Multiscale Modeling of Piezoelectric Materials

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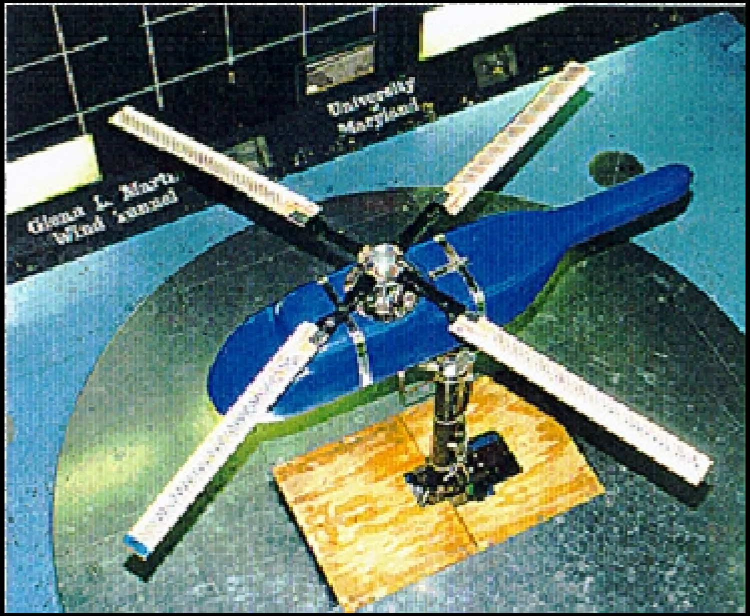
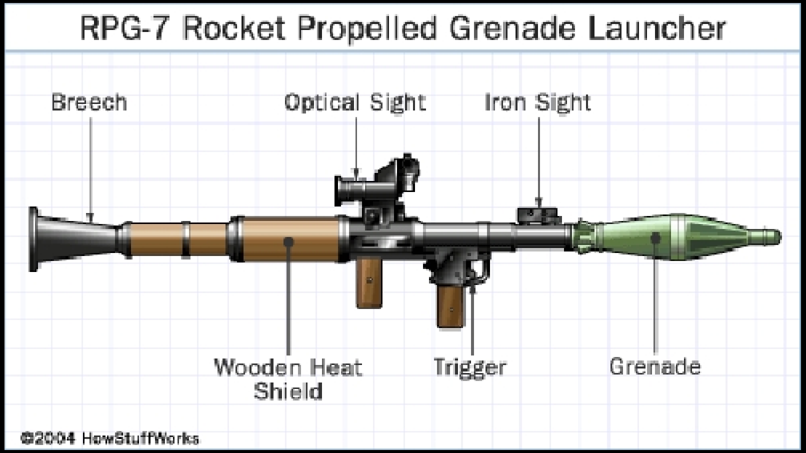
Outline

- Introduction to Piezoelectric Materials
- Piezoelectric Materials – Overview
- PZT Monoclinic Structure
- Atomistic Elasticity Tensor
- Variational Multiscale Approach

