Georgia Institute of Technology

Grand Challenge Multiscale Projects:
Multiscale Materials Design

David L. McDowell

The George W. Woodruff School of Mechanical Engineering
School of Materials Science & Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0405

ORNL Workshop on Multiscale Simulation:
Atomistic to Continuum
April 4, 2005

Outline

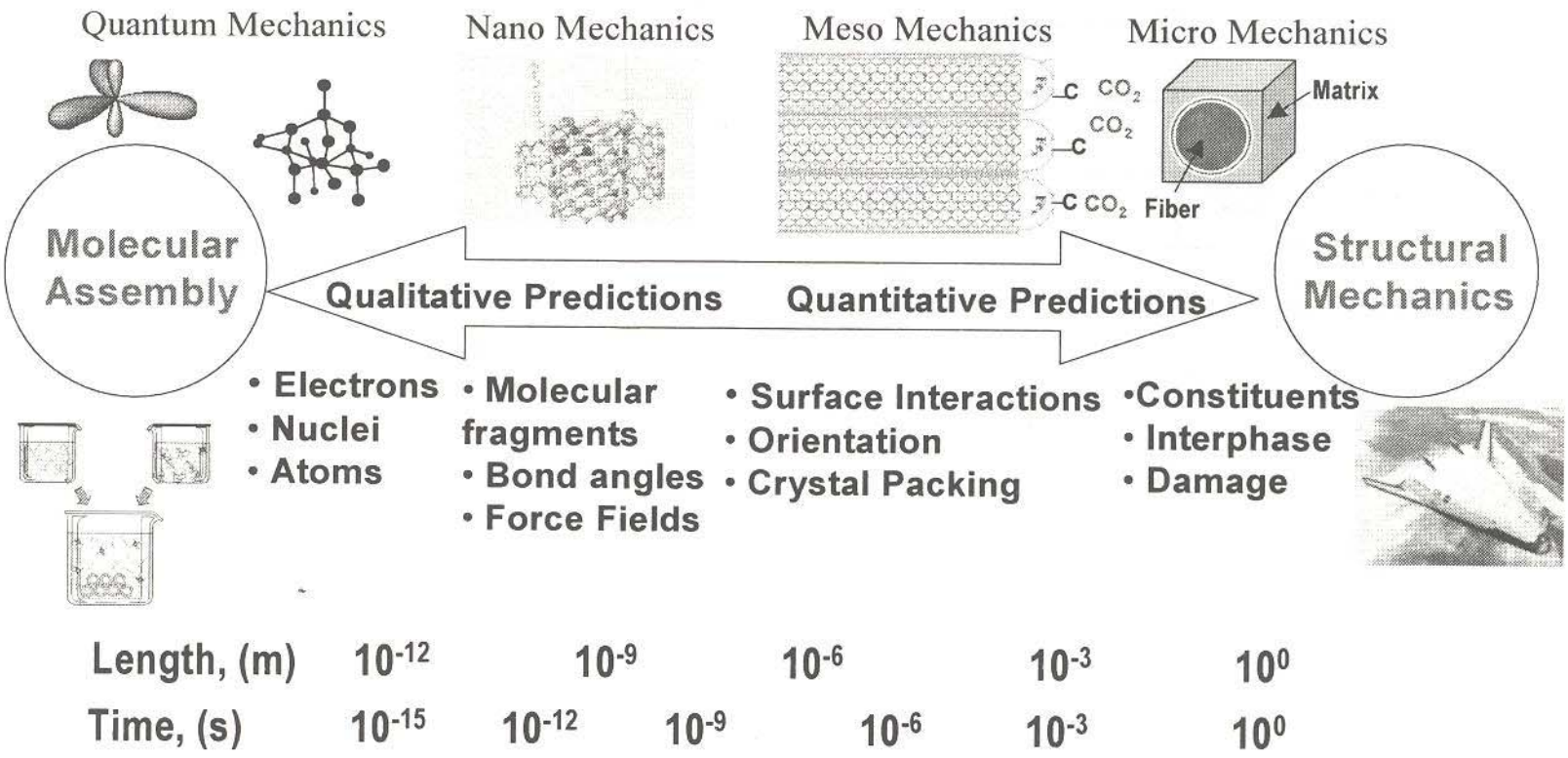
- Aspects of Multiscale Modeling
- Elements of Systems-Based Materials Design
- AFOSR MURI Example
- Future Horizons: Grand Challenges
- PSU-GT CCMD

McDowell Research

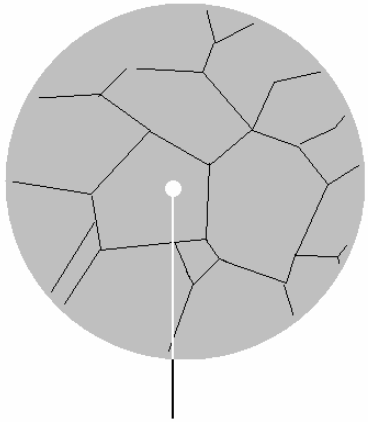
- Novel computational methods for material microstructure-property relations
  - atomistics (nanostructured materials)
  - atomistic/continuum FE couplings
  - FE-based process-structure and structure-property (hierarchical fatigue/fracture)
  - multiscale discrete dislocation/continuum modeling
- Systems-based materials design
- Various classes of cellular and heterogeneous materials

Multiscale Simulation

Gates, T.S. and Hinkley, J.A., Computational Materials: Modeling and Simulation of Nanostructured Materials and Systems, NASA/TM-2003-212163, 2003.

