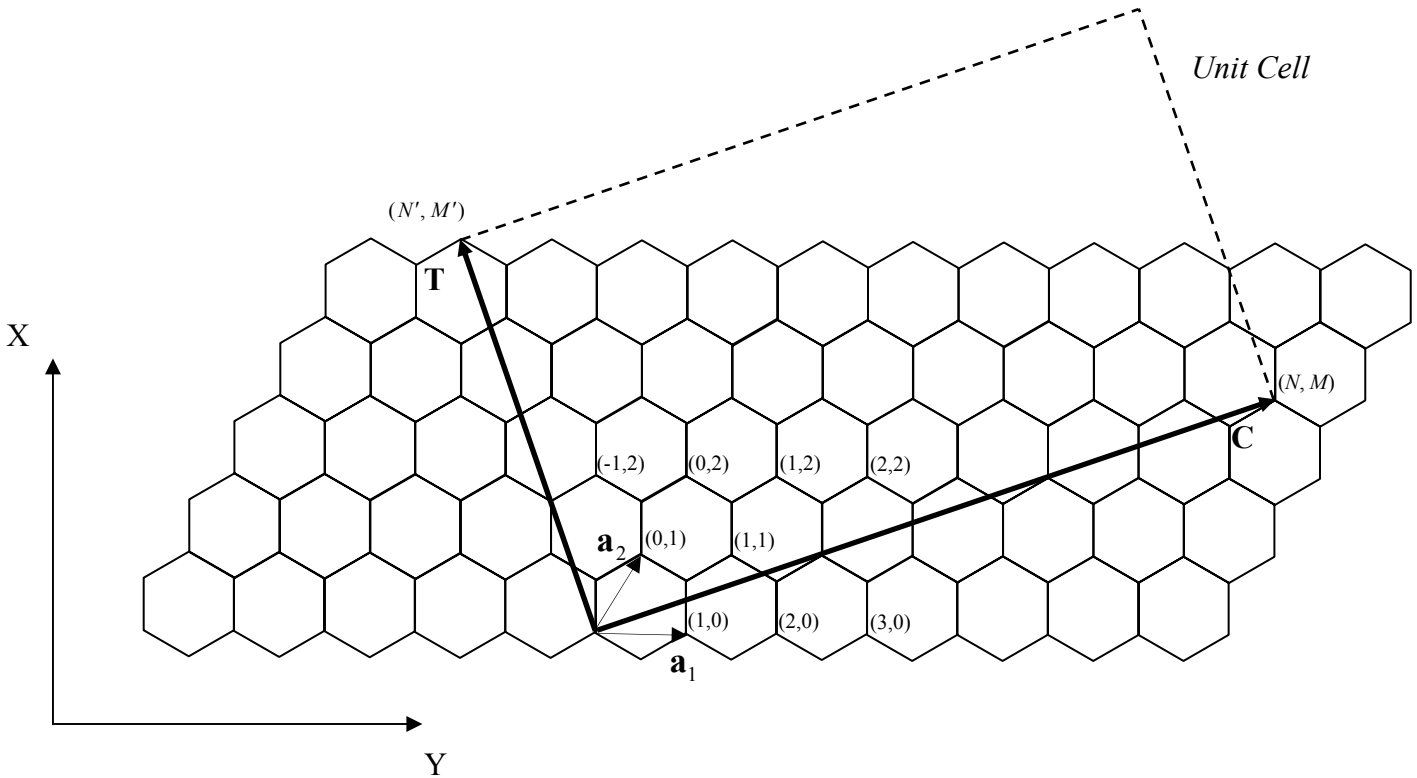
- Yet to look beyond single nanotube modeling:

  • collections of nanotubes

  • bulk solids composed entirely of, or in part by, nanostructures

Exact Mapping

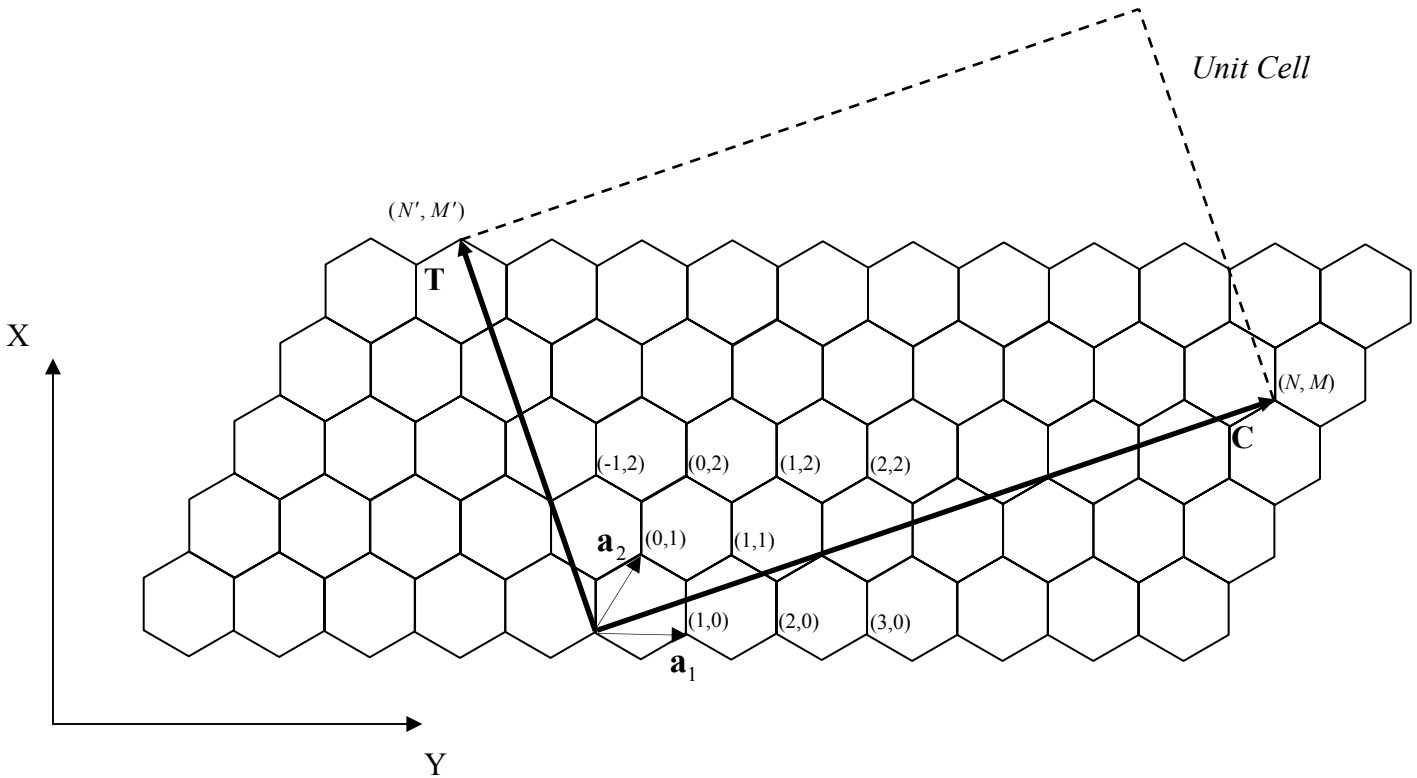
- **Motivated by Important Dependence on Chirality and Continuum Necessity For An Analytical Description of Deformation (F)**



Exact Mapping

- **Desired:** $\Psi : (n, m; N, M) \in Z^2 \times Z^2 \mapsto (x, y, z) \in R^3$

where *(x,y,z)* **define a cylindrical manifold** ***N***



Exact Mapping

- **Approach:**
  - **Apply a zero-charlity *(N,0)* cylindrical mapping to a coordinate system *(c,t)* aligned with *C* and *T*.**
  - **Apply a coordinate transformation (second mapping) which locates (X,Y,Z) coordinates in terms of *(c,t)***
  - **Express coordinates *(c,t)* in terms of *(n,m;N,M)***

$$\mathbf{r} = n\mathbf{a}_1 + m\mathbf{a}_2 = c\mathbf{e}_c + t\mathbf{e}_t$$

Basis

$$\mathbf{a}_1 = l_0\mathbf{i}$$

$$\mathbf{a}_2 = \frac{1}{2}l_0\mathbf{i} + \frac{\sqrt{3}}{2}l_0\mathbf{j}$$

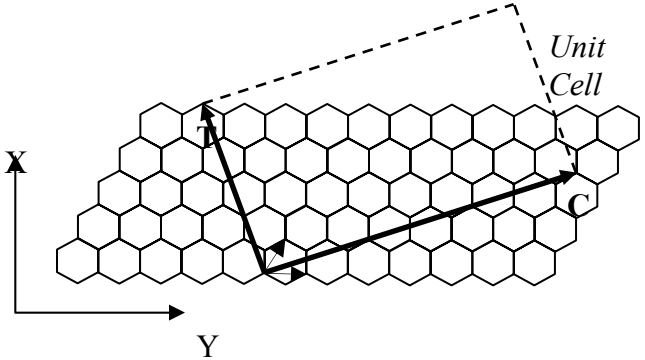
$$\mathbf{a}^i \cdot \mathbf{a}_j = \delta^i{}_j$$