Introduction

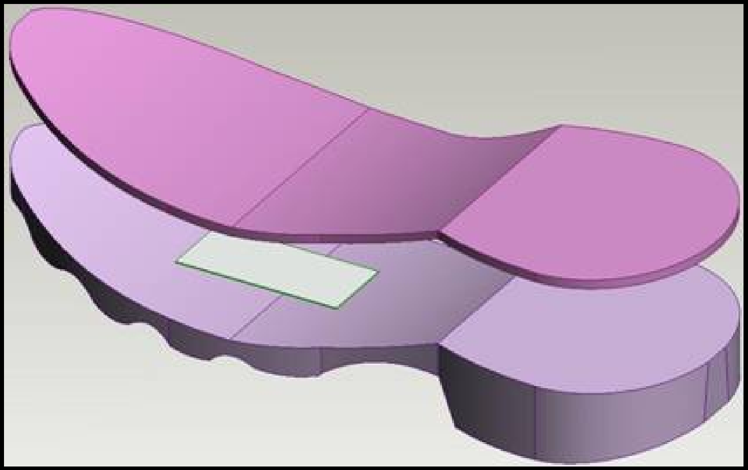


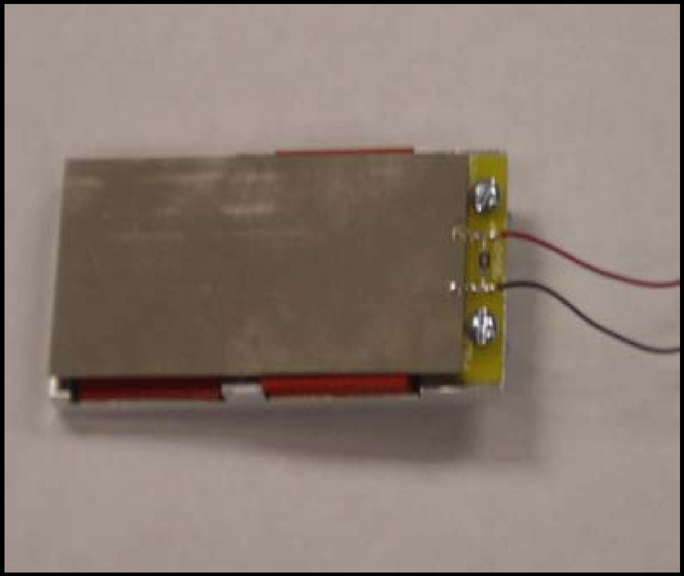


Booster → Piezo Fuse → Gunpowder Flash → Nitro Propellant

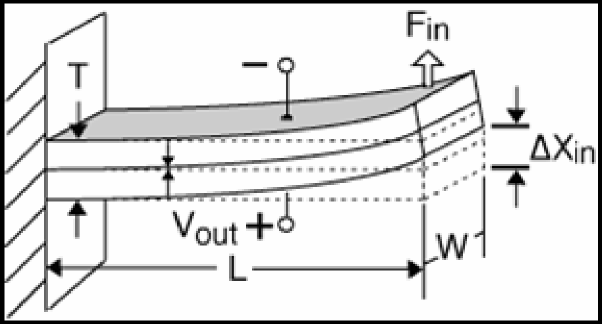
Smart controllable rotor twist research at the University of Maryland's Glen L. Martin wind tunnel.

