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UNIVERSITY

## **Bridging of the Scales, Multiscale Modeling & Simulation of Uncertain Archetype Motion**

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### **Stochastic Multiscale Analysis Workshop**

Banff, Canada

March 27 – April 1, 2011

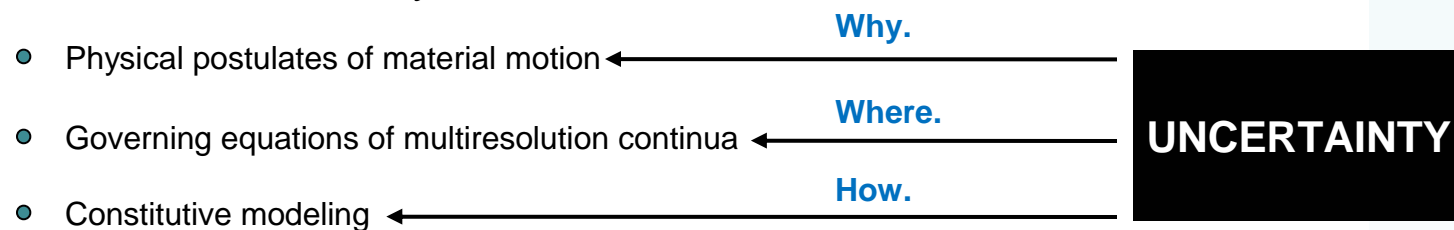
# Outline

## ■ Overarching Theme

## ■ Current research projects

- Digital 3D, design of high strength alloys. Transportation application.
- Polymer nanocomposite design. Transportation and military applications.
- Microsystem gyroscope design. Deep space application.
- Post-yield bone mechanics. Clinical application.
- Nanomedicine delivery and diagnostic mechanics. Medical application.

## ■ Mathematical machinery

- Physical postulates of material motion ← **Why.**
  - Governing equations of multiresolution continua ← **Where.**
  - Constitutive modeling ← **How.**
- 
- UNCERTAINTY**

## ■ Discussion

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## □ Mathematical machinery

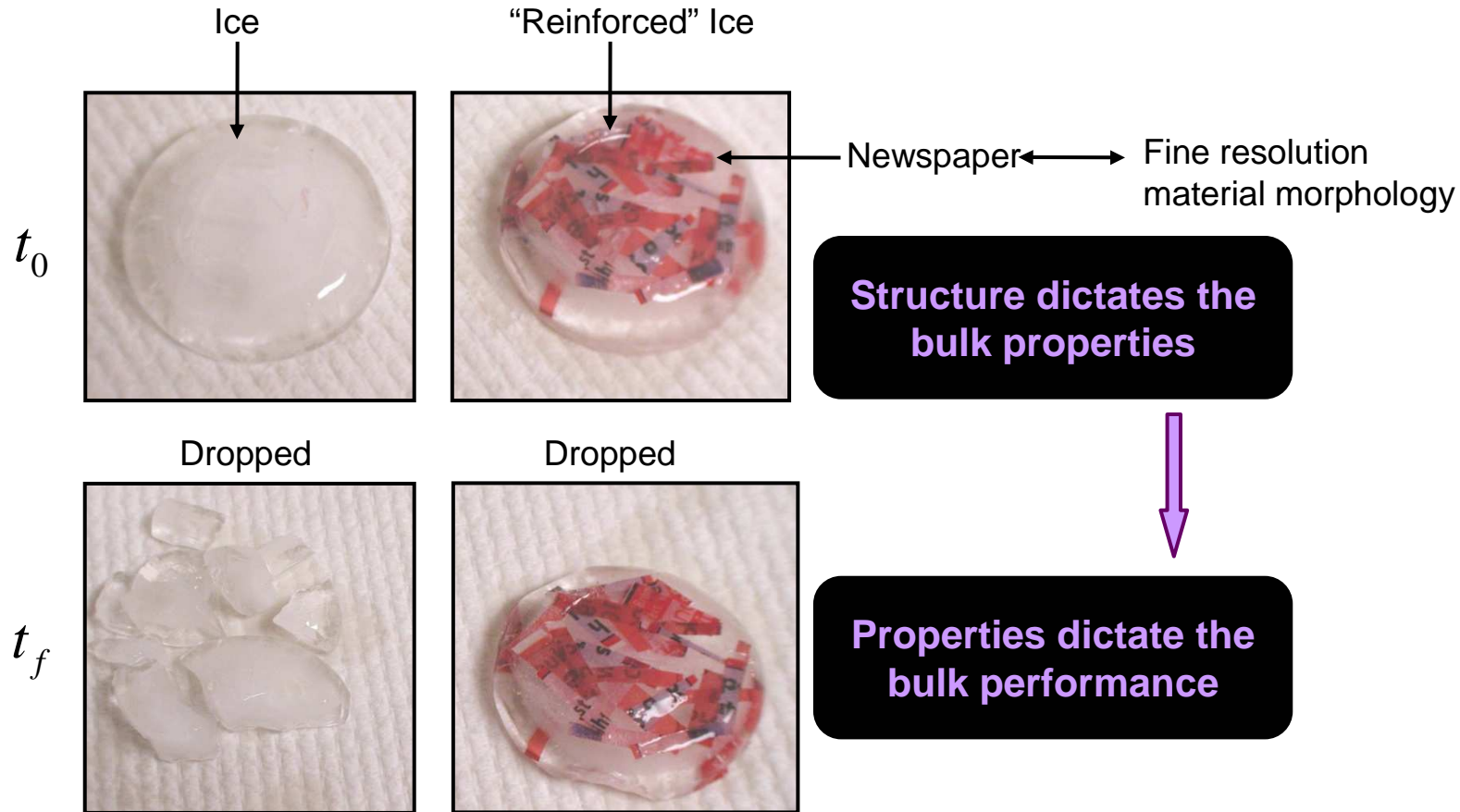
- Physical postulates of material motion ← **Why.**
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- Constitutive modeling ← **How.**

**UNCERTAINTY**

## □ Conclusions

# Multiresolution Mechanics of Materials. Why Important?

## A Macroscale Demonstration



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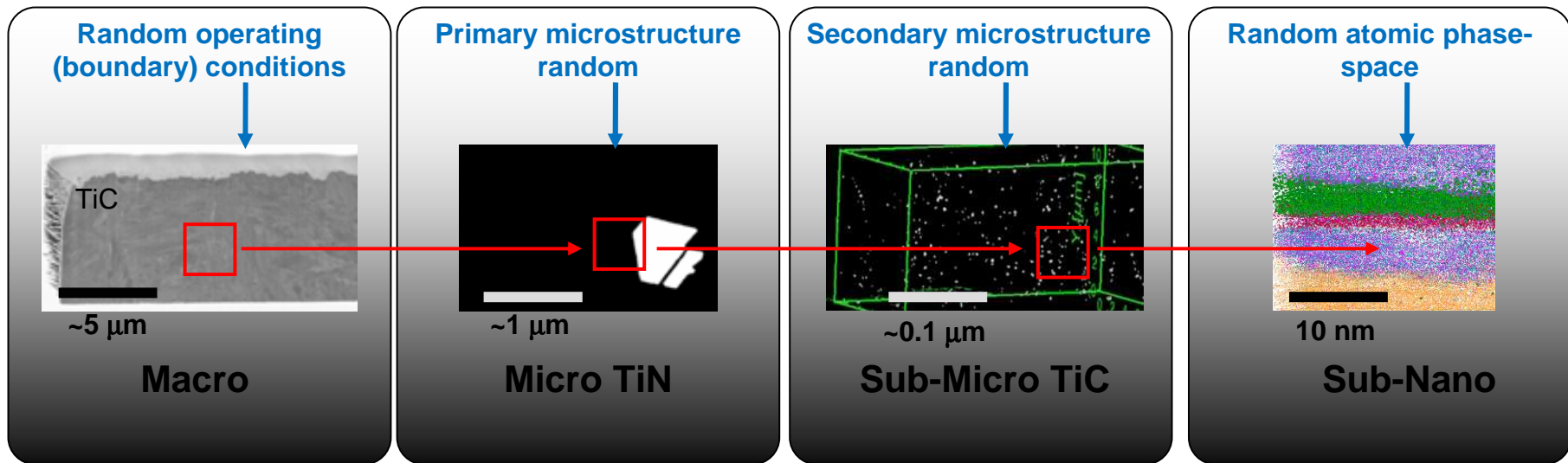
- Physical postulates of material motion ← Why.
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- Constitutive modeling ← How.

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## ☐- Conclusions

# High Strength Steel Alloy Design

- **Goal.** Deliver high strength steels for transportation applications
- **Schedule.** 2005--2010 and beyond
- **Collaborators.** *Multiple* faculty at *multiple* universities with *multiple* industry/public entities.



Increasing resolution, decreasing spatial scale, increasing uncertainty

Small Number of degrees of freedom – suitable for average behavior

Discrete behavior of TiN primary inclusions begins to be observed

Discrete behavior of TiC secondary particles is observed

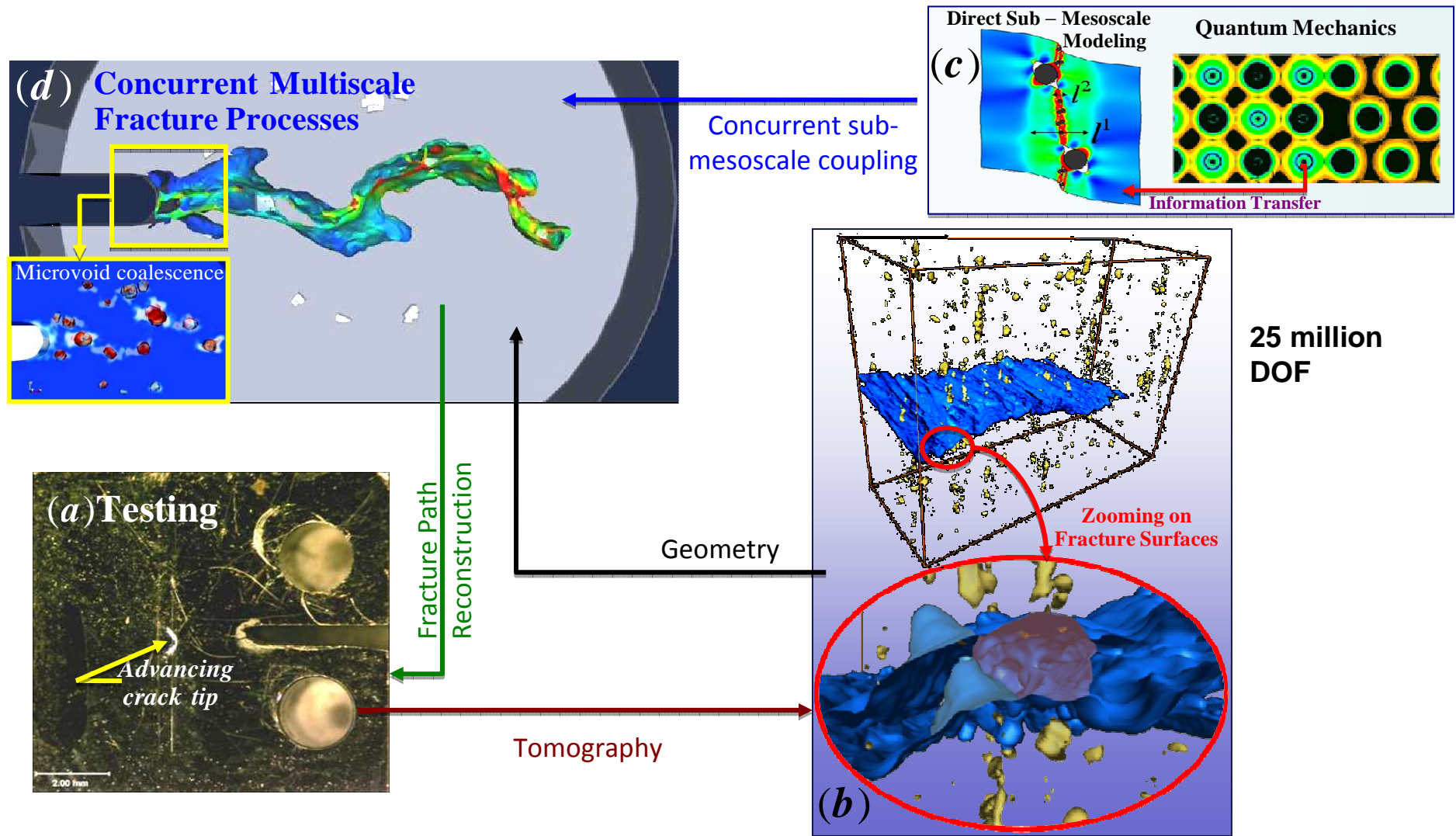
Very fine resolution – material interface is observed

- True system size: 10,000 secondary particles, 1,000 primary particles, **>1 billion DOF**
- Feasible system size: 115 primary particles, **>25 million DOF**

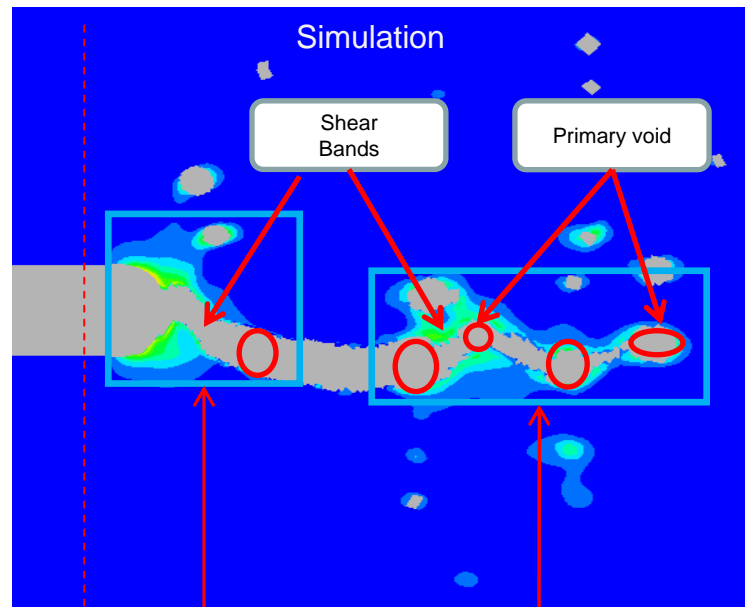
# High Strength Steel Alloy. Fracture Process Prediction

Tian et al simulation of ductile fracture process

Predictive multiscale modeling of microstructured alloy aims to increase toughness without sacrificing performance (strength and weight) for transportation applications