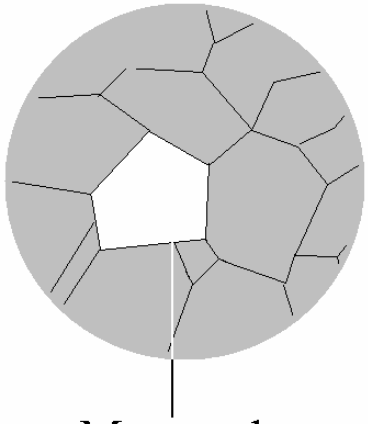


Multiscale Homogenization



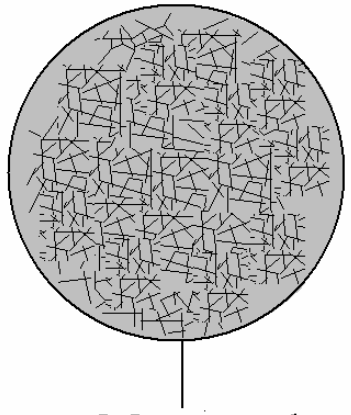
Microscale
O (0.1 - 10 μm)
Distributed dislocations
(Bilby et al., 1957)

$${}^{\mu}\mathbf{f} = {}^{\mu}\mathbf{f}^{e}\,{}^{\mu}\mathbf{f}^{p}$$



Mesoscale
O (10 - 250 μm)
Crystal plasticity
(Rice, 1971; Asaro, 1983)

$$\mathbf{f} = \mathbf{f}^{e}\,\mathbf{f}^{p}$$



Macroscale
O (250-10^4 μm)
Macroscopic plasticity
(Lee & Liu, 1967;
Bammann & Johnson, 1987)

$$\mathbf{F} = \mathbf{F}^{e}\mathbf{F}^{p}$$

Polycrystalline Materials

Scale-dependent decomposition

Polycrystal Theory

$$\mathbf{F} \equiv \frac{1}{v_{ref}} \int_{s_{ref}} \mathbf{x} \otimes \mathbf{ds}_{ref} = \frac{1}{v_{ref}} \int_{v_{ref}} \frac{\partial \mathbf{x}}{\partial \mathbf{X}} dv_{ref} = \frac{1}{v_{ref}} \int_{v_{ref}} \mathbf{f} dv_{ref}$$

$$\mathbf{F} = \underbrace{\mathbf{F}^{\mathbf{e}}}\, \tilde{\mathbf{F}}^{\mathbf{i}} \bar{\mathbf{F}}^{\mathbf{p}} \qquad \dot{\bar{\mathbf{F}}}^{\mathbf{p}} \bar{\mathbf{F}}^{\mathbf{p}-1} \equiv \frac{1}{v_{ref}} \int_{v_{ref}} \dot{\mathbf{f}}^{\mathbf{p}} \mathbf{f}^{\mathbf{p}-1} dv_{ref}$$

net recoverable stretch and lattice rotation, may be compatible over RVE, not necessarily at macroscale (after Bilby & Smith, 1956)

$$\tilde{\mathbf{F}}^{\mathbf{i}} \equiv \tilde{\mathbf{F}} \bar{\mathbf{F}}^{\mathbf{p}-1} = \frac{1}{v_{ref}} \left(\int_{v_{ref}} \tilde{\mathbf{f}}^{\mathbf{e}} \tilde{\mathbf{f}}^{\mathbf{p}} dv_{ref} \right) \bar{\mathbf{F}}^{\mathbf{p}-1}$$

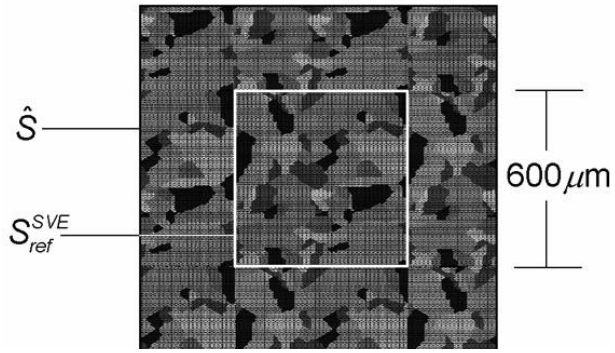
$\mathbf{F}\,\mathbf{F}^{\mathbf{e}-1}$

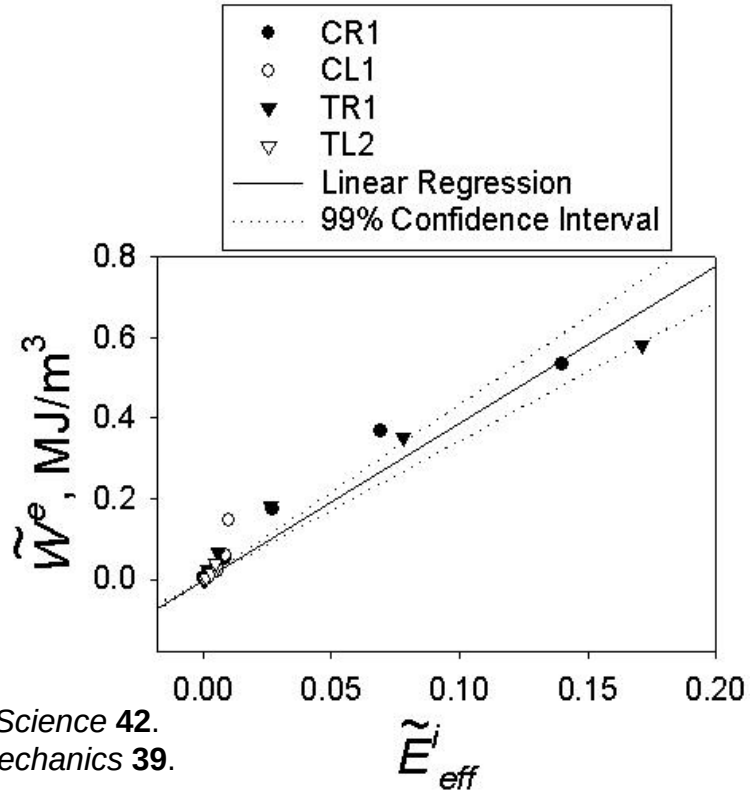
residual elasticity

$\tilde{\mathbf{F}}^{\mathbf{i}}$ accounts here for integranular incompatibility.