Introduction

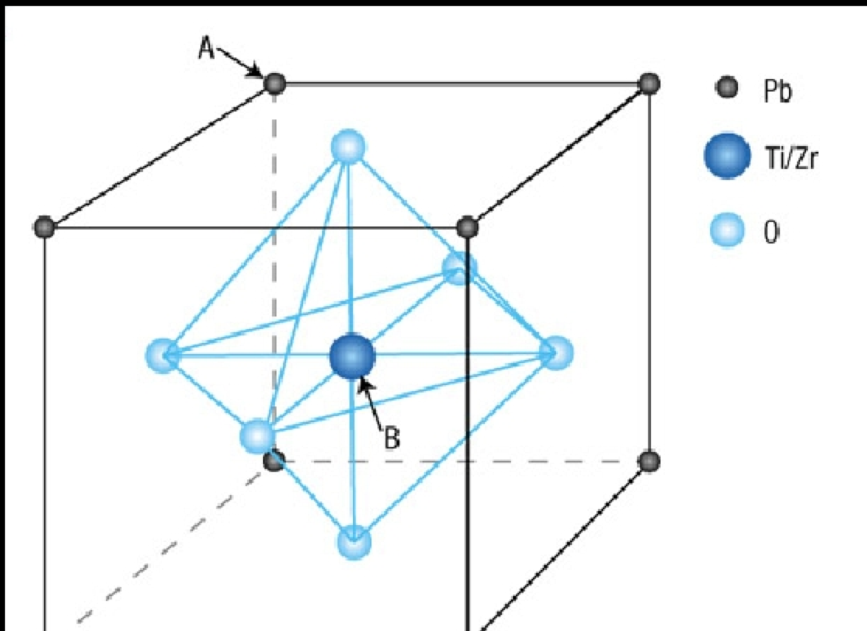




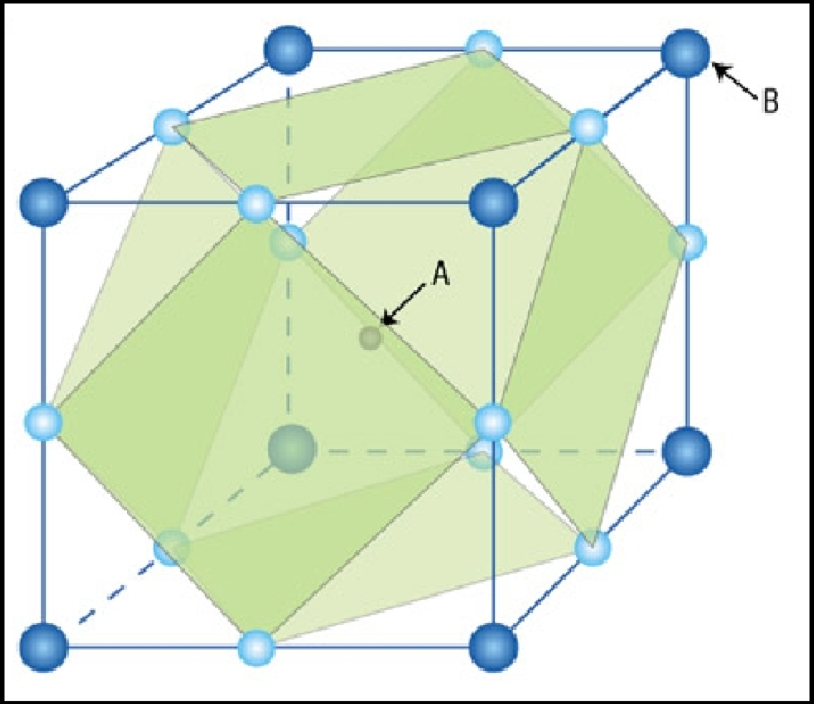
Piezoelectric research at USMA conducted by cadets using piezoelectric boards in an attempt to generate electricity using the natural gait of a soldier's step.



PZT Monoclinic Structure



Figures from www.nature.com



$$PbZr_{0.52}Ti_{0.48}O_3$$

Perovskite Structure ABO_3

Constitutive Equation
(Solid Mechanics – Continuum)