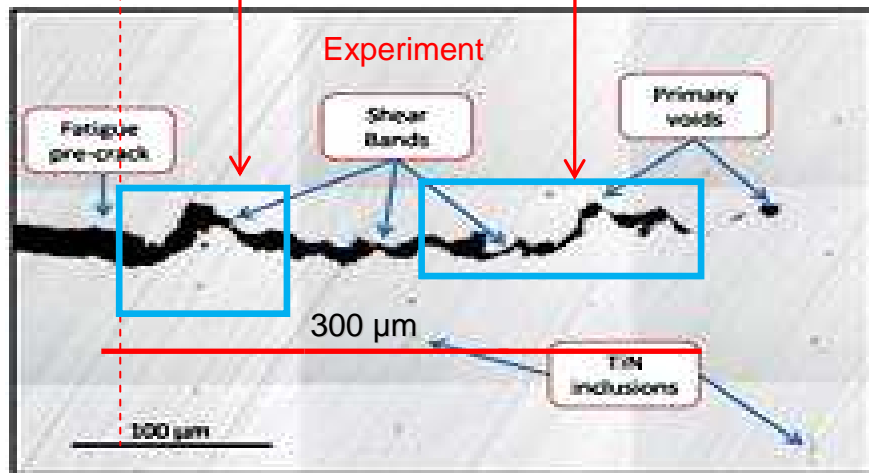
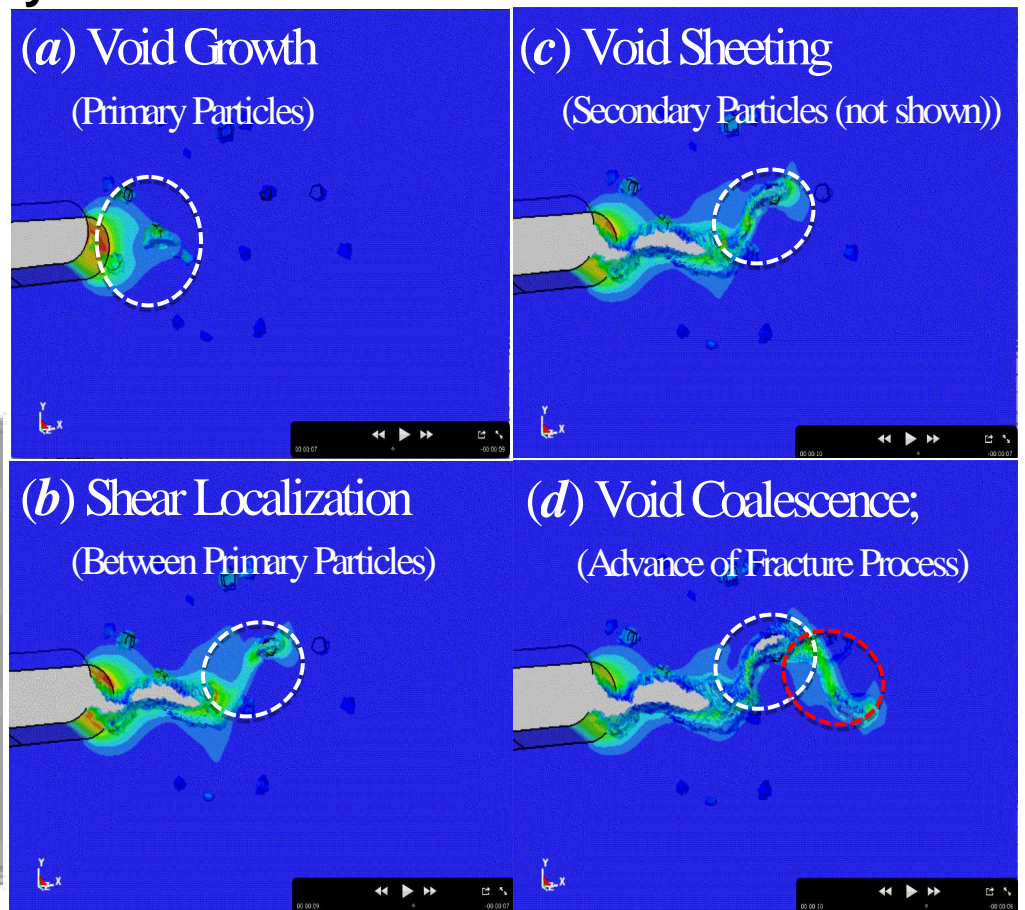
# High Strength Steel Alloy. Validation with Experiments



## 115 primary particles

- Notch size
- Features of zig-zag pattern are captured
- Experiments has more zig-zags

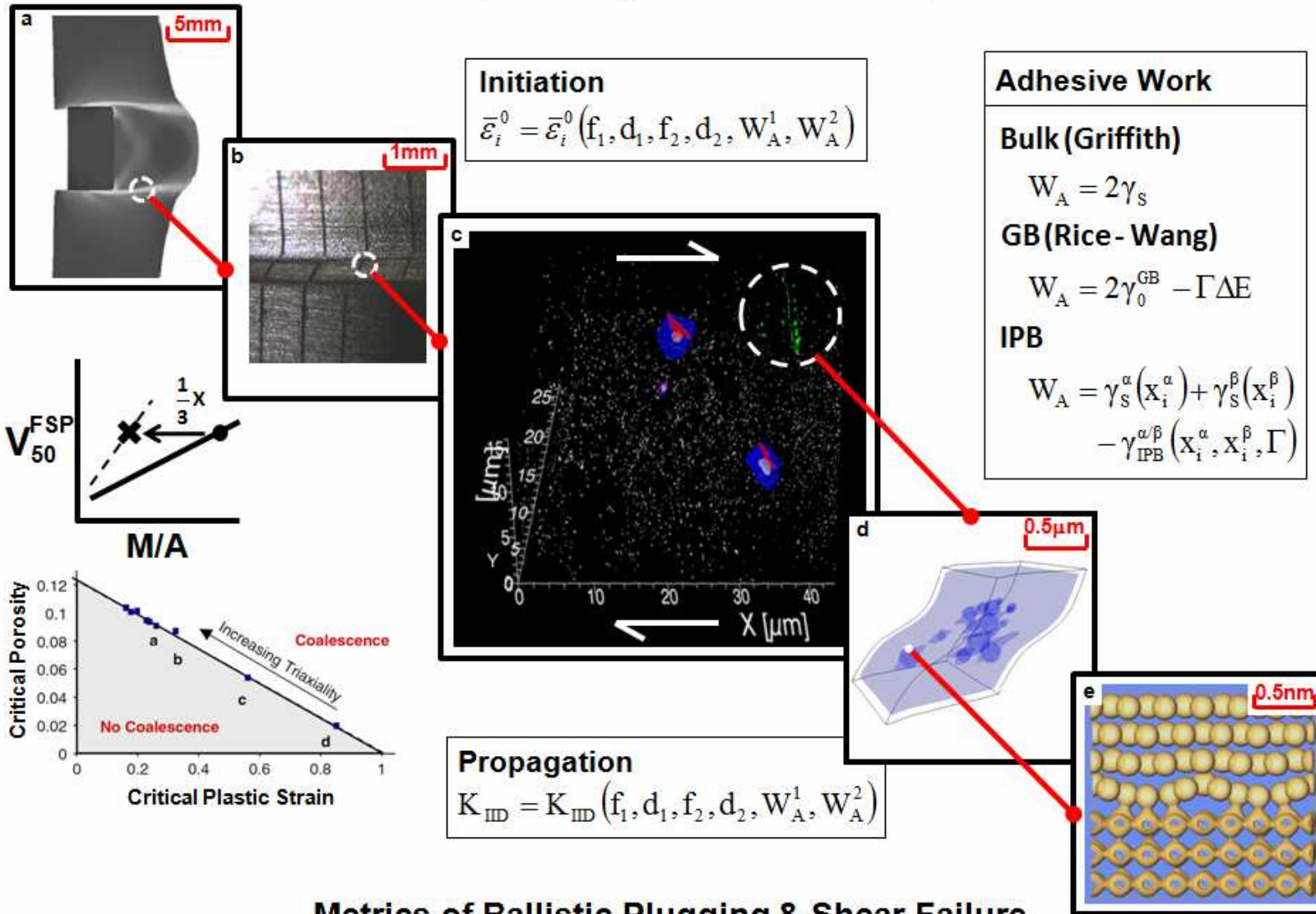
## Physics of Reconstruction of Fracture Process





# Design of High Strength Steel Alloy. Ballistic Protection & Dynamic Fracture

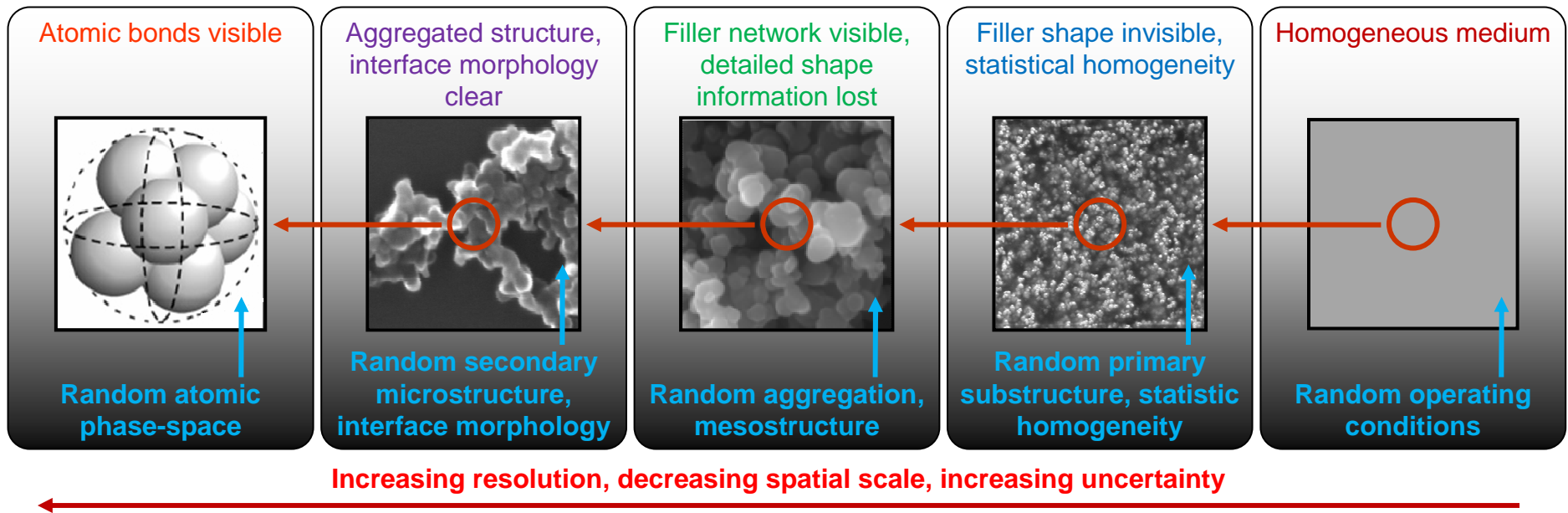
Performance  $\Rightarrow$  Properties  $\Rightarrow$  Structure



Metrics of Ballistic Plugging & Shear Failure

# Polymer Nanocomposite Material Design

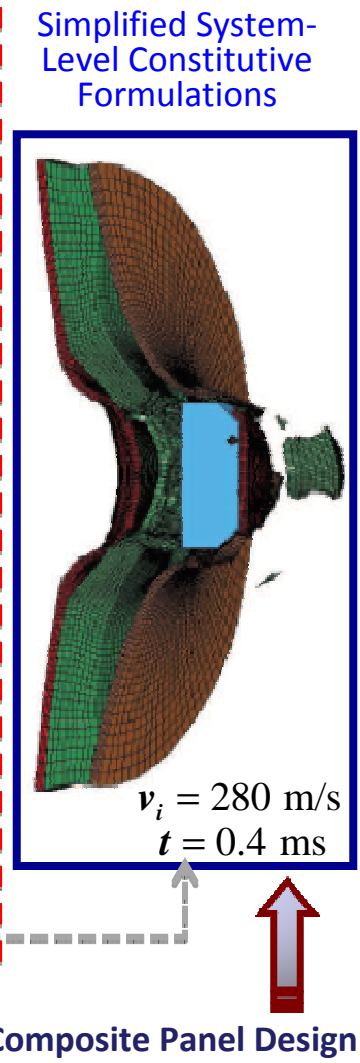
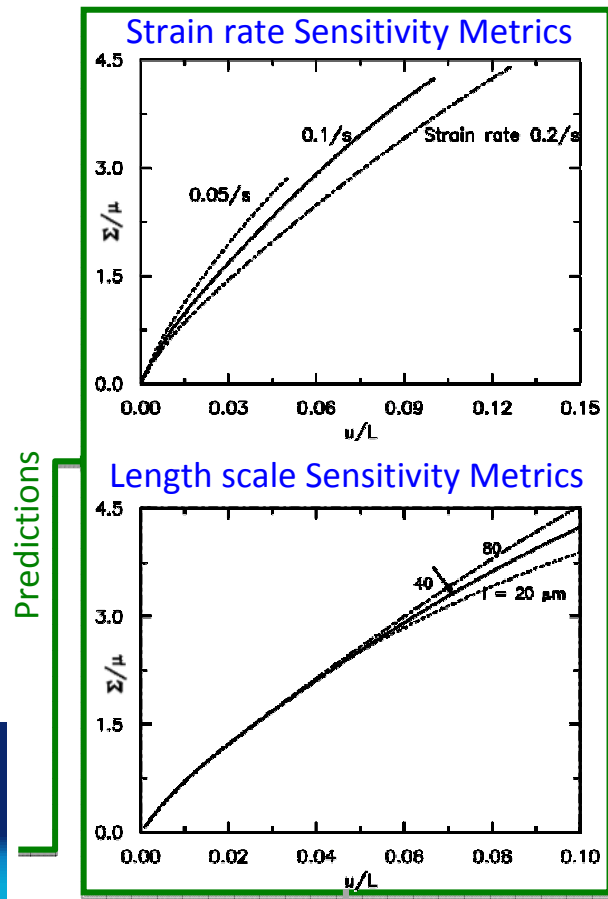
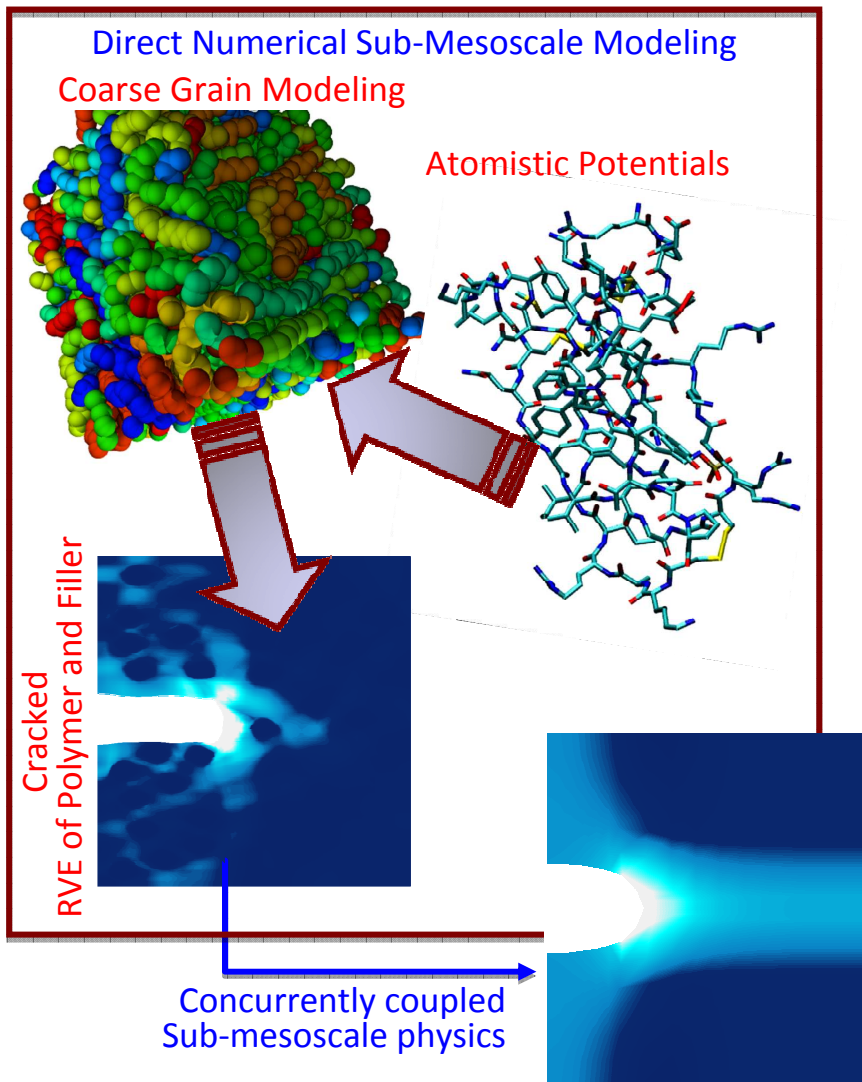
- **Goal.** Increase transportation materials performance (1), ballistic protection (2), and fracture toughness (3)
- **Schedule.** 2008-current
- **Collaborators.** 5 faculty at NU, Prof. Kruger ETH Zurich, Goodyear Tire & Rubber Co, ARO, NSF