Embeds effects of residual elastic strains necessary to accomodate moments of plastic strain at the fine scale.

Can also incorporate kinematical fields that are not associated with slip, e.g. initial GB structure, twin structure, etc.



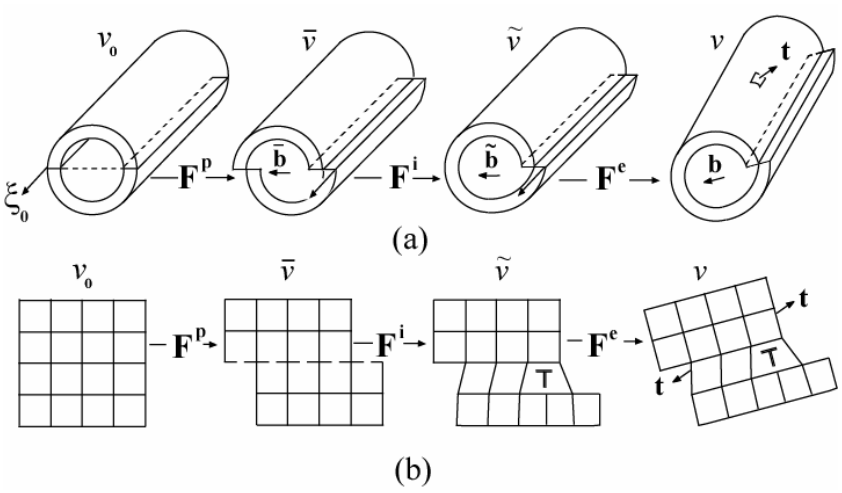


Clayton, J.D. and McDowell, D.L., 2003, *Int. J. Plasticity* **19**.
Clayton, J.D., Bammann, D.J., and McDowell, D.L., 2004, *Int. J. Engineering Science* **42**.
Clayton, J.D., Bammann, D.J., and McDowell, D.L., 2004, *Int. J. Non-linear Mechanics* **39**.

Disclinations: micropolar kinematics

Deformation gradient

$$\mathbf{F} = \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{i}}\mathbf{F}^{\mathrm{p}} \qquad \mathbf{F}^{\not\mathcal{L}} \equiv \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{i}}$$



Lattice directors

$$\mathbf{d}_a = \left(F^{\not\mathcal{L}-1}\right)^{\bar{\alpha}}_{.a}\overline{\mathbf{d}}_{\bar{\alpha}}$$

$$\nabla_b \mathbf{d}_a = \mathbf{d}_{a,b} - \Gamma^{..c}_{ba}\mathbf{d}_c$$

Connection

Micromorphic rotation variable

$$\Gamma^{..a}_{cb} \equiv F^{\not\mathcal{L}\,a}_{.\bar{\alpha}} F^{\not\mathcal{L}-1\bar{\alpha}}_{.b,c} + Q^{..a}_{cb} = \overline{\Gamma}^{..a}_{cb} + Q^{..a}_{cb}$$

Torsion tensor: net dislocations

$$T^{..a}_{cb} \equiv \Gamma^{..a}_{cb} - \Gamma^{..a}_{bc} = \overline{T}^{..a}_{cb} + 2Q^{..a}_{[cb]}$$

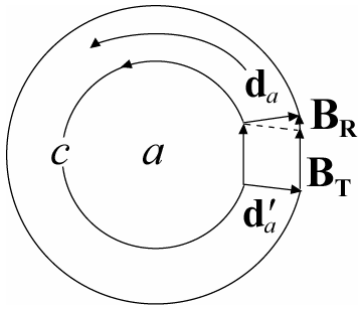
$$2\alpha^{ad} \equiv \varepsilon^{dbc}T^{..a}_{bc} \qquad \boldsymbol{\alpha} = \sum_j \left(\rho^j_+ - \rho^j_-\right)\mathbf{b}^j_+ \otimes \boldsymbol{\xi}^j$$

Total Burgers vector

$$B^a \equiv \frac{1}{2}\varepsilon^{dbc}\int_a \left(T^{..a}_{bc} - R^{...a}_{ecb}x^e\right)n_d\,da$$

$$= \int_a \left(\alpha^{ad} + C^{\not\mathcal{L}-1af}\varepsilon_{fgb}\theta^{gd}x^b\right)n_d\,da$$

$$= \underbrace{B_T{}^a}_{\text{dislocations}} + \underbrace{B_R{}^a}_{\text{disclinations}}$$



$$C^{\not\mathcal{L}}{}_{ab} \equiv \mathbf{d}_a \bullet \mathbf{d}_b$$

Curvature tensor: net disclinations

$$R^{...a}_{bcd} = 2\nabla_{[c}Q^{..a}_{d]b} + Q^{..a}_{ce}Q^{..e}_{db} - Q^{..a}_{de}Q^{..e}_{cb} + T^{..e}_{cd}Q^{..a}_{eb}$$

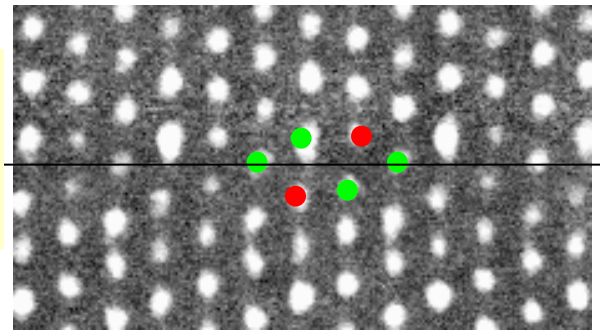
$$4\theta^{gd} \equiv \varepsilon^{gba}\varepsilon^{dce}R_{abce} \qquad \boldsymbol{\theta} = \sum_k \left(\eta^k_+ - \eta^k_-\right)\boldsymbol{\omega}^k_+ \otimes \boldsymbol{\zeta}^k$$