Hooke's Law

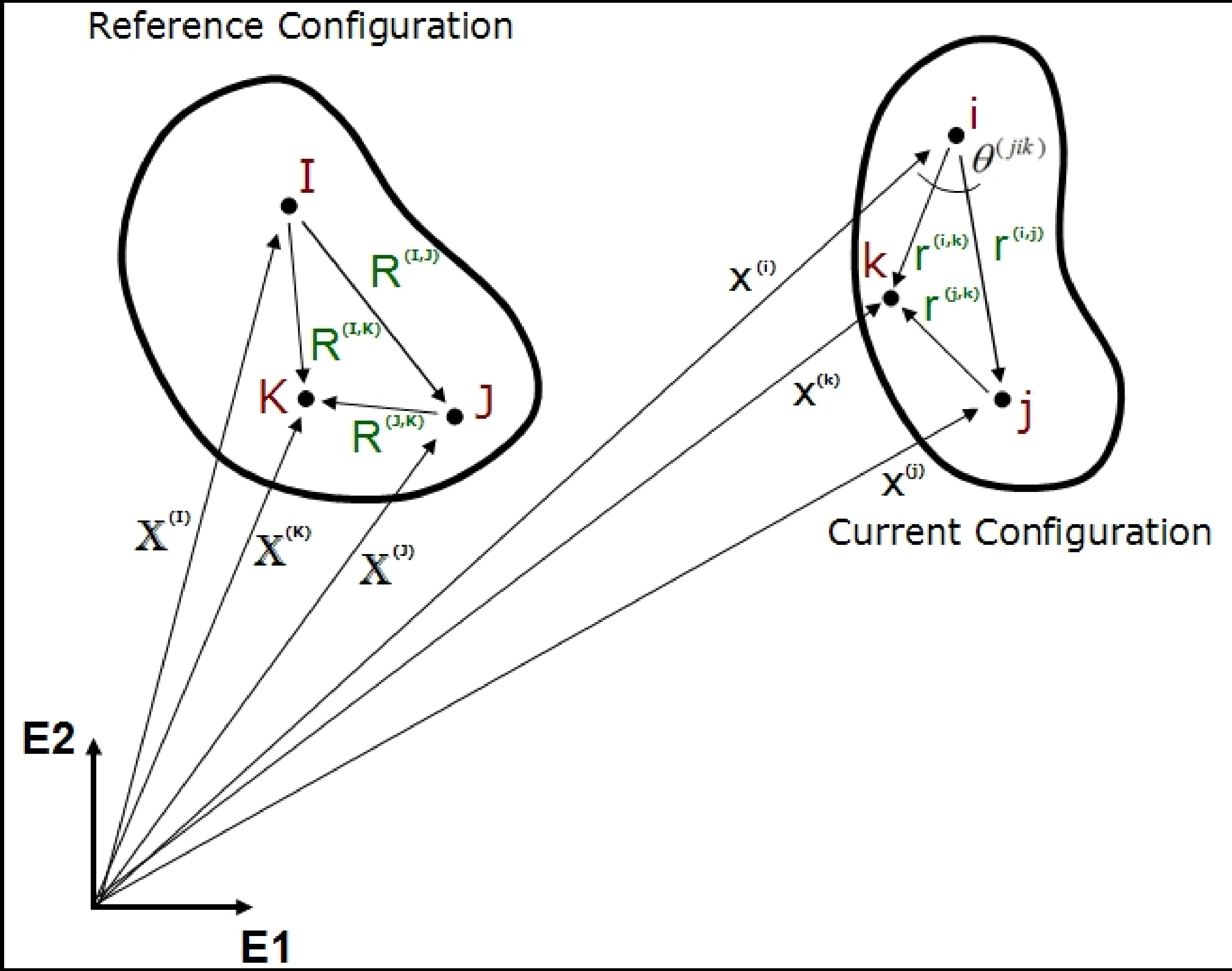
$$S_{IJ} = C_{IJKL} E_{KL}$$

Stress

Strain

Elasticity Tensor

Atomistic Position Vectors



Atomistic Elasticity Tensor

$$
\mathrm{C}_{IJKL} = \frac{\partial^2 \Phi}{\partial C_{IJ} \partial C_{KL}}
$$

Elasticity Tensor

$$
= \frac{\partial^2 \Phi}{\partial F_{mN} \partial F_{pQ}} \frac{\partial F_{mN}}{\partial C_{IJ}} \frac{\partial F_{pQ}}{\partial C_{KL}}
$$

(Chain Rule)

$$
= \left(\begin{array}{l} \dfrac{\partial^2 \Phi}{\partial r_i^{(ij)} \partial r_j^{(ik)}} \dfrac{\partial r_i^{(ij)}}{\partial F_{mN}} \dfrac{\partial r_j^{(ik)}}{\partial F_{pQ}} + \dfrac{\partial^2 \Phi}{\partial r_i^{(ij)} \partial r_j^{(ij)}} \dfrac{\partial r_i^{(ij)}}{\partial F_{mN}} \dfrac{\partial r_j^{(ij)}}{\partial F_{pQ}} \\ \qquad + \dfrac{\partial^2 \Phi}{\partial r_i^{(ik)} \partial r_j^{(ik)}} \dfrac{\partial r_i^{(ik)}}{\partial F_{mN}} \dfrac{\partial r_j^{(ik)}}{\partial F_{pQ}} + \dfrac{\partial^2 \Phi}{\partial r_i^{(ik)} \partial r_j^{(ij)}} \dfrac{\partial r_i^{(ik)}}{\partial F_{mN}} \dfrac{\partial r_j^{(ij)}}{\partial F_{pQ}} \end{array} \right) \frac{\partial F_{mN}}{\partial C_{IJ}} \frac{\partial F_{pQ}}{\partial C_{KL}}
$$