- *True* system size: ~1000 particles, >**1.2 billion** DOF
- *Feasible* system size: 40 particles, >**35 thousand** DOF
- *Multiresolution* system size: 0 particles ~**1700** DOF

# Polymer Nanocomposite Design. Energy Desipation & Dynamic Fracture

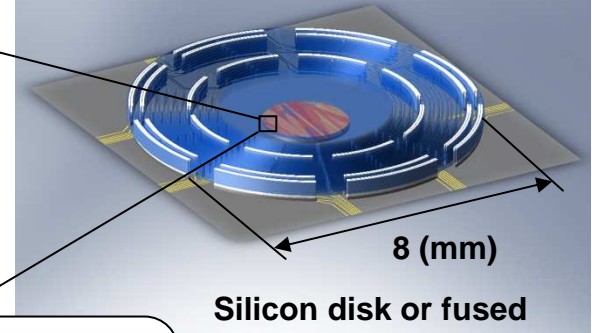
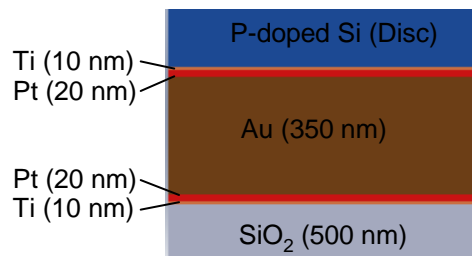
Predictive multiscale modeling of microstructured elastomer aims to guide our parallel development of system-level constitutive models to design composite sandwich plates



# Microsystem under Harsh Environment (Boeing micro-gyroscope)

- Goal. Design Boeing microsystem for harsh deep space applications.
- Schedule. 2005-2008
- Collaborators. Northwestern, Boeing

## System Description

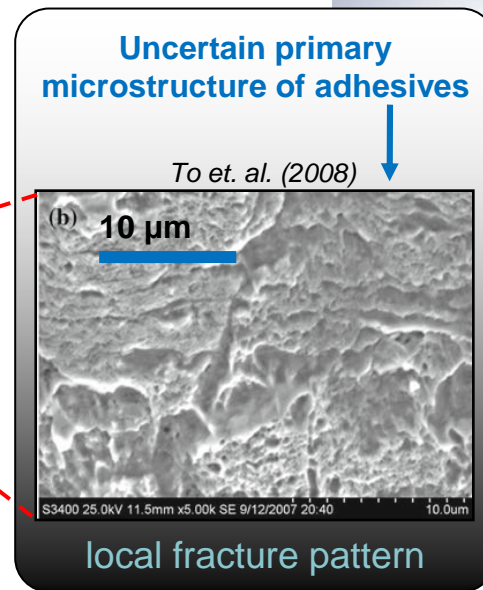
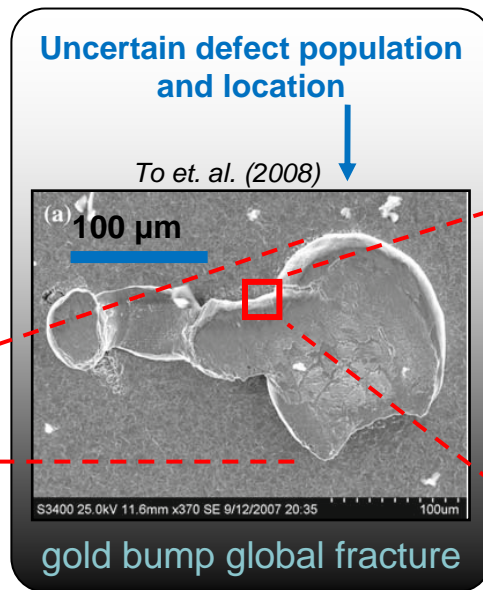
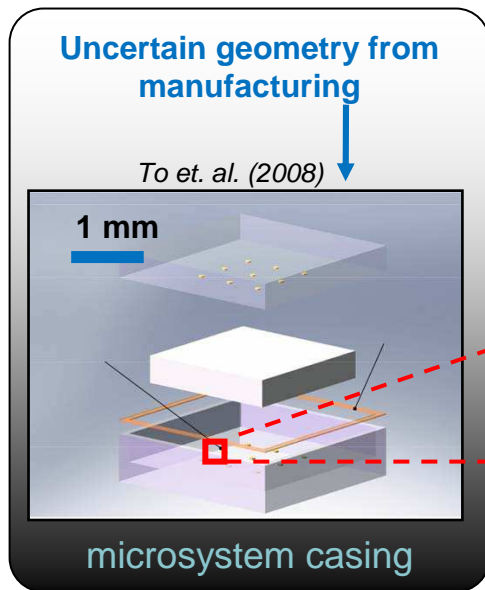


Silicon disk or fused quartz disc bonded to silicon substrate

Microsystem subjected to numerous **uncertain boundary conditions**

Aging, thermal, radiation, mechanical loading

Multiphase problem in which material structure governs phase interaction



mm

μm

nm

Increasing resolution, decreasing spatial scale, increasing uncertainty

Delamination in thermal cycling and shock

Creep

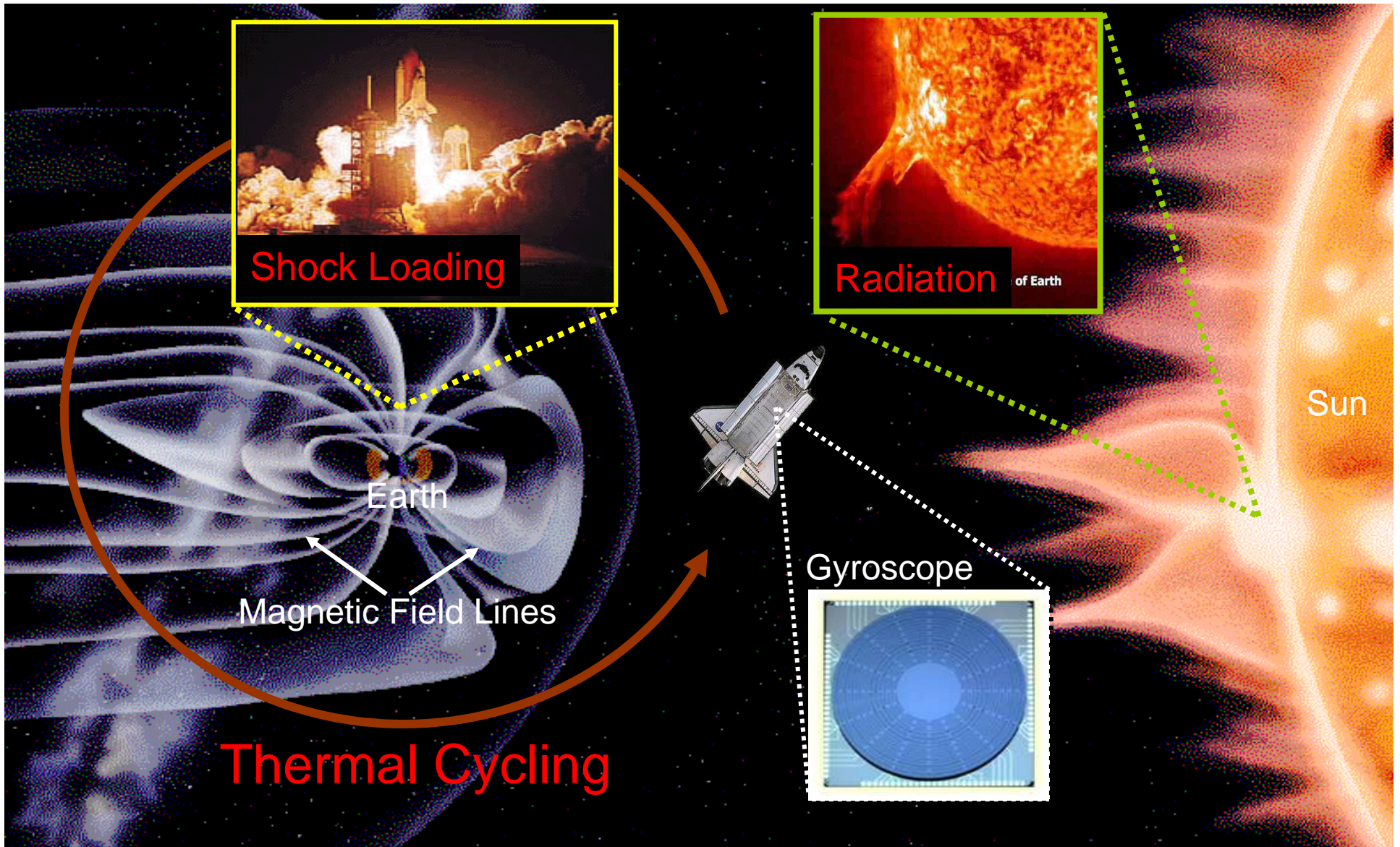
Grain boundary migration

Material interdiffusion

## Mechanisms & Phenomena

To et al (2008)

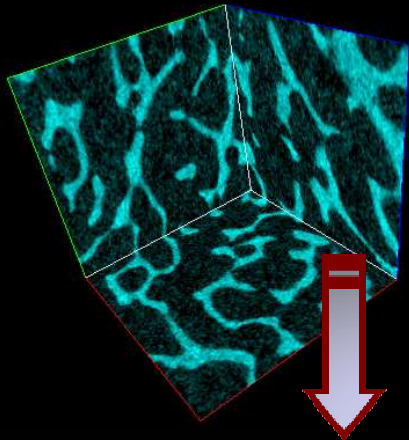
# Microsystem. Uncertain Harsh Environment!



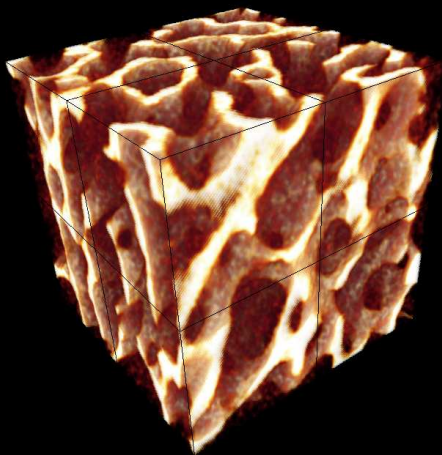
# Post Yield Bone Mechanics. Fracture Path Prediction

- *True system size*: Big bone is  $O$  (cm)
- *Feasible system size*: 3 x 3 (mm), 8 micron resolution ~20 million voxels ~22 million DOF