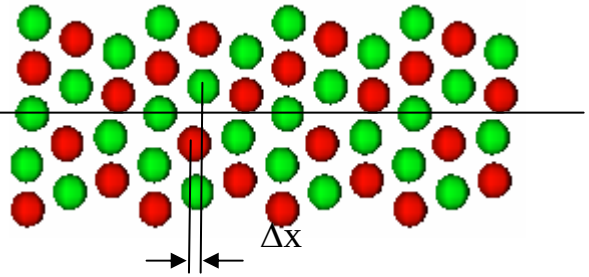
Grain Boundaries

- Interface structures
  - It is imperative that energy minimization (prior to deformation) reproduces realistic nanoscale grain boundary interface structures
  - We use published HRTEM data to confirm our energy minimization conditions

Medlin *et al.* (1993)

Aluminum

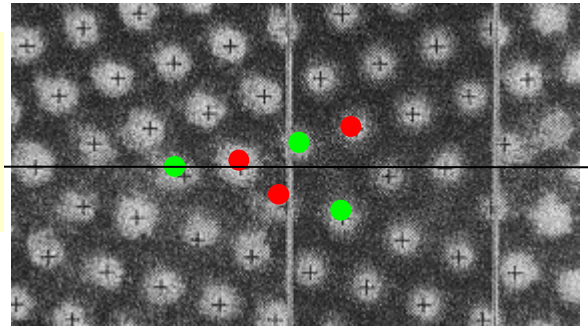


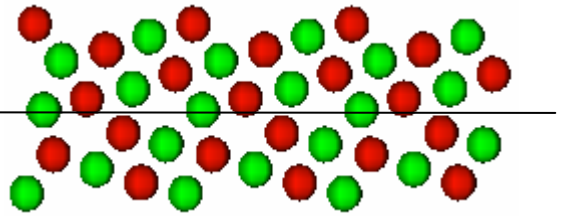


Σ3 {112} interface

Mills *et al.* (1992)

Aluminum





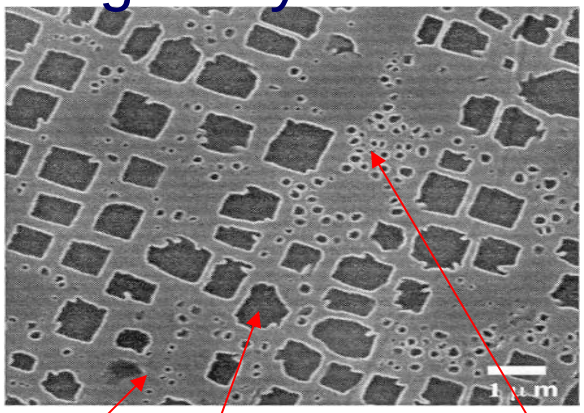
Σ9 {221} interface

Fatigue of Ni-Base Superalloys

The George W. Woodruff School of Mechanical Engineering
School of Materials Science and Engineering