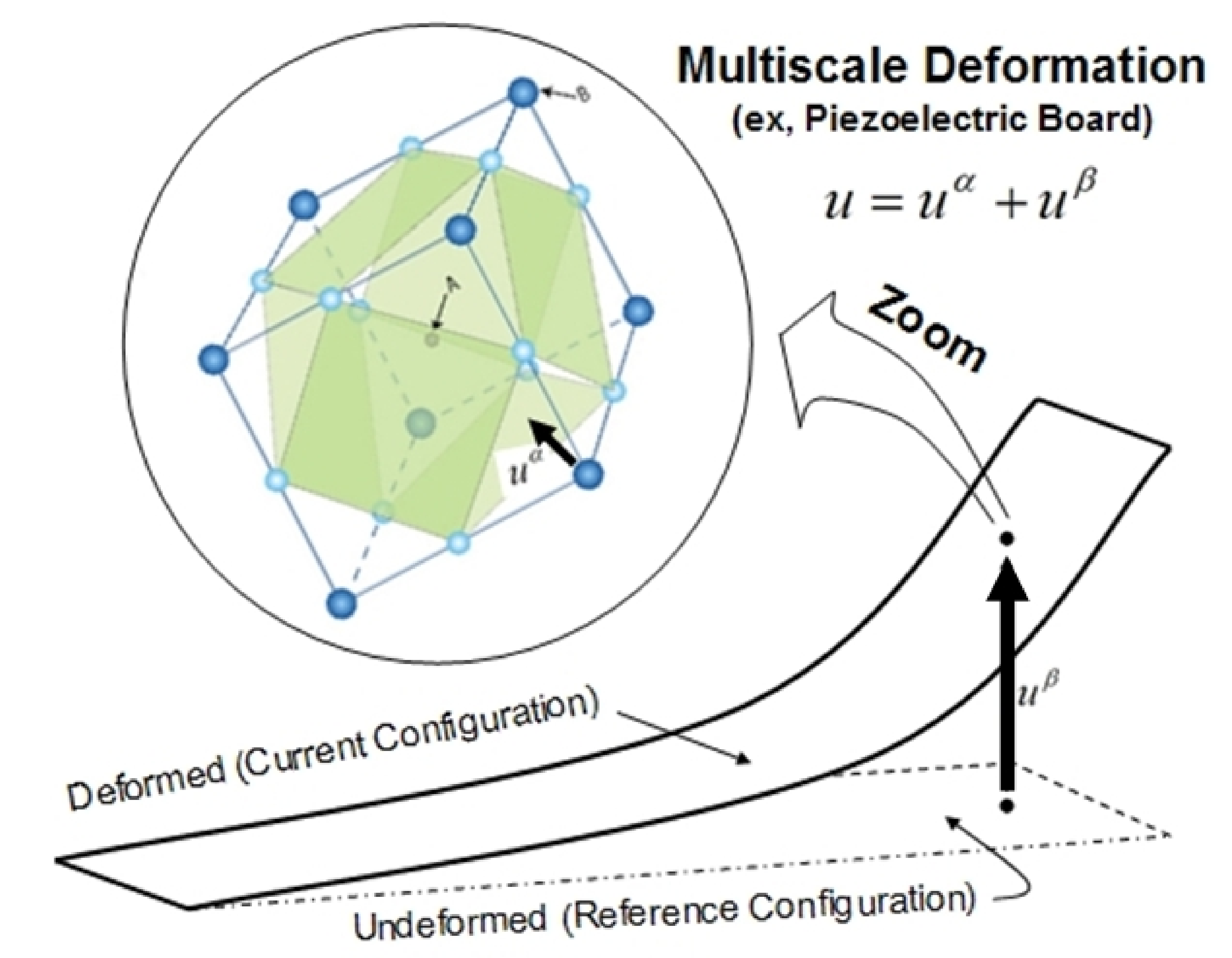
$$
\phi = \sum_{\substack{i,j \\ i<j}} v_2(r_{(ij)}) + \sum_{\substack{i,j,k \\ i<j<k}} v_3(r_{(ij)}, r_{(ik)}, r_{(jk)})
$$