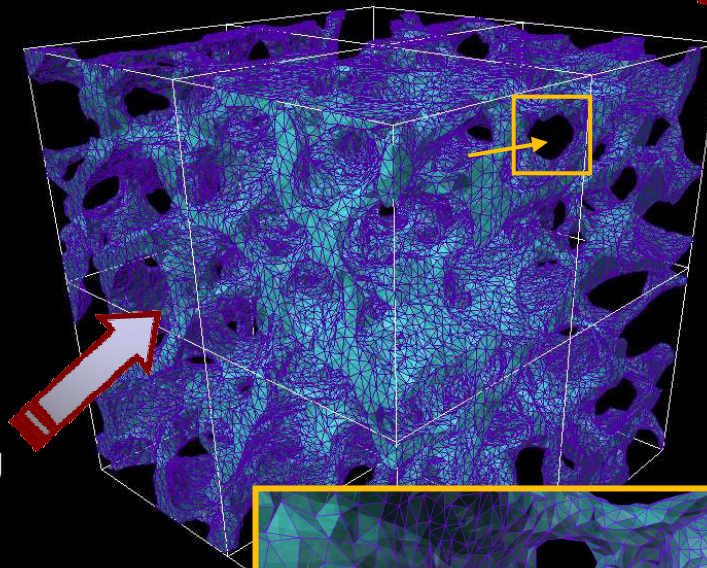
Binary image transformation



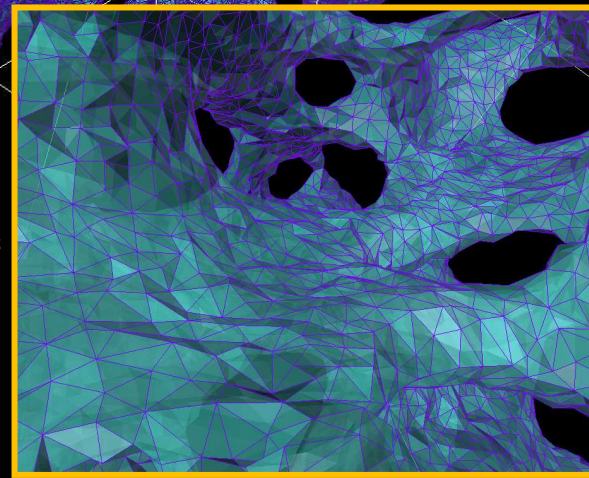
Surface identification and Rendering



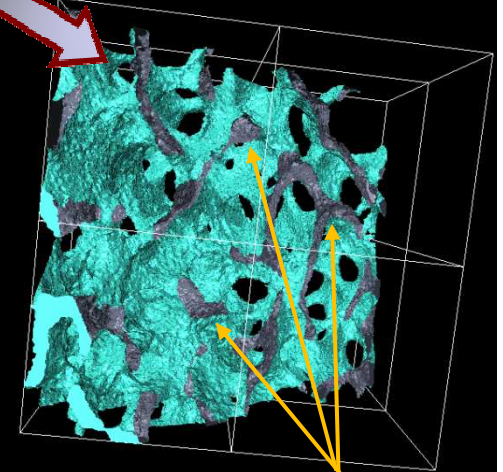
Surface and Volume Meshing



Meshed interior of connected bone structure



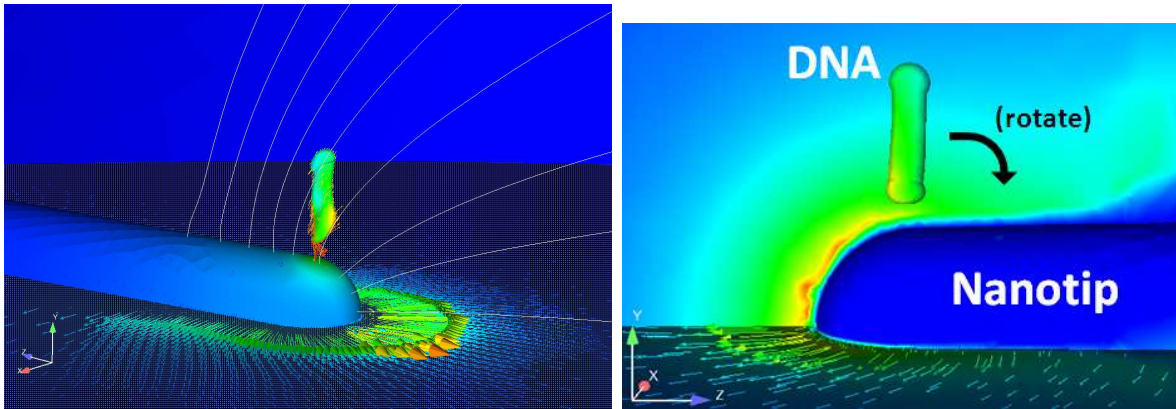
Simulation



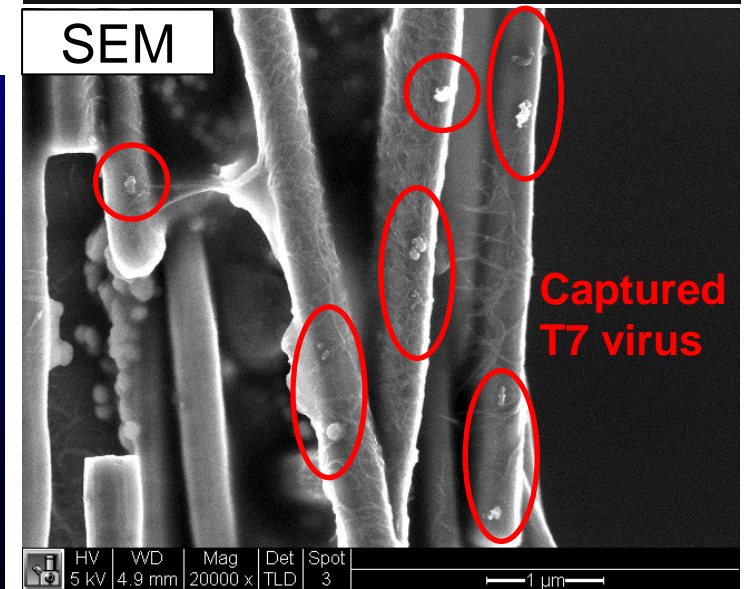
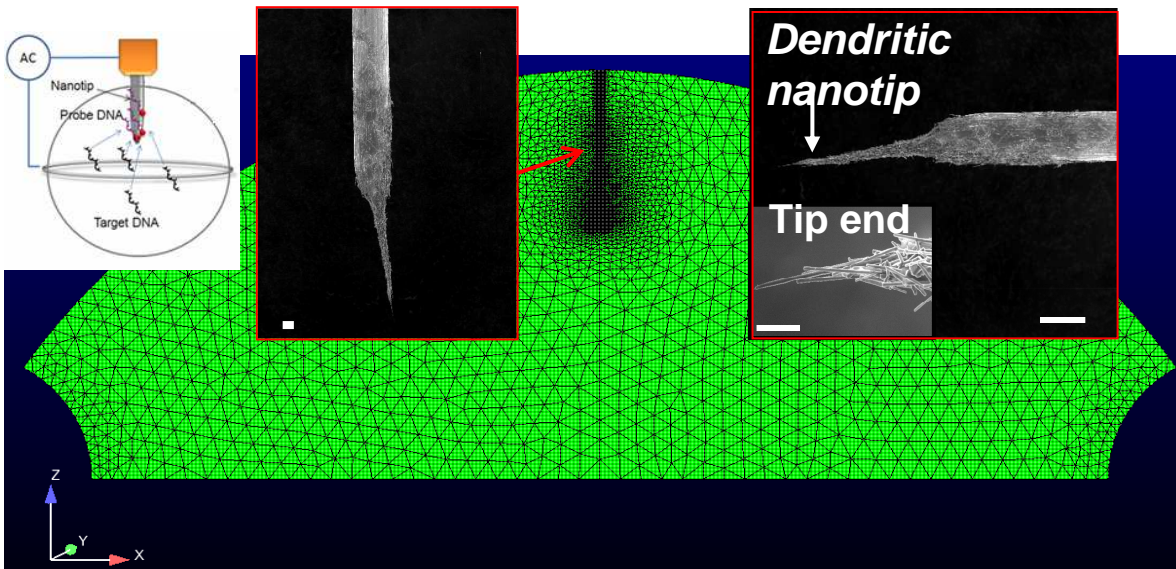
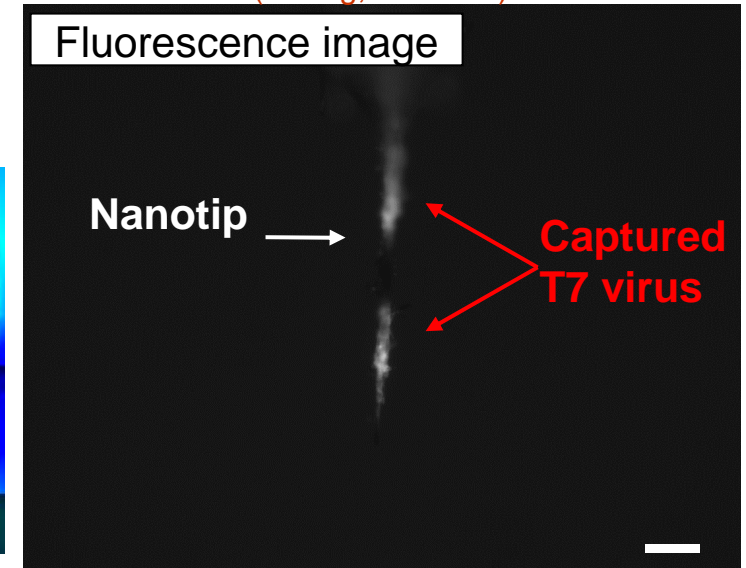
Global fracture path

# Nanotip Enrichment System for Sensing and Diagnostic

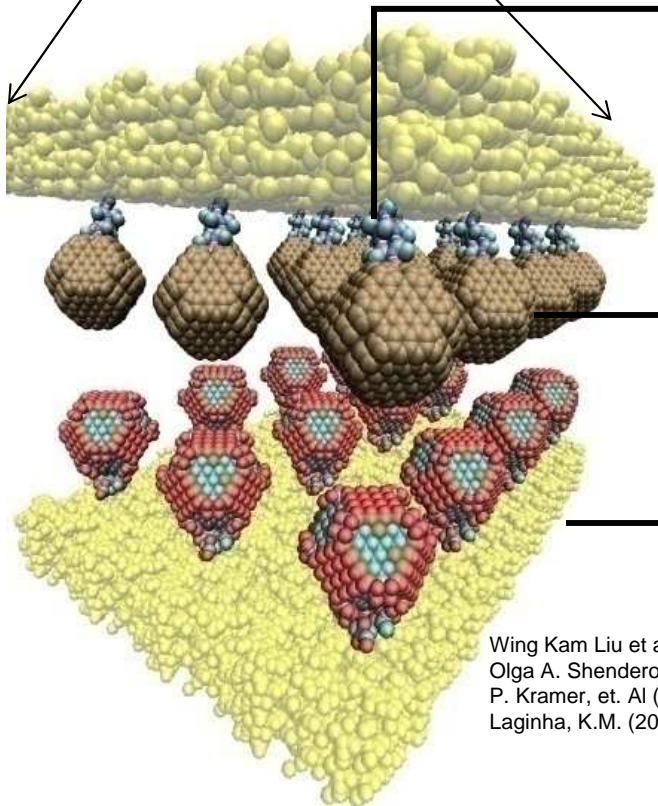
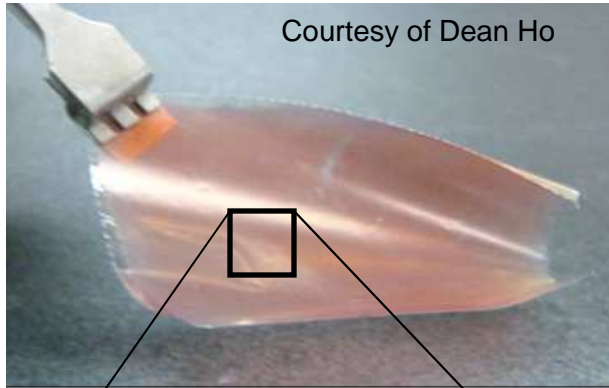
Immersed molecular electrokinetic finite element method is utilized to optimize design and determine experimental parameters for nanotip based sensor



Captured T7 virus on a nanotip  
(Chung, U. Wash)

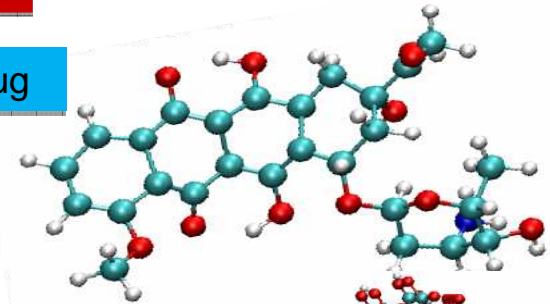


# Materials



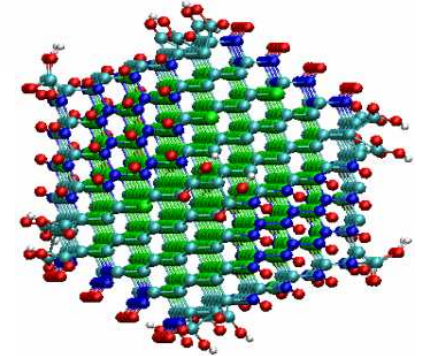
## Doxorubicin

- Anticancer Drug



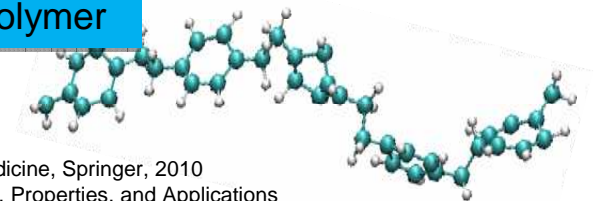
## Nanodiamond

- Drug Carrier
- 4-5 nm in dia.
- Truncated Octahedral Shape
- Graphitized Surface
- Diamond Core



## Parylene

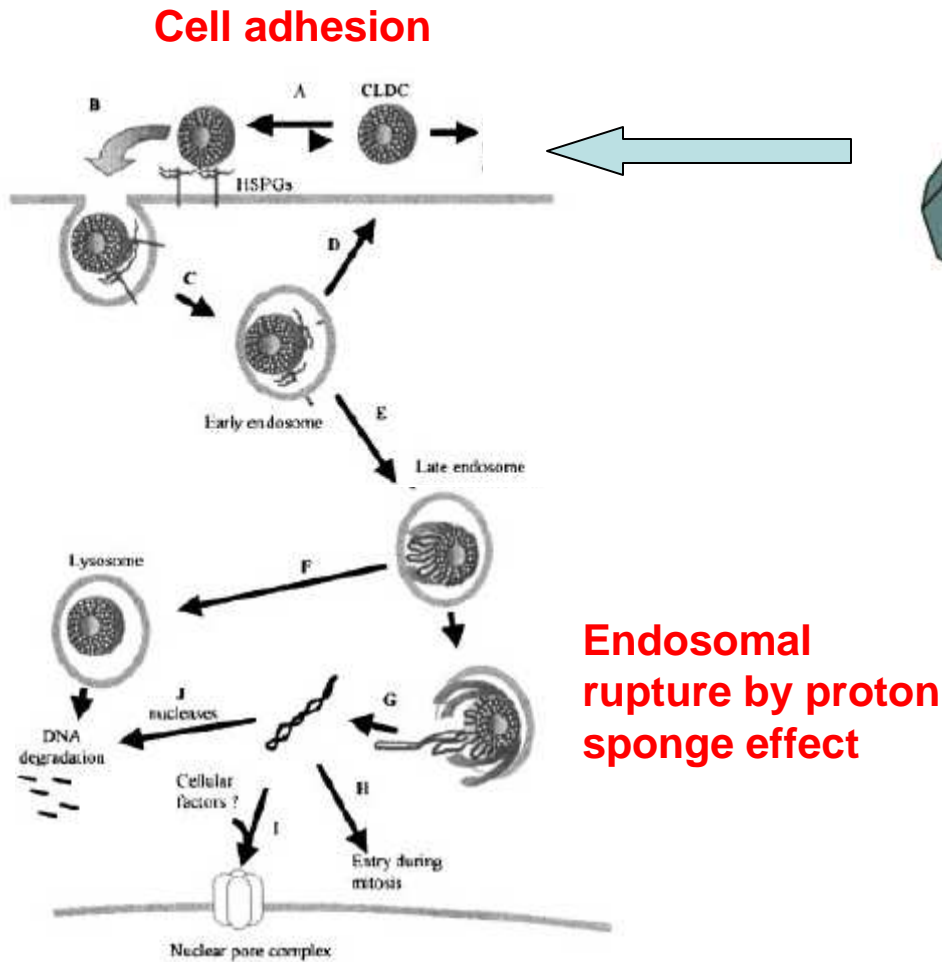
- Biocompatible Polymer



Wing Kam Liu et al. in "Nanodiamonds: Applications in Biology and Nanoscale Medicine, Springer, 2010  
Olga A. Shenderova and Dieter M. Hab, Ultrananocrystalline Diamond: Synthesis, Properties, and Applications  
P. Kramer, et. Al (2003), Journal of Polymer Science: Polymer Chemistry Edition 22 (2): 475-491.  
Laginha, K.M. (2007) Clinical Cancer Research. Vol. 11 (19).