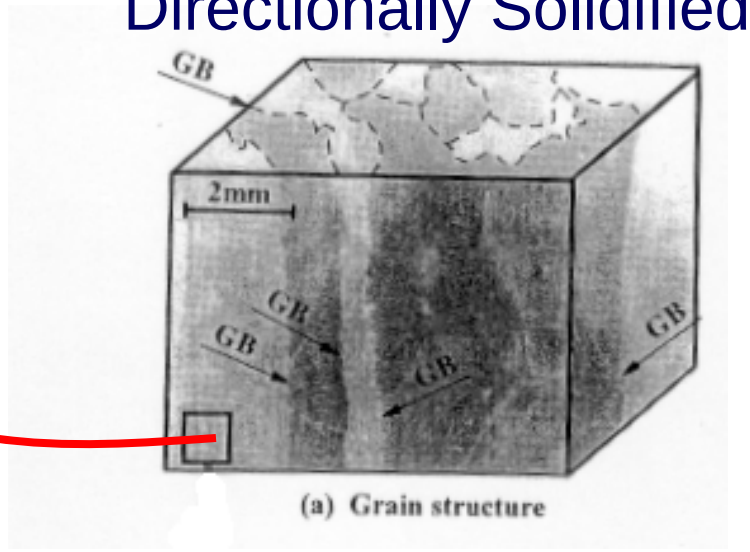
Supersolvus heat treatment

Single Crystal/Grain



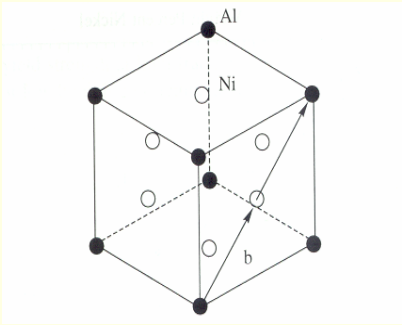
matrix γ' precipitate γ'' precipitate

Directionally Solidified



Polycrystal

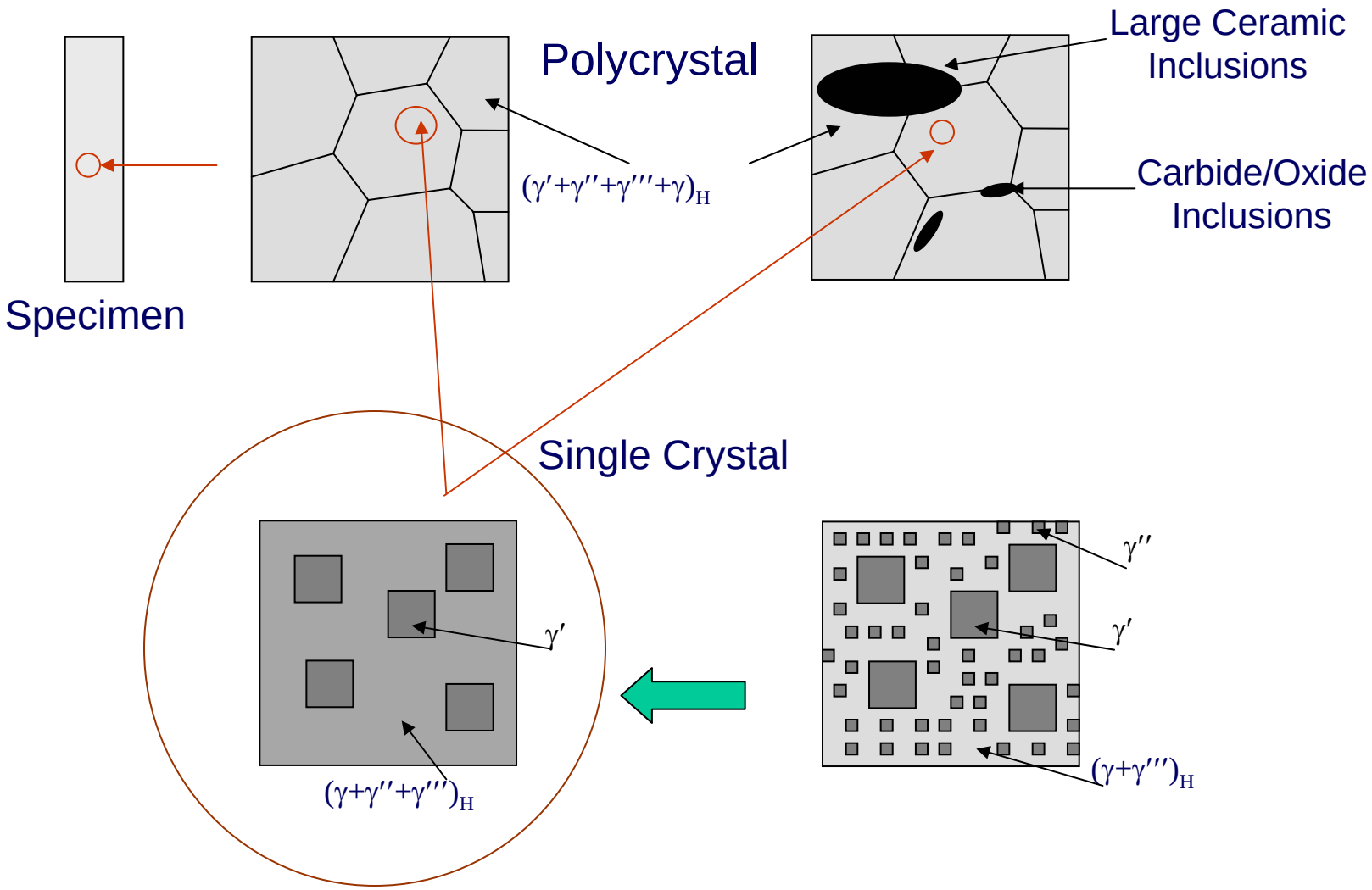
- Matrix
  - FCC γ Ni
- Precipitates
  - FCC superlattice ($L1_2$) Ni_3Al
  - V_f = 40 – 50% (DS/Poly)
    60 – 70% (SC)
  - Size γ' 50 nm – 500 nm
    γ'' 10 nm



DARPA/GE AIM

With M. Shenoy, A. Wang, R. Kumar

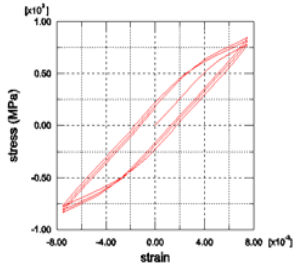
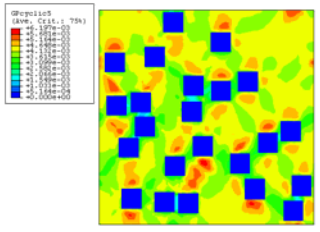
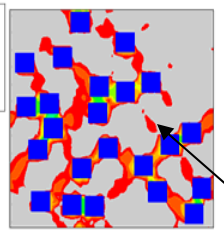
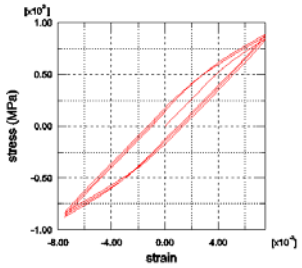
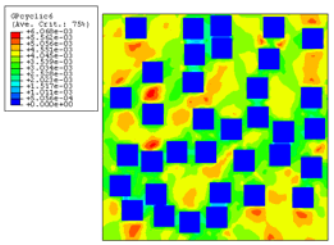
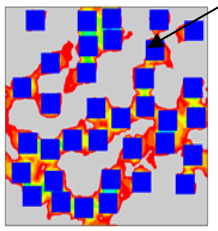
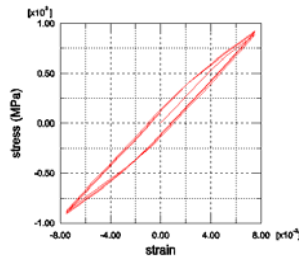
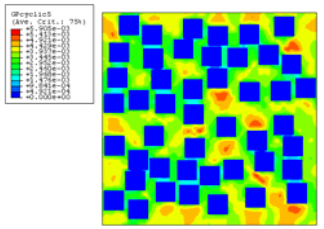
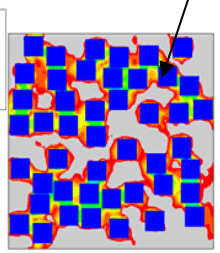
Scales of Interest