Potential Function

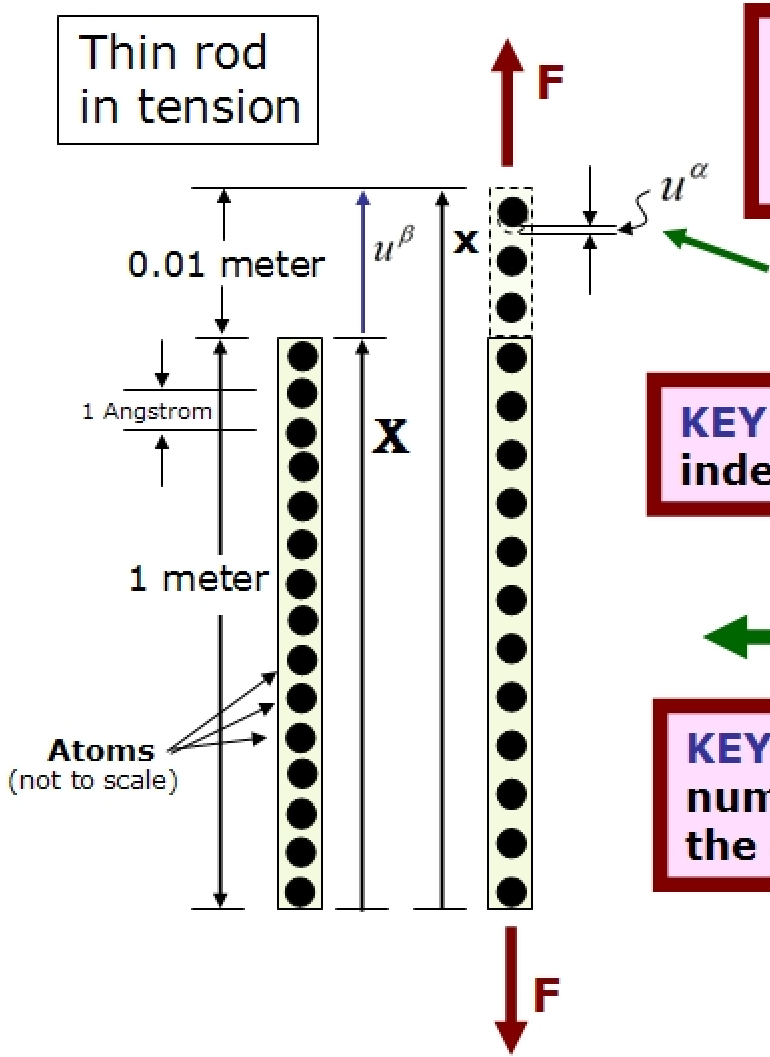
$$
(\mathbf{r})_i = (\mathbf{FR})_i = r_i = \sum_I F_{iI} R_I = F_{iI} R_I
$$

Cauchy-Born Rule

Multiscale Deformation



Multiscale Deformation



KEY POINT #1: The magnitude of u^α is on the Angstrom scale. The magnitude of u^β is on the meter scale.

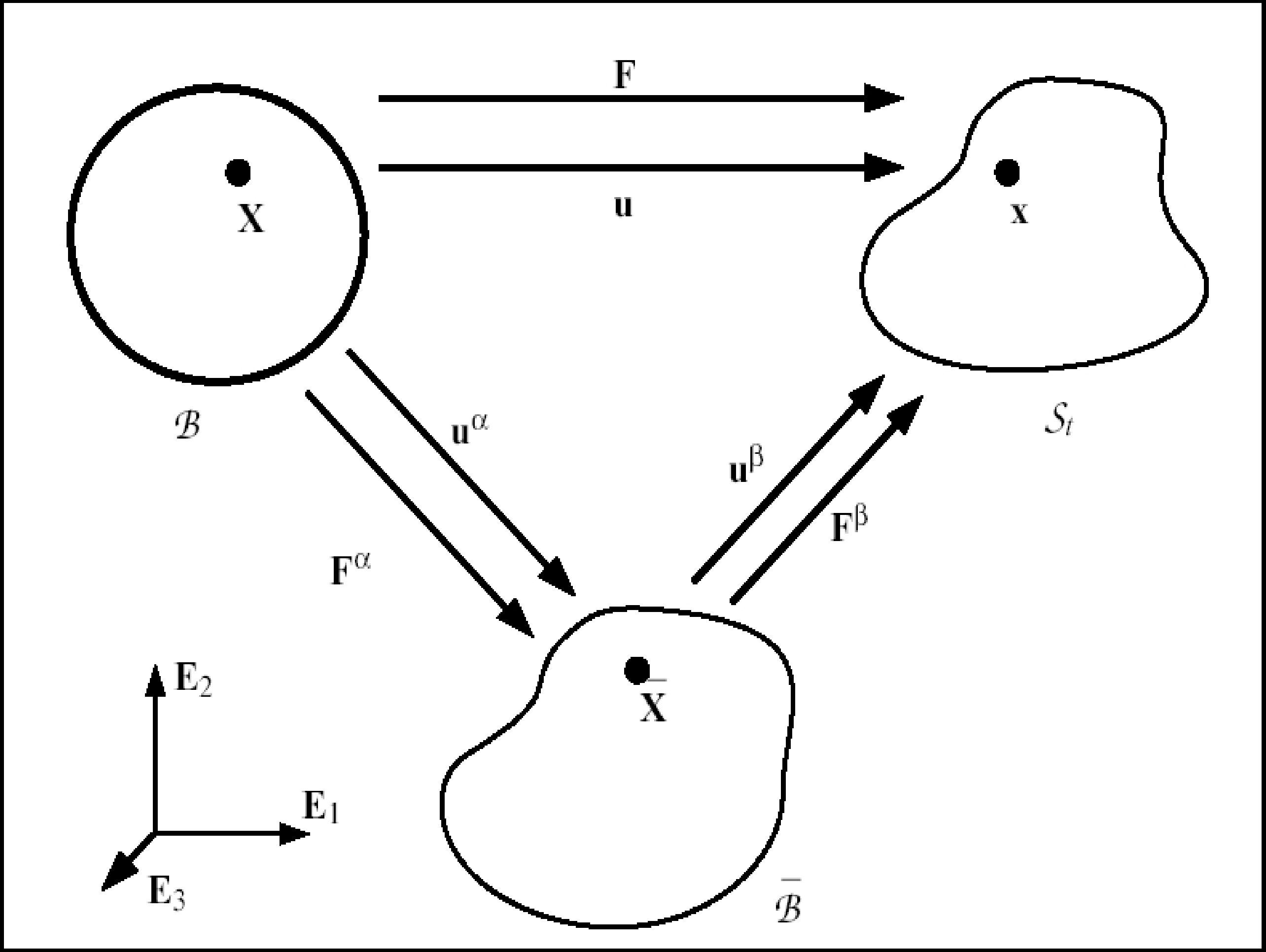
Local strain is 0.01 $\frac{\text{Angstrom}}{\text{Angstrom}}$