# Extracellular and Intracellular behaviors of ND complex



## Synthesis of ND complex



## 3 important phenomena in gene delivery

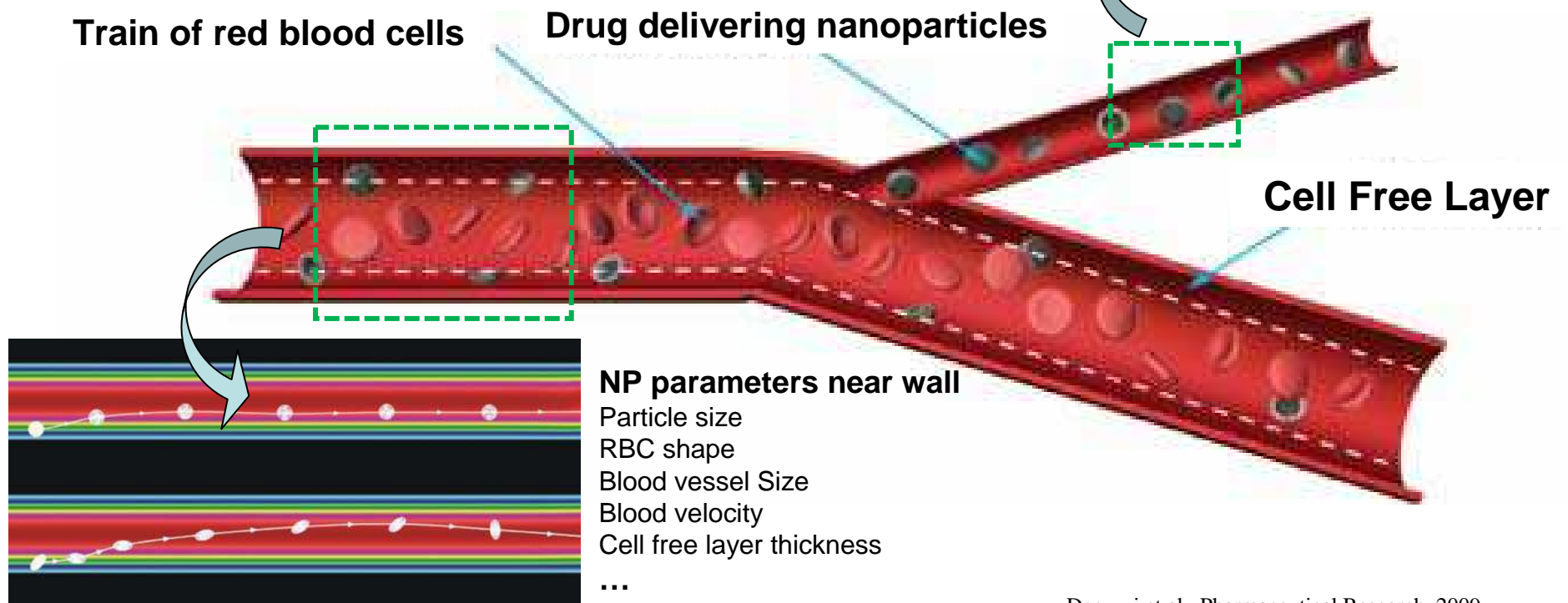
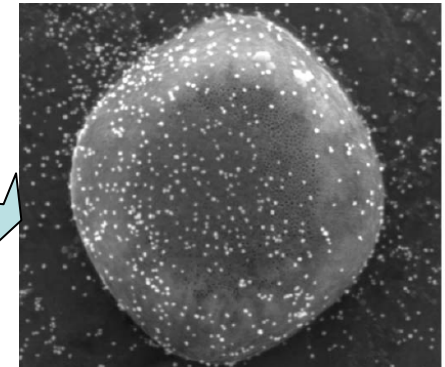
- 1) Synthesis of ND complex
- 2) Cell adhesion of ND complex (extracellular behavior)
- 3) Endosomal rupture : H<sup>+</sup> entry into the endosome leads into swelling and rupture of endosome (intracellular behavior)

Christopher M. Wiethoff, Russel Middaugh, "Barrier to Nonviral Gene Delivery", J of Pharmaceutical sciences, vol 92, No2, 2003

# Cell-Nanoparticle in blood vessel

Particles (rejected by the red blood cells)

- Tend to accumulate in close proximity to the walls (as platelets)
  - Easy to leave larger vessels in favor of the smaller.
  - High particle accumulation in the micro capillary bed
- **Nanoparticles to release drugs or therapeutic agents fast and accurately arrive at target cells.**



Decuzzi et al., Pharmaceutical Research, 2009

# Cell-Nanoparticle in blood vessel

## Basic Properties for Simulation

### RBCs

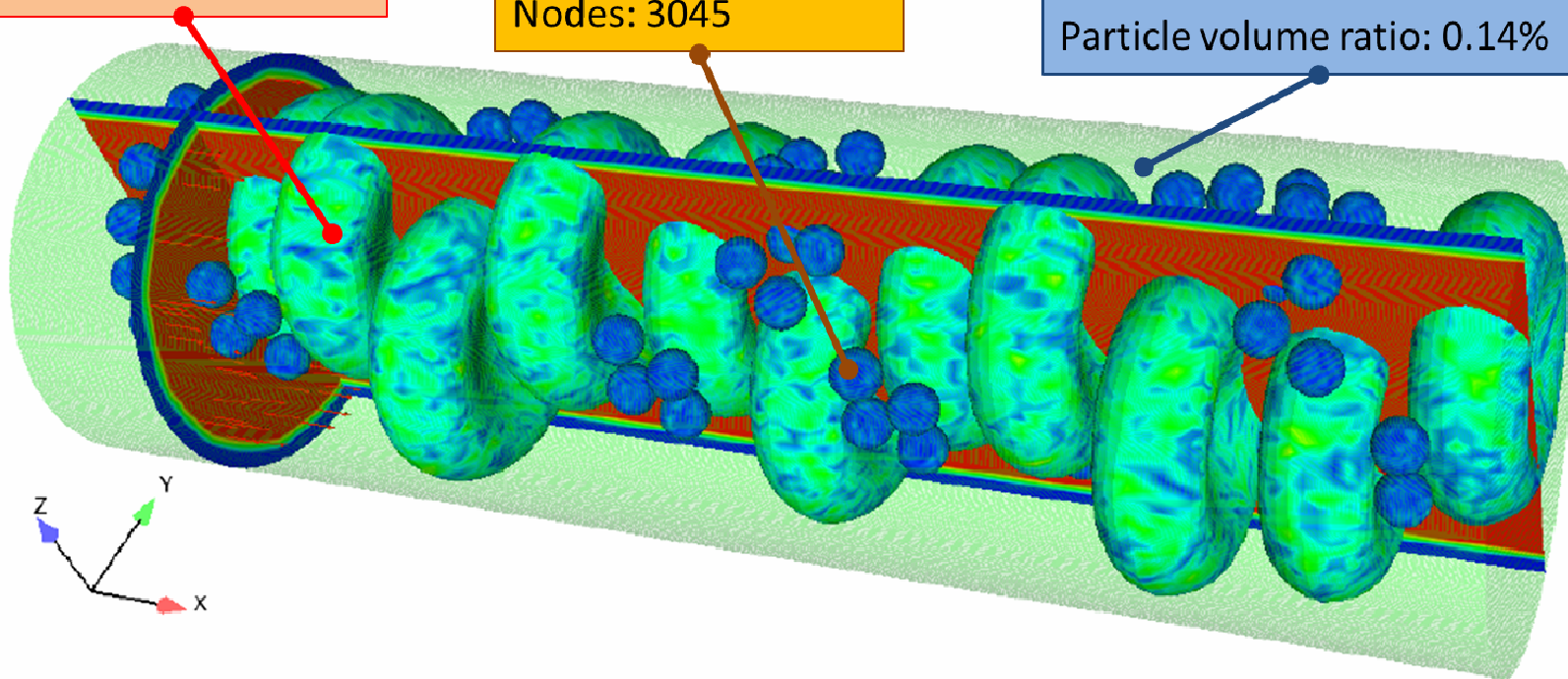
Radius:  $3\mu\text{m}$   
Width:  $2\mu\text{m}$   
Volume:  $\sim 56.55\mu\text{m}^3$   
Mesh size:  $0.2\mu\text{m}$   
Elements: 2304  
Nodes: 4612

### Particles

Radius:  $0.5\mu\text{m}$   
Volume:  $0.5249\mu\text{m}^3$   
Mesh size:  $0.1\mu\text{m}$   
Elements: 2816  
Nodes: 3045

### Channel

Radius:  $6\mu\text{m}$   
Length:  $36\mu\text{m}$   
Volume:  $4071.50\mu\text{m}^3$   
Mesh size:  $0.6\mu\text{m}$   
Elements: 21360  
Nodes: 23729  
RBC volume ratio: 15.28%  
Particle volume ratio: 0.14%



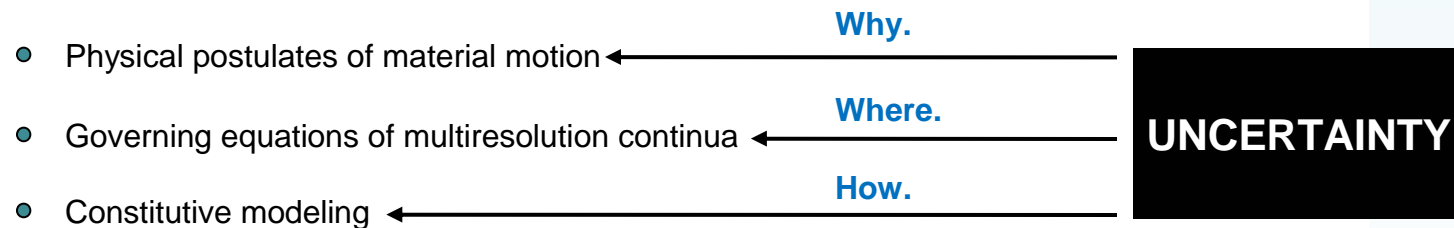
# Outline

## ☐- Overarching Theme

## ☐- Current research projects

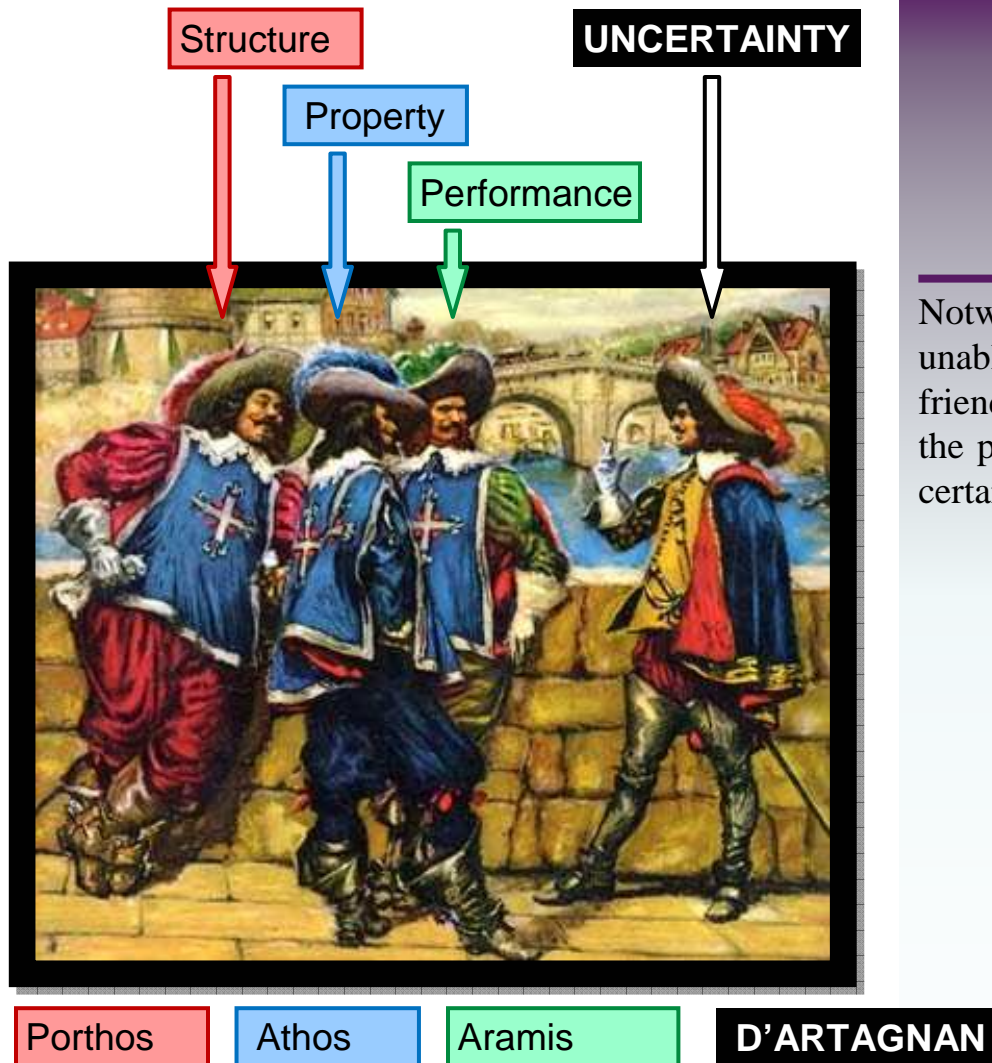
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  - Constitutive modeling ← **How.**
- 
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## ☐- Conclusions

# Overarching Theme



Notwithstanding all the pains he took, D'Artagnan was unable to learn any more concerning his three new-made friends. He formed, therefore, the resolution of believing for the present that all was said of their past, hoping for more certain and extended revelations in the future.