$$\Longrightarrow$$

Dual Basis

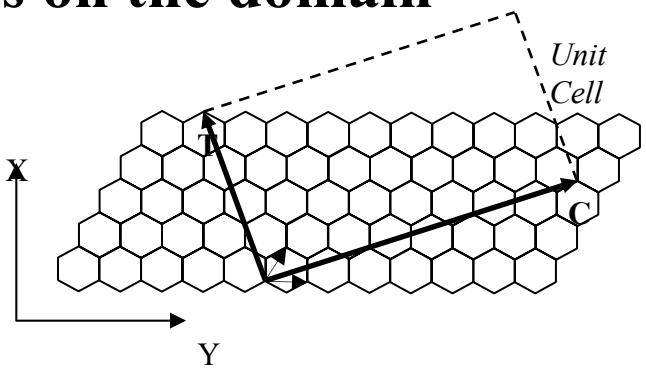
$$\mathbf{a}^1 = \frac{1}{l_0}\left(\mathbf{i} - \frac{\sqrt{3}}{3}\mathbf{j}\right)$$

$$\mathbf{a}^2 = \frac{1}{l_0}\left(\frac{2\sqrt{3}}{3}\mathbf{j}\right)$$

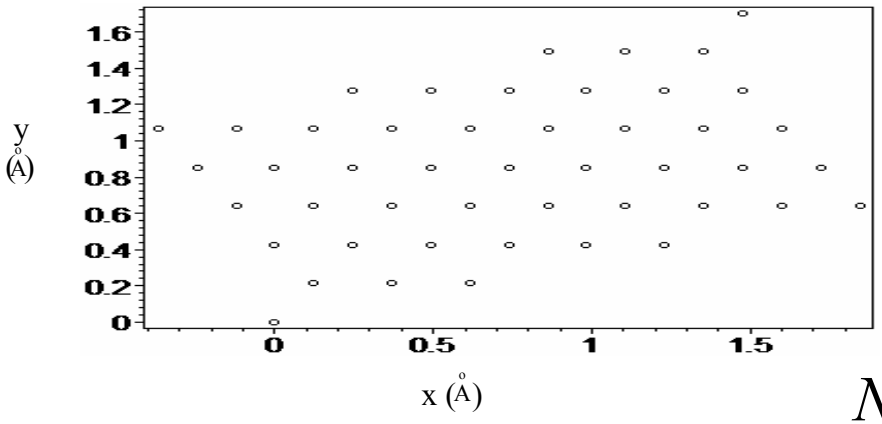


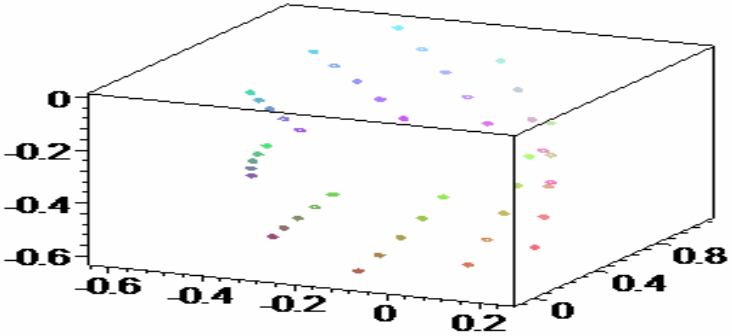
Exact Mapping

- **Unit Cell:**
  - **Mapping is not one-to-one until bounds on the domain $(n,m) \in Z^2$ are defined**
  - **Developed in the paper**