Effects of Primary Cooling γ′ Volume Fraction

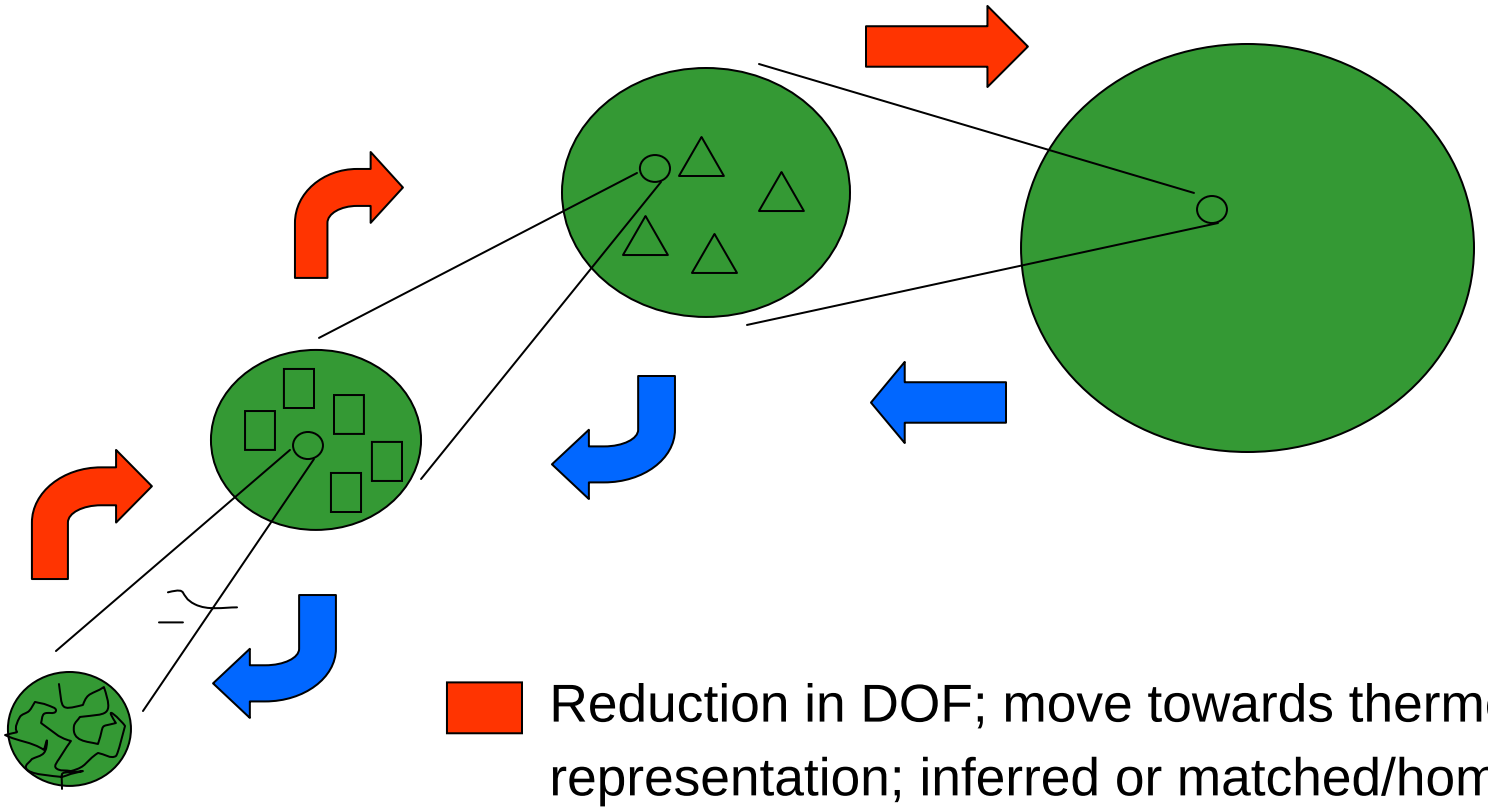
Precipitate Size = 0.3 μm

(Realization 1)

$\gamma' - V_f$	Stress-Strain Curve	Contours of $\Delta\gamma_{\theta}^{PC}$	Contours of $\Delta\gamma^{PC*}$
0.2		 $\Delta\gamma_{\theta,\max}^{PC} = 0.619\%$	 $\Delta\gamma^{PC*} = 0.400\%$
0.3		 $\Delta\gamma_{\theta,\max}^{PC} = 0.607\%$	 $\Delta\gamma^{PC*} = 0.367\%$
0.4		 $\Delta\gamma_{\theta,\max}^{PC} = 0.591\%$	 $\Delta\gamma^{PC*} = 0.365\%$

Percolation limits

Multiscale Simulation - DOF



Reduction in DOF; move towards thermodynamic representation; inferred or matched/homogenized

Increase in DOF; move towards dynamical representation; computed or measured

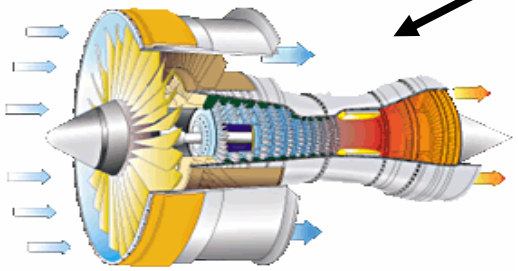
Concurrent or Hierarchical

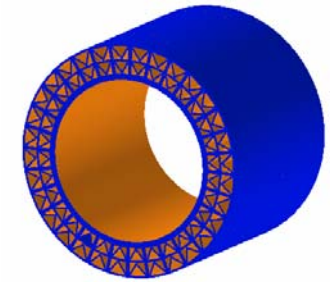
Why Do Multiscale Modeling?