Alexander Dumas  
*The Three Musketeers*  
1844

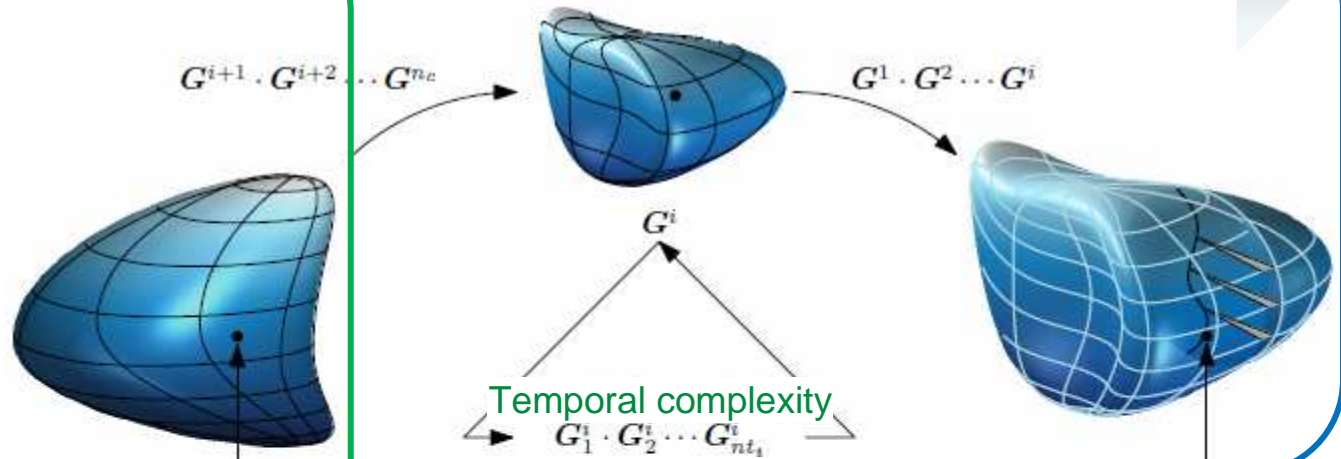
# Multiscale Machinery. Physical Postulates

Behavioral complexity

Configurational complexity

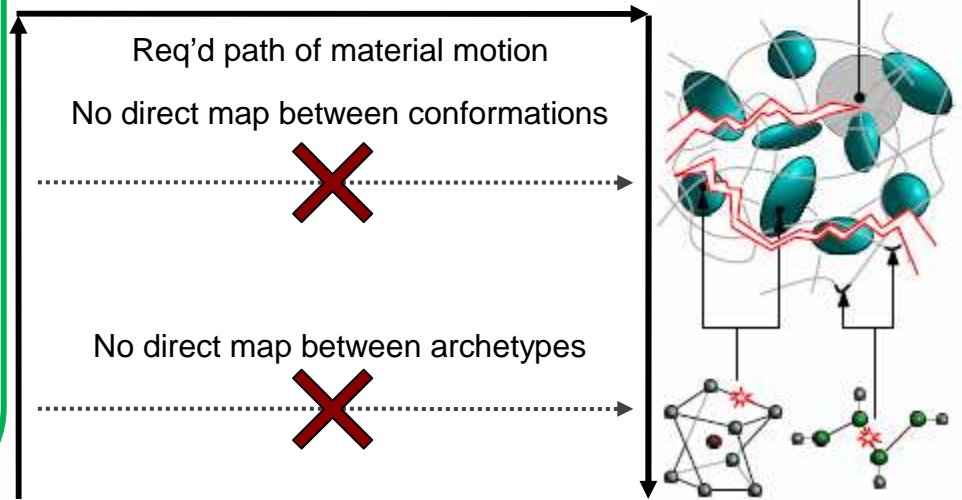
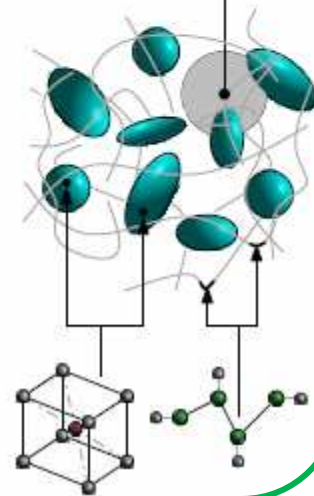
Structural complexity

Continuum configuration



Archetype conformation

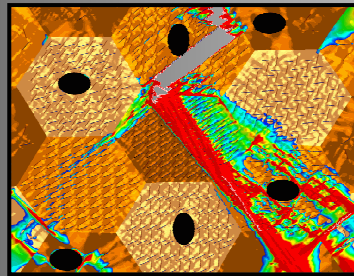
Archetype definition



# Archetypes and Conformation. Examples

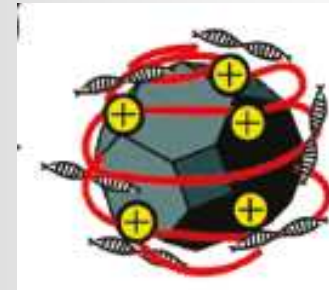
## POLYCRYSTALLINE METAL

**Hierarchy**  
of conformational  
structures



Granular structure

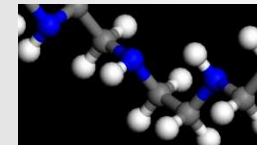
## GENE DELIVERY SYSTEM



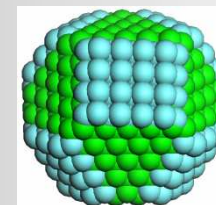
**Conformation**  
of archetypes into  
mesostructure



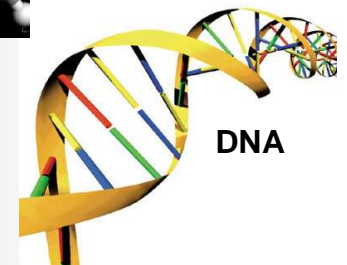
Subgranular structure



PEI

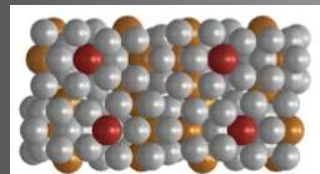


Nanodiamond

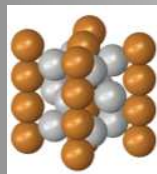


DNA

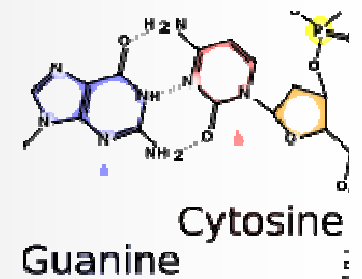
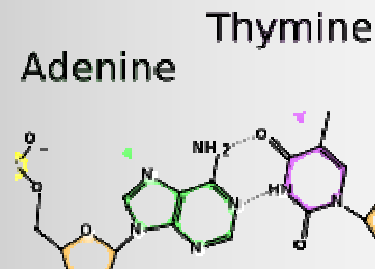
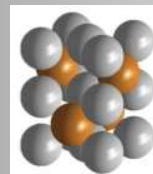
**Archetypes**  
Building blocks  
Space filling units



Dispersoids

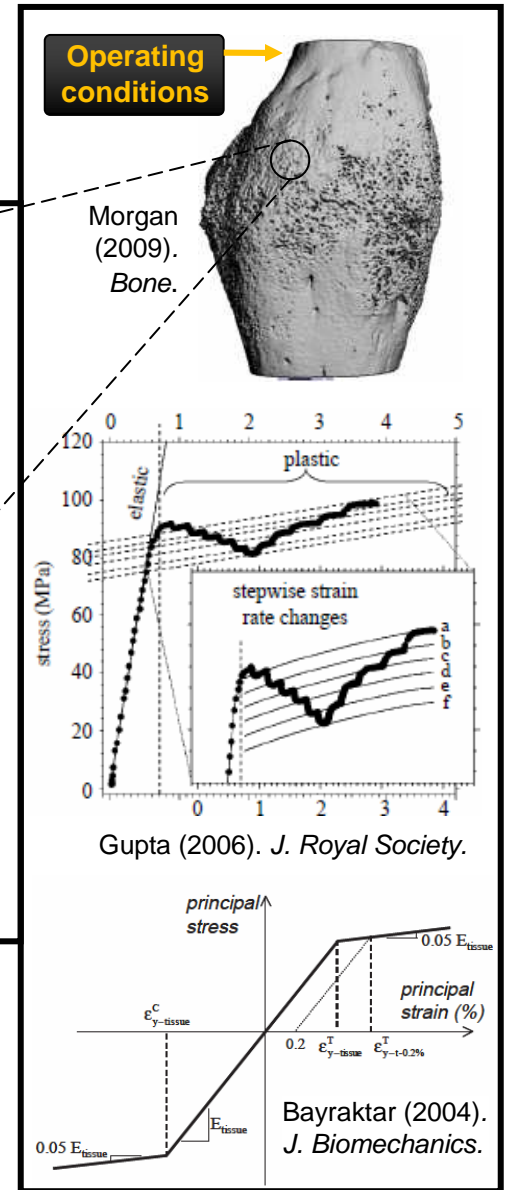
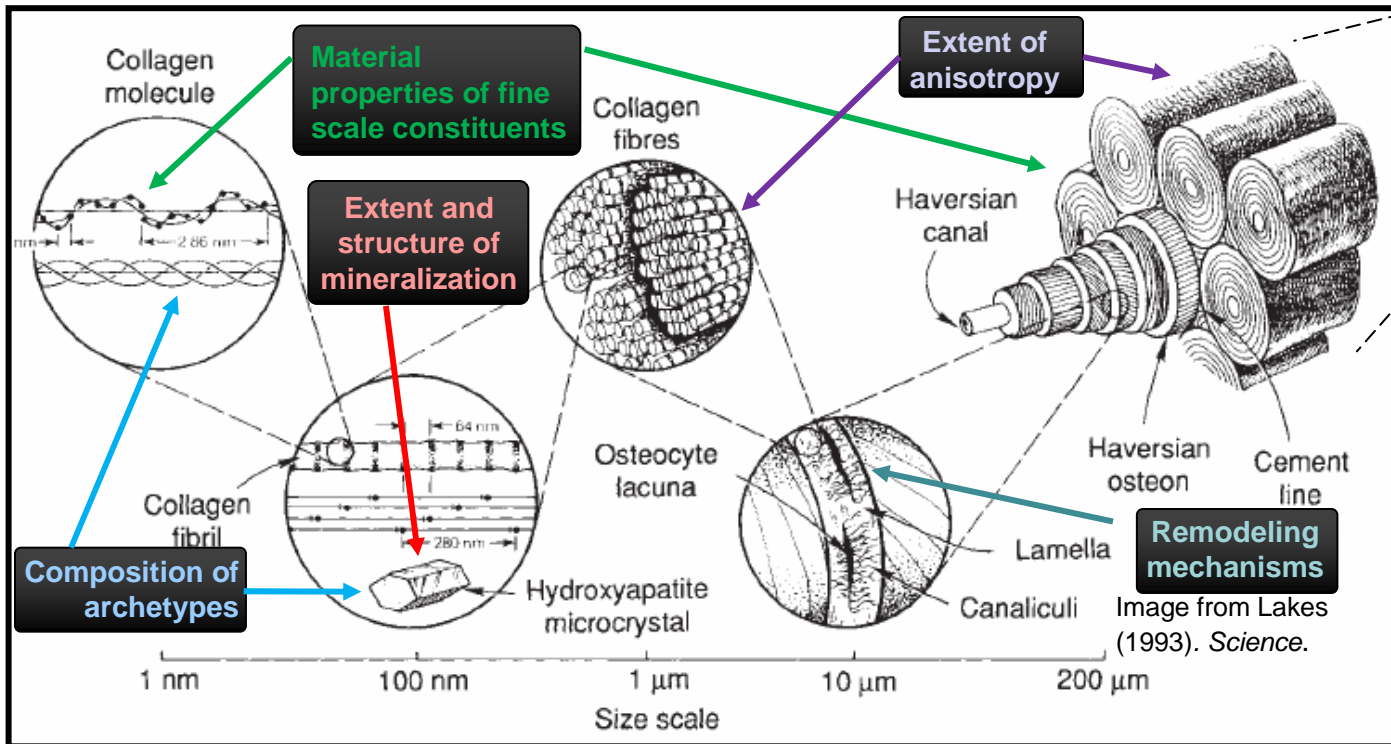


Precipitate crystals



# Post Yield Bone Mechanics

- **Goal.** Predict post yield behavior, fracture path likelihood in spongy bone
- **Schedule.** 2010-current
- **Collaborators.** Iwona Jasiuk U-Illinois, Elise Morgan Boston University



Increasing resolution, decreasing spatial scale, increasing uncertainty

Microscopic Mechanisms



Macroscopic rate dependent plasticity



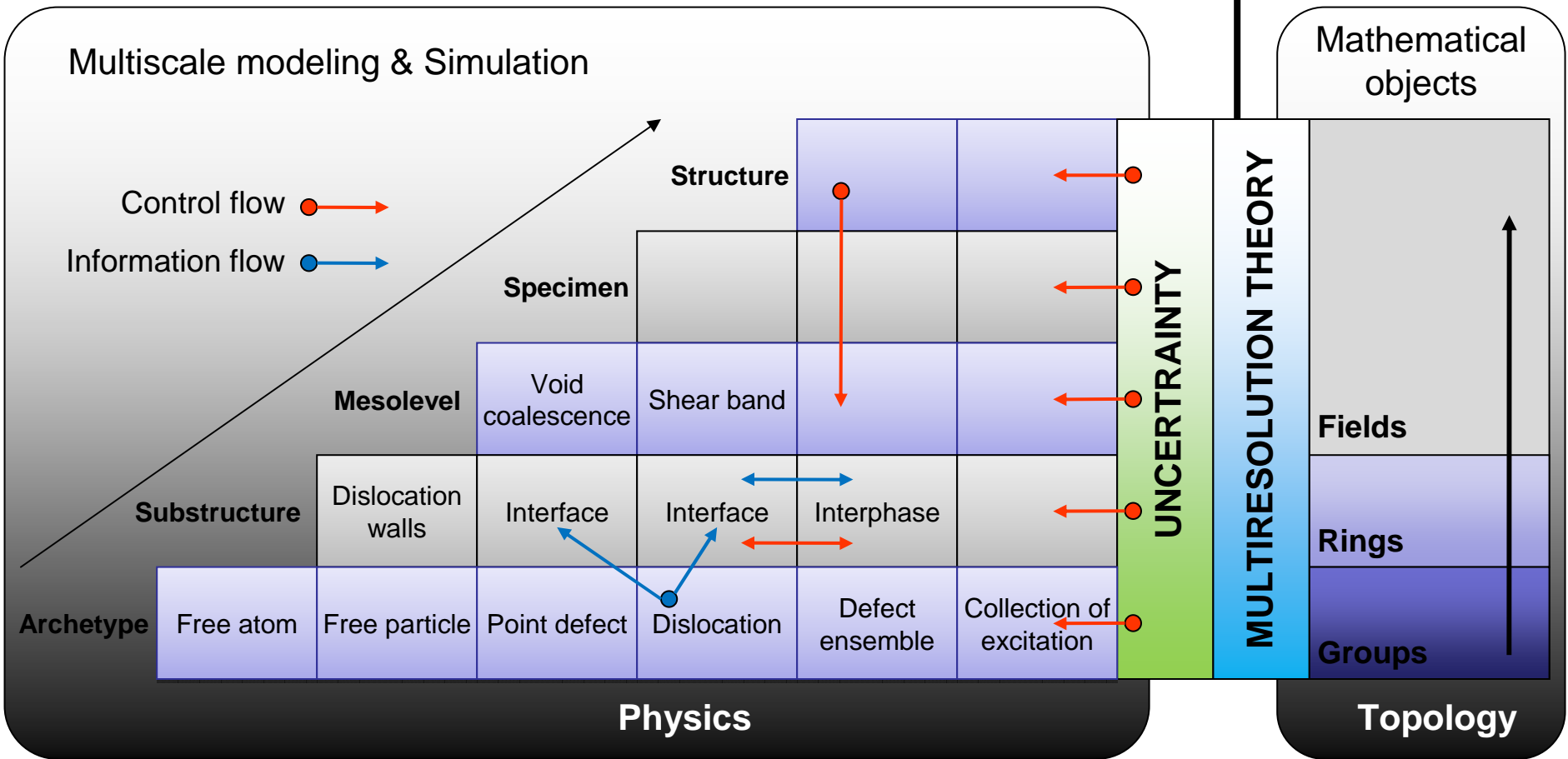
# Multiscale Machinery. Physical Postulates

Computational Theories

Space-time discretization

High-performance computing

## Scale-Bridging Theory



# Uncertainty Types

- Random multiscale conditions
  - Inherent structural variation (batch to batch randomness, random field)
  - Uncertain multiscale boundary conditions (chaotic environments)
  
- Lack of knowledge, lack of information
  - Misunderstood physics
  - Insufficient physical experiments
  - Model inadequacy
  
- Limited computational resource

**STOCHASTIC PDE's**



Greene, M.S., Y. Liu, et al. (2011).  
Computational uncertainty analysis in multiresolution materials via stochastic constitutive theory.  
*CMAME* **200(1-4): 309-325.**

# General Stochastic Formulation

Write general partial differential equation governing evolution of some system

$(\Omega, \mathfrak{F}, P)$  Probability space

$\Omega$  Could be infinite dimensional

Ghanem (1999) Xiu (2009)  
 Ghanem & Spanos (1991)  
 Xiu & Karniadakis (2002)  
 Xiu (2006)  
 Acharjee (2006)

## Uncertainty

(1) Stochastic differential operators.