KEY POINT #2: Strain is scale independent. It's equal to 0.01

Global strain is 0.01 $\frac{\text{meter}}{\text{meter}}$

KEY POINT #3: An enormous number of u^α experienced by all the atoms over a region sums up to u^β .

Multiscale Kinematics



$$u = u^\alpha + u^\beta$$

$$u := x - X$$

$$u^\alpha := \bar{X} - X$$

$$u^\beta := x - \bar{X}$$

$$F = F^\beta F^\alpha$$

$$F := \frac{dx}{dX}$$

$$F^\beta := \frac{dx}{d\bar{X}}$$

$$F^\alpha := \frac{d\bar{X}}{dX}$$

Pertinent Equations

Conservation of Linear Momentum

$$\nabla \cdot \sigma(u^{\alpha}, u^{\beta}) + b = \rho \frac{d^2 u^{\beta}}{dt^2}$$

$$\sigma = \frac{1}{J} F^{\beta} S F^{\beta^T}$$

Hooke's Law

$$S = C : E^{\beta}$$

Lagrange Strain

$$E^{\beta} = \frac{1}{2}\left(F^{\beta^T} F^{\beta} + I\right)$$

$$F^{\beta}(u^{\alpha}, u^{\beta}) = I + \frac{\partial u^{\beta}}{\partial \overline{X}} \left(\frac{\partial u^{\alpha}}{\partial X}\right)^{-1}$$