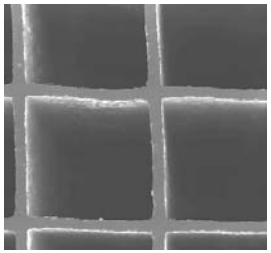
- Address phenomena occurring at different length and time scales
- Fine scale behavior is often relevant to phenomena that depend on extremal characteristics – fracture, fatigue, turbulence; mean field homogenization unsuited for this task → variable resolution modeling
- Practical limitations on computing time, DOF
- Engineering applications demand it

→ **Materials Design**

Shift from Emphasis on *Product Design* to *Product-Process-Material System Design*

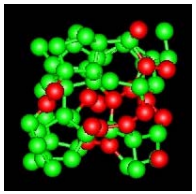






**(Cochran, et al)

**(Randle, WWW)



**(Piscanec et al, WWW)

Courtesy of C.C. Seepersad, SRL

System Specifications

System
Subsystems
Components
Parts

Material Specifications

Macro
Meso
Molecular
Quantum

Materials Design: A Realistic Perspective

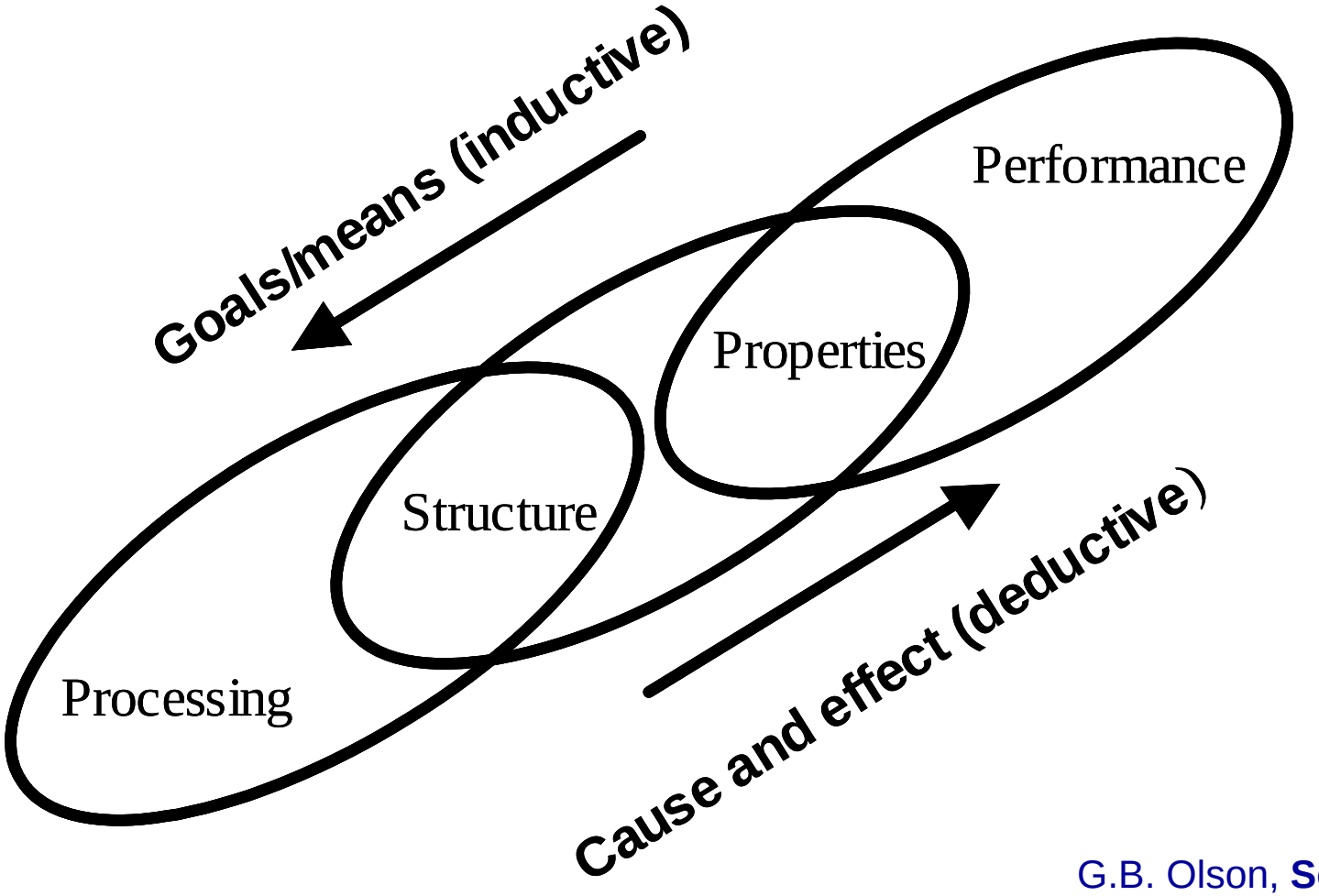
Empirical design

- *Constrained initial conditions (composition, process path)*
- *Meander through scales and phenomena by "intelligent tweaking"*
- *Get as far as you can towards desirable properties*

Systems design

- *To what degree can empirical path be replaced by simulation informing decisions? 15%? 30%?*
- *To what extent can multiple phenomena be considered simultaneously rather than sequentially?*
- *To what extent can constraints on the design problem be relaxed (including initial) and multiple objectives considered?*