- Random field coefficients
- Material properties
- Dimension reduction req'd

(2) Uncertain environment, i.e. random boundary or initial conditions.

- Mechanical loads unknown
- Temperature field unknown
- Current state of system uncertain

(3) Uncertain domain.

- Rough edges from processing
- Micro/tele scope finite resolution

### Governing Equation

$$[\mathbf{T}] \mathbf{v}(\mathbf{x}, t, \omega) + [\bar{\mathbf{S}} + \mathbf{S}_\omega] \mathbf{v}(\mathbf{x}, t, \omega) = \mathbf{0}$$

↑ Temporal operator      ↑ Mean spatial operator      ↑ Random spatial operator

$$[\bar{\mathbf{B}} + \mathbf{B}_\omega] \mathbf{v}(\mathbf{x}, t, \omega) = \mathbf{0}$$

↑ Boundary condition

$$\mathbf{v}(\mathbf{x}, t = 0, \omega) = \mathbf{v}_0(\mathbf{x}, \omega)$$

↑ Initial condition

### Equation Domain

$$\text{in } D(\omega) \times (0, T] \times \Omega$$

↑ Time domain      ↑ Spatial domain      ↑ Random domain

$$\text{in } \partial D(\omega) \times [0, T] \times \Omega$$

↑ Spatial boundary

$$\text{in } D(\omega) \times \{t = 0\} \times \Omega$$

# Stochastic Formulation for Solid Mechanics

## General

$$[T + \bar{S} + S_Z] \mathbf{v}(\mathbf{x}, t, \mathbf{Z}) = \mathbf{0}$$

in  $D(\omega) \times (0, T] \times \Omega$

- Uncertainty parameterization technique required
- KL transformation, Polynomial Chaos Expansion
- Dimension reduction methodology

## Solid Mechanics

Composition operation

$$[T + \bar{S}](\mathbf{v}) = [-T + N \circ f \circ g \circ h](\mathbf{v})$$

- $[T](\bullet) = \text{acceleration} \triangleq \partial_t(\bullet)$
- $[N](\bullet) = \text{balance law} \triangleq \bar{\nabla} \cdot (\bullet)$
- $[f](\bullet) \triangleq \text{constitutive law}$
- $[g](\bullet) = \text{objectivity} \triangleq \text{sym}(\bullet)$
- $[h](\bullet) = \text{compatibility} \triangleq \bar{\nabla}(\bullet)$

Solution (vector) space

$$\mathbf{v}(\mathbf{x}, t, \mathbf{Z})$$

Tensor space

$$\nabla \mathbf{v}(\mathbf{x}, t, \mathbf{Z})$$

Symmetric tensor space

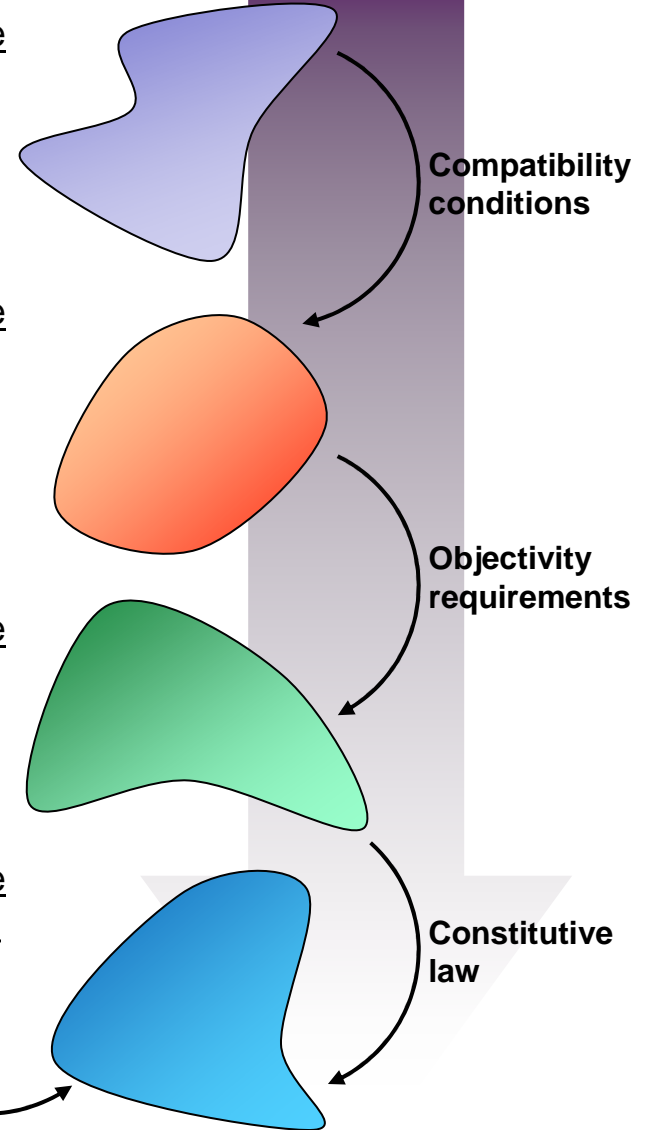
$$\text{sym}[\nabla \mathbf{v}(\mathbf{x}, t, \mathbf{Z})]$$

Stress tensor space

$$\sigma\{\text{sym}[\nabla \mathbf{v}(\mathbf{x}, t, \mathbf{Z})]\}$$

**Balance Law**

acts on stress space



# Stochastic Formulation for Multiresolution Continua

## Solid Mechanics

$$[T + \bar{S} + S_Z](\mathbf{v}) = [-T + N \circ (\bar{\mathbf{f}} + \mathbf{f}_Z) \circ \mathbf{g} \circ \mathbf{h}](\mathbf{v})$$

Macroscopic stress

$$-\rho \dot{\mathbf{v}} + \left[ \boldsymbol{\sigma} - \sum_{n=1}^{N-1} \boldsymbol{\beta}^n \right] \cdot \bar{\nabla} + \mathbf{b} = \mathbf{0}$$

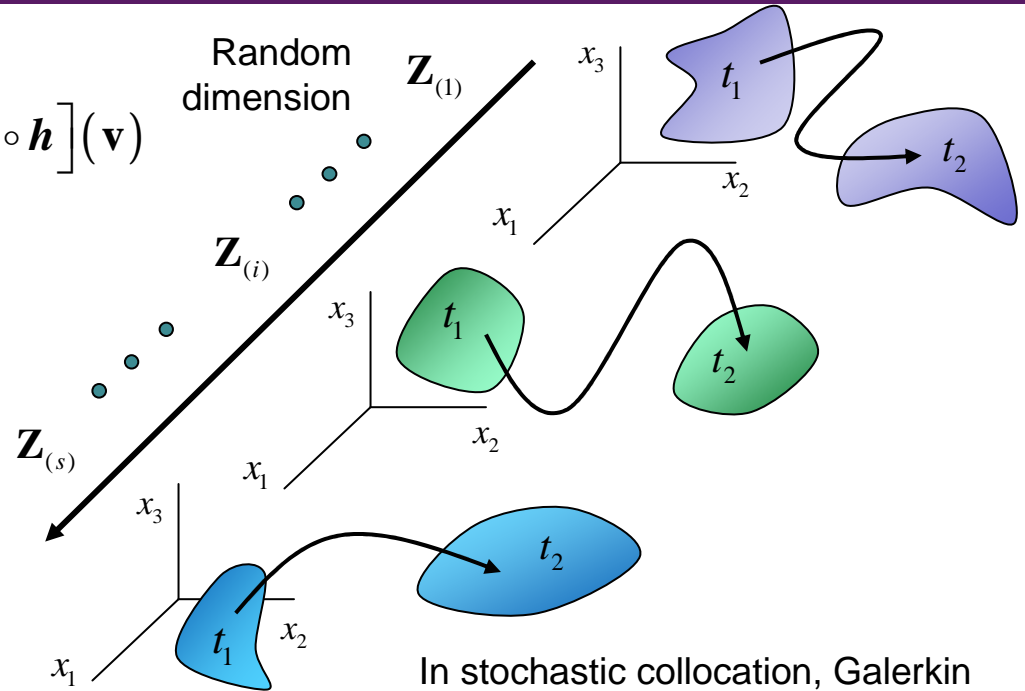
Temporal operator      Spatial operator

$$-\dot{\gamma} \cdot \mathbf{I}^n + \bar{\boldsymbol{\beta}}^n \cdot \bar{\nabla} - \boldsymbol{\beta}^n + \mathbf{B}^n = \mathbf{0}, \quad n = 1, 2, \dots, N$$

Boundary condition

$$\left[ \boldsymbol{\sigma} - \sum_{n=1}^{N-1} \boldsymbol{\beta}^n \right] \cdot \mathbf{n} = \mathbf{t}$$

$$\bar{\boldsymbol{\beta}}^n \cdot \mathbf{n} = \mathbf{T}^n, \quad n = 1, 2, \dots, N$$



In stochastic collocation, Galerkin projection, **random dimension discretized** like space and time

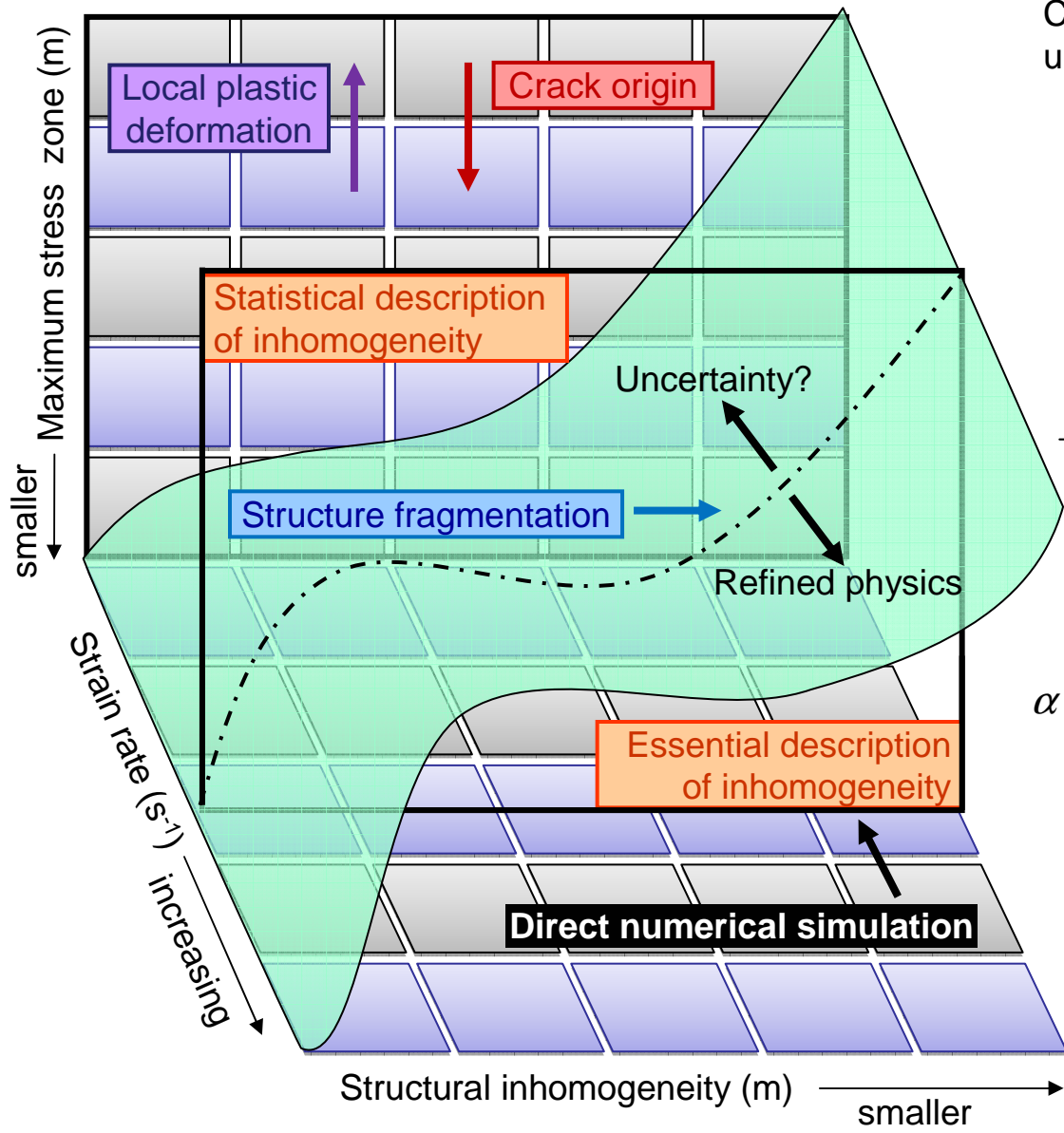
### RANDOM SOLUTIONS

VELOCITY      MICRO-VELOCITY GRADIENT

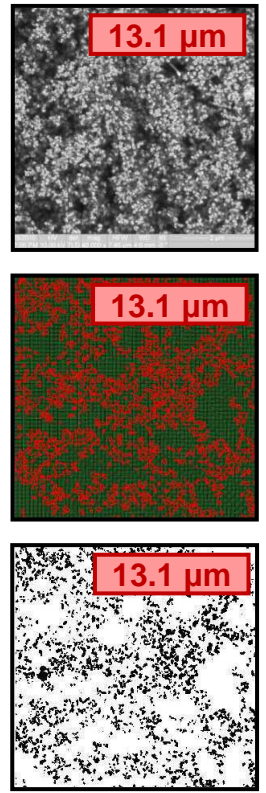
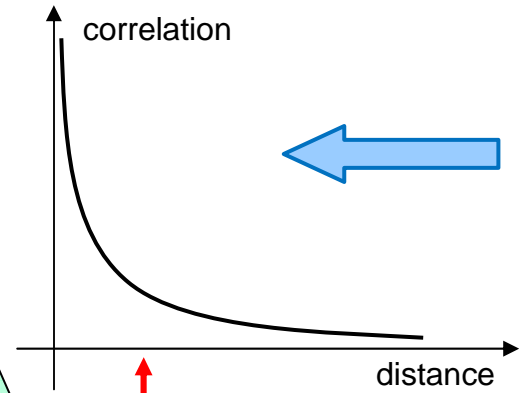
$$\boldsymbol{\sigma}, \boldsymbol{\beta}^n, \boldsymbol{\beta}^n = \mathbf{f}_\sigma, \mathbf{f}_\beta, \mathbf{f}_{\bar{\beta}} \left( \text{sym} \nabla \mathbf{v}(\mathbf{x}, t, \mathbf{Z}), \underline{\underline{\mathbf{L}^n}}(\mathbf{x}, t, \mathbf{Z}) - \mathbf{L}, \nabla \mathbf{L}^n(\mathbf{x}, t, \mathbf{Z}) \right)$$