- **Results:**





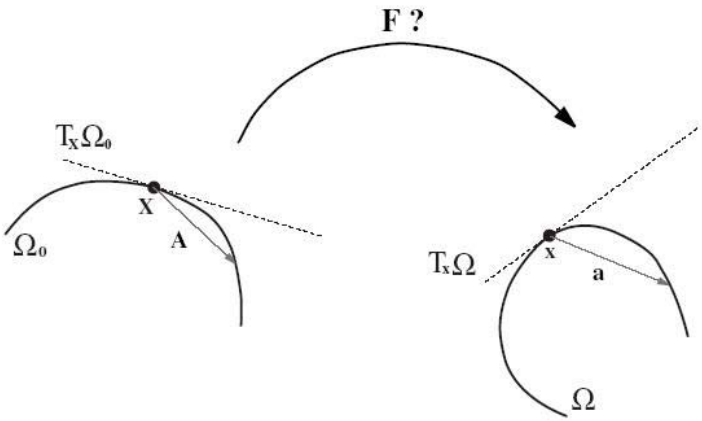
N=6, M=3

Higher-Order Born Rule

- **Traditional Born Rule is a Tangent Map**

$$\mathbf{r}_i = \mathbf{F} \cdot \mathbf{R}_i$$

$$\mathbf{F} = \frac{\partial \mathbf{r}}{\partial \mathbf{R}} = F_{iJ}\, \mathbf{e}_i \otimes \mathbf{e}_J = \frac{\partial x_i}{\partial X_J} \mathbf{e}_i \otimes \mathbf{e}_J$$



Courtesy of Arroyo Marino (2002)

- **Inappropriate for Studying Curved Manifolds**

Higher-Order Born Rule

- **Exact Relationship:**

$$\mathbf{dr} = \mathbf{F} \cdot \mathbf{dR}$$

- **Integrate Once and Taylor Expand F**

$$\mathbf{r} = \int \mathbf{F} \cdot \mathbf{dR} \qquad \mathbf{F}(\mathbf{R}) = \mathbf{F}(\mathbf{0}) + \left.\frac{\partial \mathbf{F}}{\partial \mathbf{R}}\right|_{\mathbf{R}=\mathbf{0}} \cdot \mathbf{R} + O(\mathbf{R}^2)$$

- **Results in a Higher-Order Rule**

$$\mathbf{r} = \mathbf{F}(\mathbf{0}) \cdot \mathbf{R} + \mathrm{K} \cdot \int \mathbf{R} \cdot \mathbf{dR} + O(\mathbf{R}^2)$$

Higher-Order Born Rule

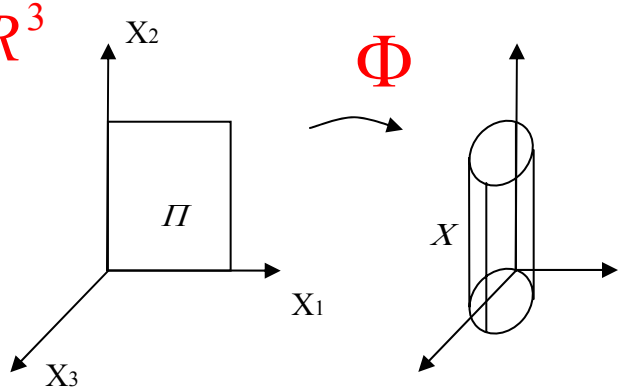
- **Performance – Cylindrical Mapping**

$$\Phi : (X_1, X_2, X_3) \in R^3 \rightarrow (x_1, x_2, x_3) \in R^3$$

$$x_1 = \Phi_1(X_1, X_2, X_3) = r\sin(X_1 / r)$$

$$x_2 = \Phi_2(X_1, X_2, X_3) = X_2$$

$$x_3 = \Phi_3(X_1, X_2, X_3) = r\cos(X_1 / r) - r$$



- **Deformation Gradient**

$$F = \begin{bmatrix} \cos(X_1/r) & 0 & 0 \\ 0 & 1 & 0 \\ -\sin(X_1/r) & 0 & 0 \end{bmatrix}$$

$$\mathrm{K}_{311} = -1/r$$

- **Result of Map**

$$\mathbf{r} = X_1\mathbf{e}_1 + X_2\mathbf{e}_2 - \frac{1}{r}\frac{X_1^{\,2}}{2}\mathbf{e}_3 + O(\mathbf{R}^2)$$

Future Work

- **Complete Hybrid Continuum-Atomistic Framework**
  - **Scale-linking through Higher-Order Born Rule**
  - **Equivalence of Atomic Potentials with Hyperelastic Strain Energy**
  - **Loading description at the bulk-scale**
  - **Plasticity, phase transition, and fracture**
  - **Capability to analyze materials composed entirely of, or in part by, nanostructures**