Newton's 2nd Law

$$F = m\ddot{u}^{\alpha}$$

$$F = q_o E$$

Coulomb's Law

$$F = \frac{1}{4\pi\varepsilon_o} \frac{q q_o}{r^2}$$

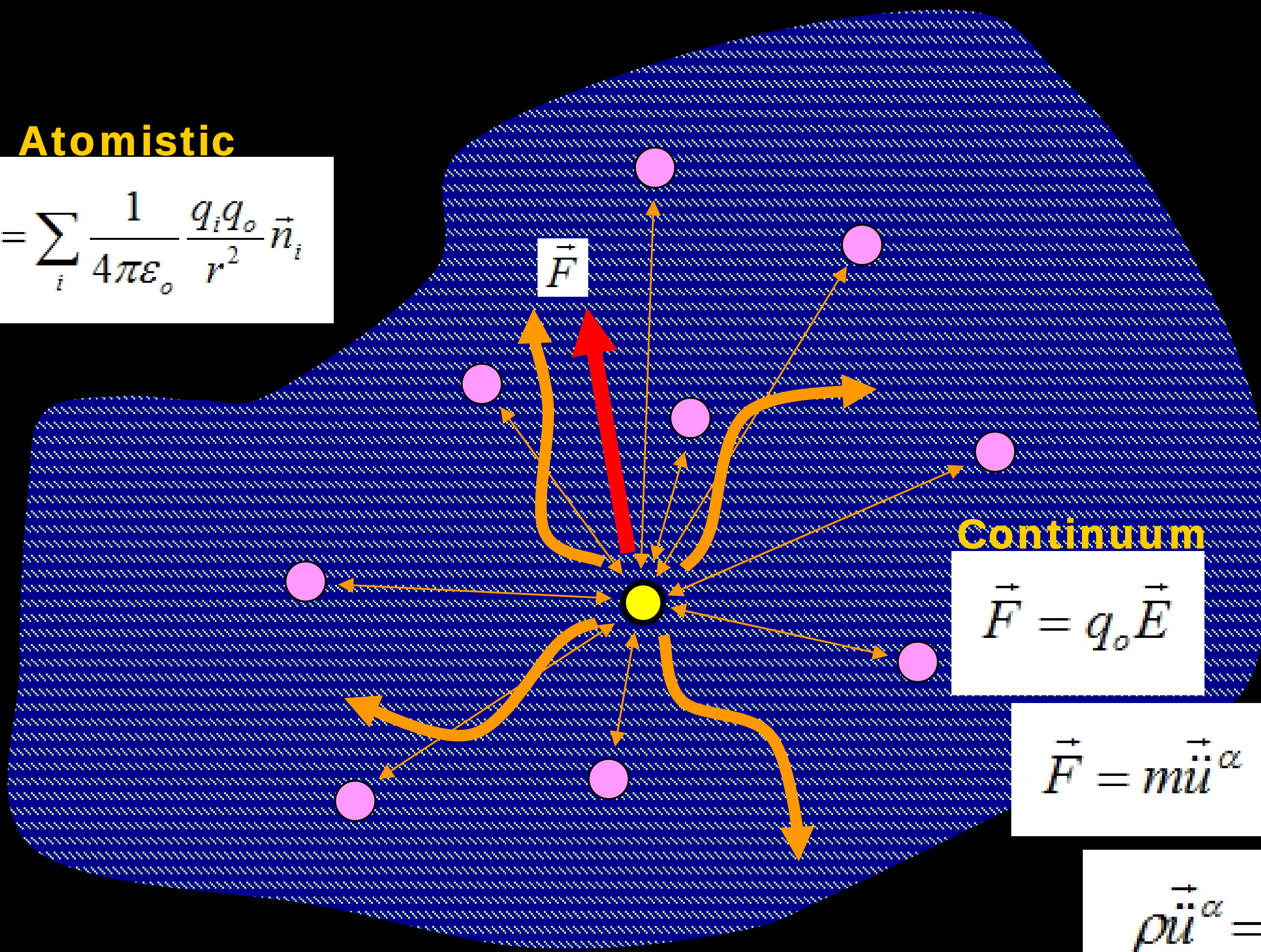
Gauss's Law

$$\varepsilon_o \oint E \cdot ds = q$$

Charges and Electric Field

Atomistic

$$\vec{F} = \sum_i \frac{1}{4\pi\varepsilon_o} \frac{q_i q_o}{r^2} \vec{n}_i$$



Continuum

$$\vec{F} = q_o \vec{E}$$

$$\vec{F} = m\ddot{\vec{u}}^{\alpha}$$

$$\rho\ddot{\vec{u}}^{\alpha} = \frac{q_o}{V}\vec{E}$$

Variational Multiscale Equations

$$\mathcal{G}_1 := \int_{S_t} \nabla w^{\beta} : \sigma(u^{\alpha}, u^{\beta}) dS_t - \int_{S_t} (w^{\beta} \cdot b) dS_t - \int_{\partial S_t} (w^{\beta} \cdot t) d\partial S_t - \int_{S_t} (w^{\beta} \cdot \rho \ddot{u}^{\beta}) dS_t = 0$$

Unknowns $\{u^{\alpha}, u^{\beta}\}$

$$\mathcal{G}_2 := \int_{S_t} w^{\alpha} \cdot (\rho \ddot{u}^{\alpha} - \tilde{q} E) dS_t = 0$$

Unknowns $\{u^{\alpha}, E\}$

$$\mathcal{G}_3 := \int_{S_t} w^{E} \cdot \left(\frac{1}{\mu} \nabla \times \nabla \times E \right) dS_t + \int_{S_t} w^{E} \cdot \left(\varepsilon \ddot{E} + \gamma \dot{E} \right) dS_t = 0$$

Unknowns $\{E\}$

Questions?