Constitutive law an implicit function of a denumerable set of random variables

# Stochastic Formulation and Length Scales



Consideration of length scale effects and uncertainty intimately related



**KL Expansion**

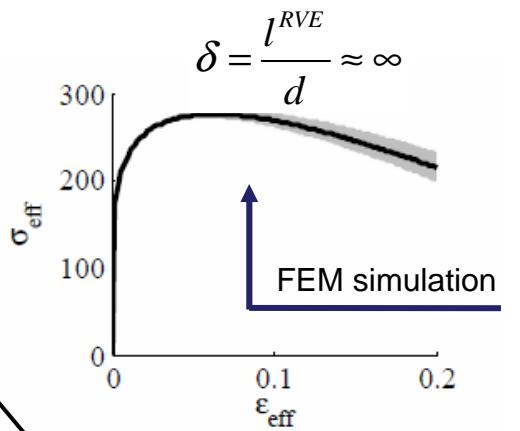
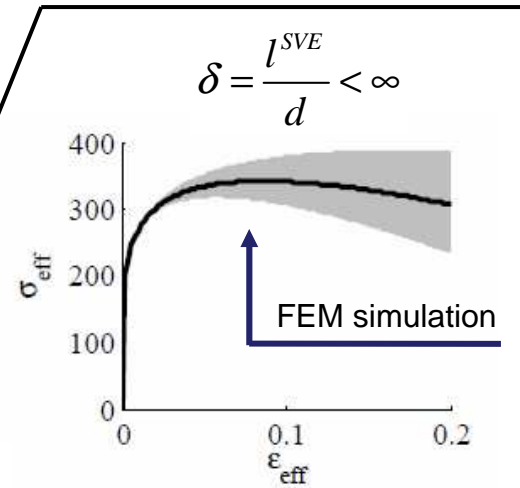
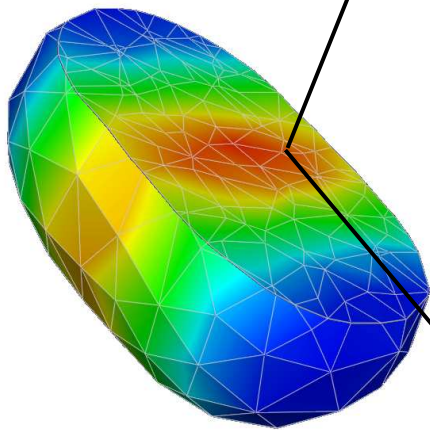
$$\alpha(\mathbf{x}, t, \omega) = \sum_{i=1}^P \sqrt{\lambda_i} \xi_i(\omega) \psi_i(\mathbf{x}, t)$$

**Number of terms is intractable if correlation length is small relative to macroscopic domain**

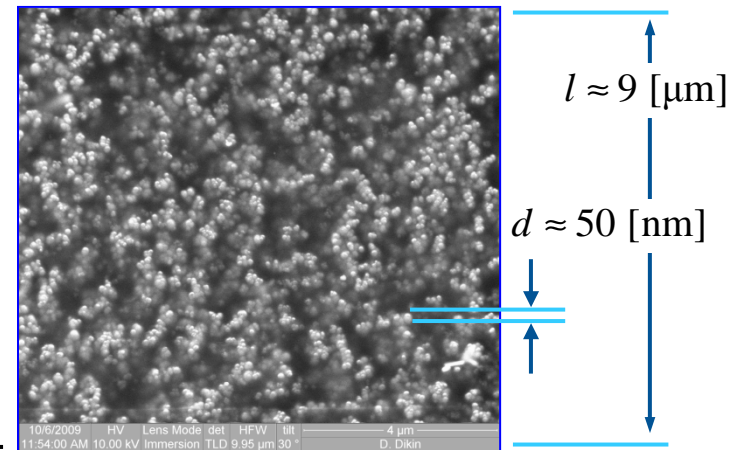
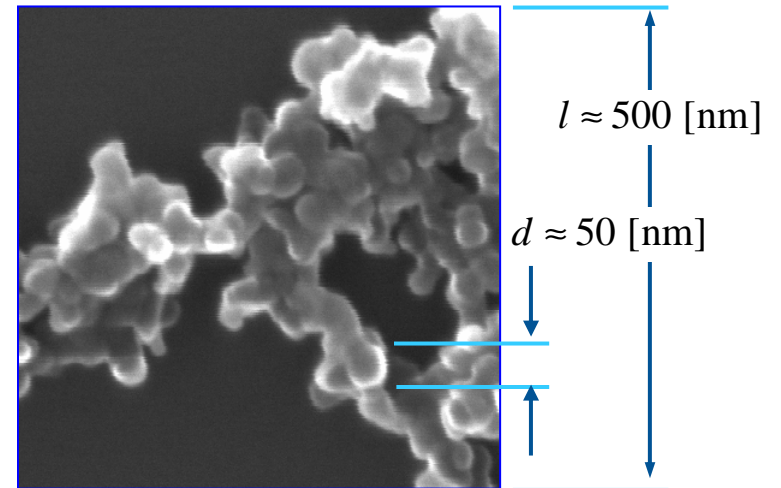
# Stochastic Constitutive Theory

- Denumerable set of random variables are structural descriptors of microstructure
- Unique stress distributions averaged to provide constitutive behavior

## MACRO-SCALE SIMULATION



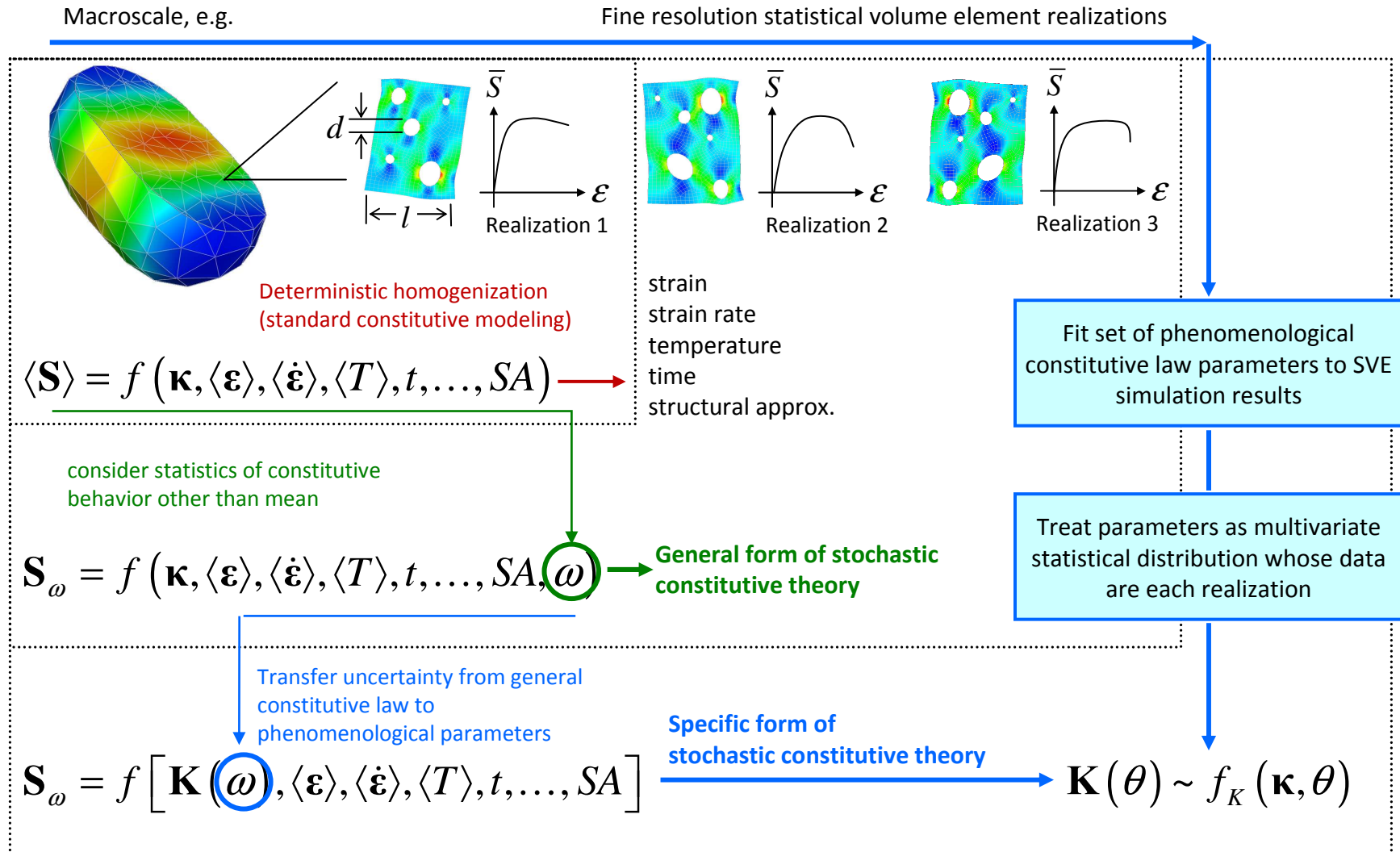
## MICRO-SCALE VOLUME ELEMENTS



SEM images provided by D. Dikin (2010)

# Stochastic Constitutive Theory

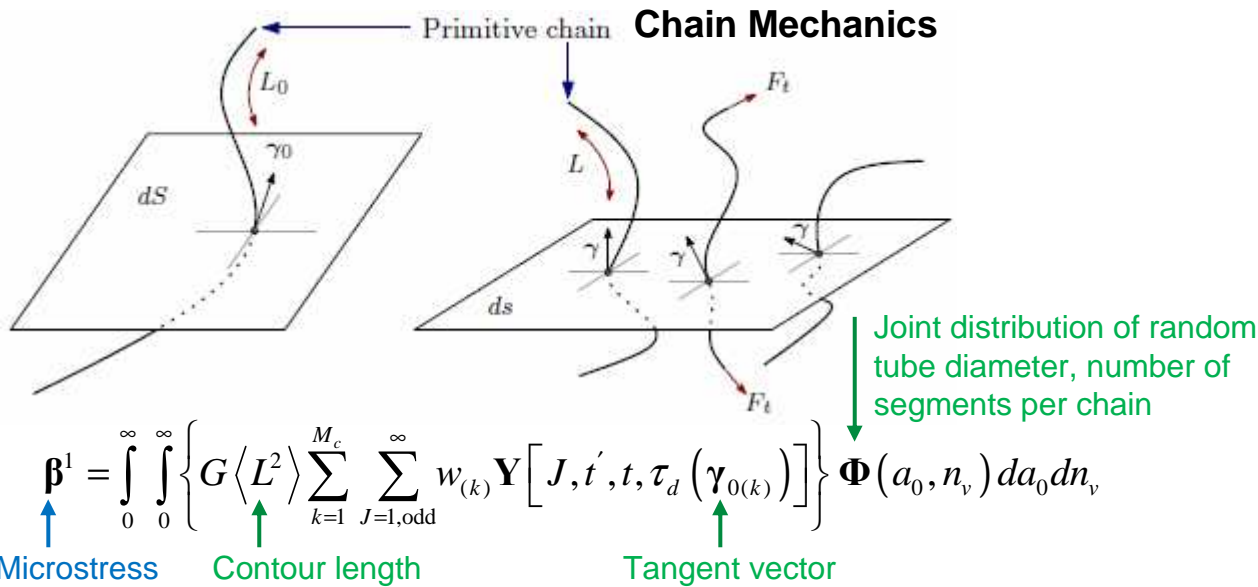
For multiscale analysis, deterministic fine scale simulations create randomness



Greene (2010)



# Examples of Constitutive Law. Mechanistic Nonlinear Viscoelasticity

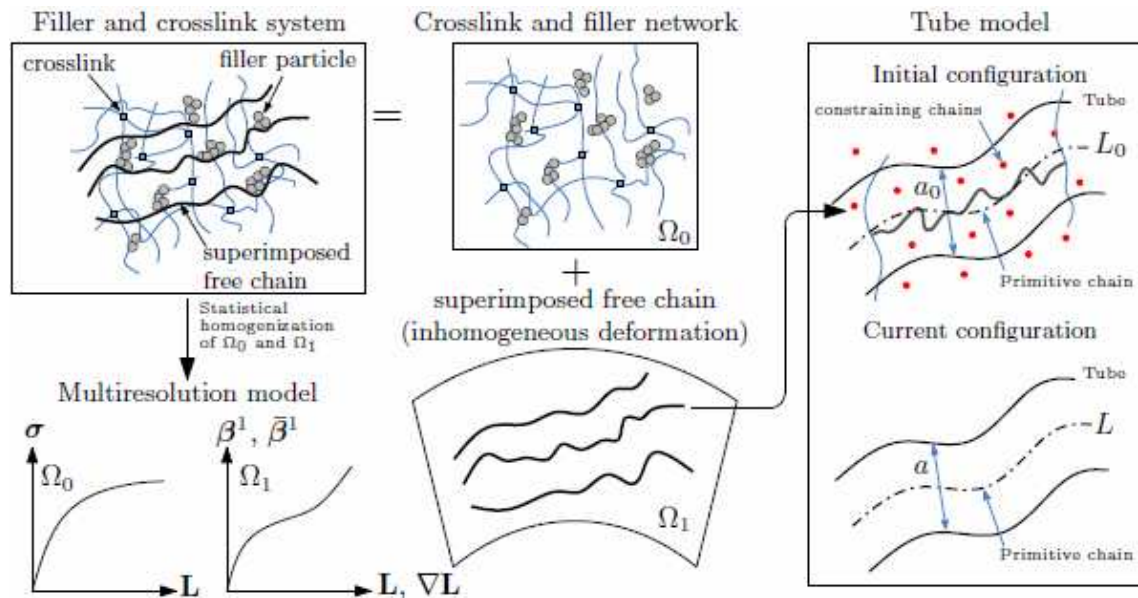


## Operating conditions

$T$	TEMPERATURE
$\omega$	FREQUENCY

## Polymer chemistry (real chains)

$N$	CHAINS PER UNIT VOLUME
$\rho$	POLYMER DENSITY
$b$	MONOMER-MONOMER DISTANCE
$n$	MONOMERS PER CHAIN



## Polymer physics

$D_c$	DIFFUSION CONSTANT
$\tau_d$	RELAXATION TIME

Predicted from MD simulations

$$\tau_d = \frac{\left( \frac{nb^2}{a} \right)^2}{D_c \pi^2}$$

# Outline

## ☐- Overarching Theme

## ☐- Current research projects

- D3D, design of high strength steels. Aerospace application.
- Polymer nanocomposite design. Automotive application.
- Post-yield bone mechanics. Clinical application.
- Microsystem gyroscope design. Deep space application.
- Nanotip enrichment. Medical application

## ☐- Mathematical machinery

- Physical postulates of material motion ← **Why.**
  - Governing equations of multiresolution continua ← **Where.**
  - Constitutive modeling ← **How.**
- UNCERTAINTY**

## ■- Conclusions

## Discussion

- - Engineering systems are complex and large, reduction of uncertain dimension may not always be possible
- - Is there a tradeoff in analysis of uncertainty and higher fidelity models?
- - When is computational uncertainty analysis worthwhile?
- - Link between material microstructure and material property critical to understanding random property fields.
- - Thumbs up for archetypes and multiresolution theory

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# Closure



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**QUESTIONS**



**MANY THANKS!**