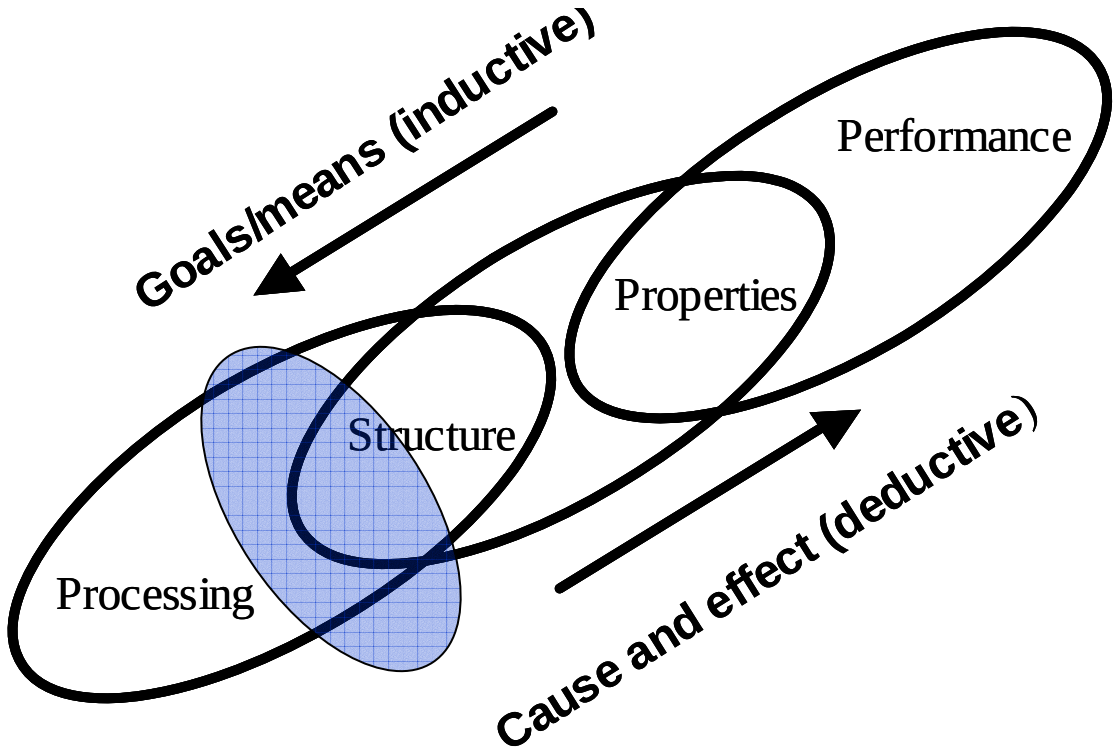
Olson's Hierarchical Conception: Materials by Design



G.B. Olson, **Science**, 29 Aug., 1997, Vol. 277

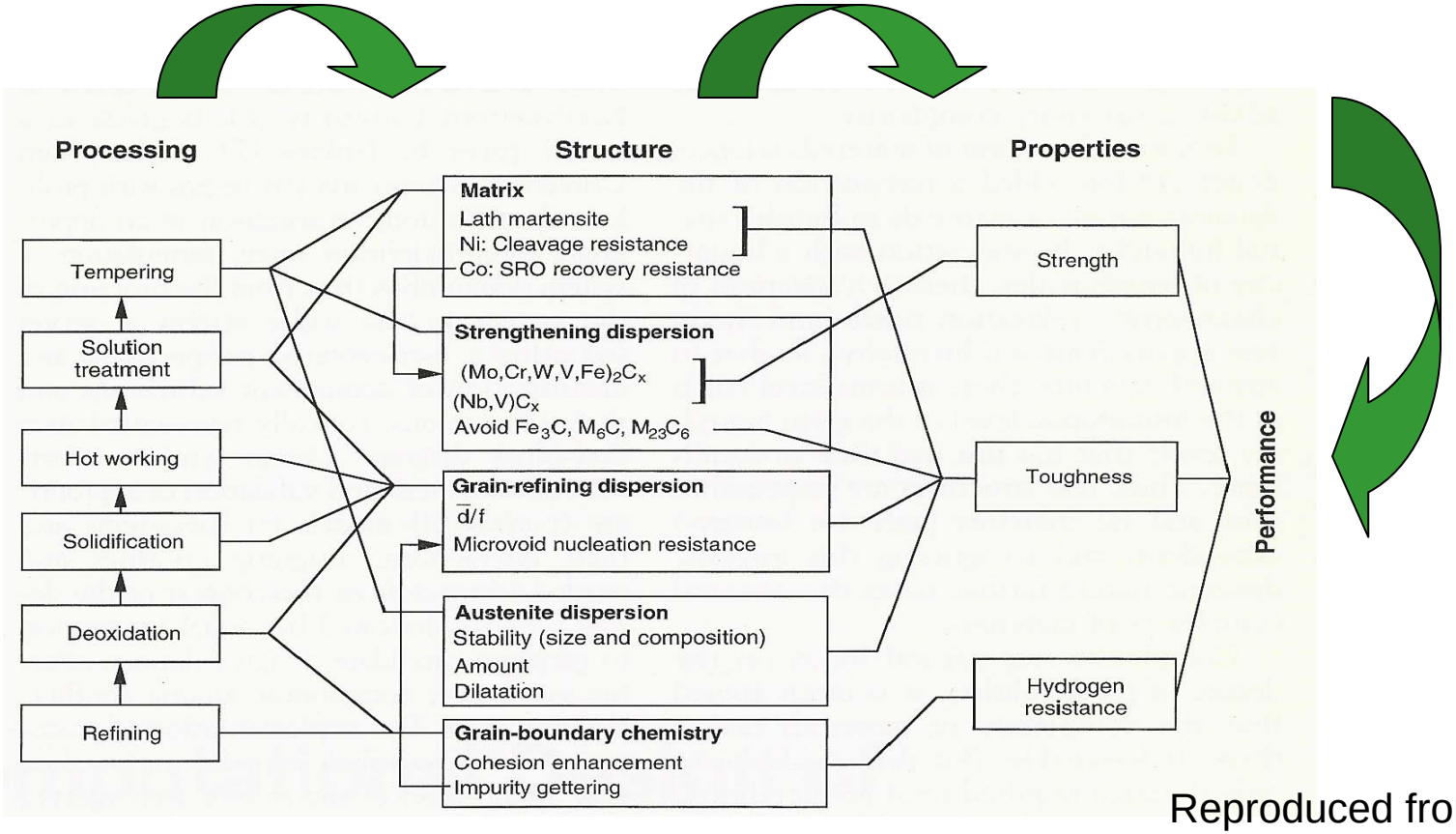
Types of Mappings in Materials Design

Property-performance mappings - Relate feasible properties to response functions that are relevant to imposed performance requirements.



Example

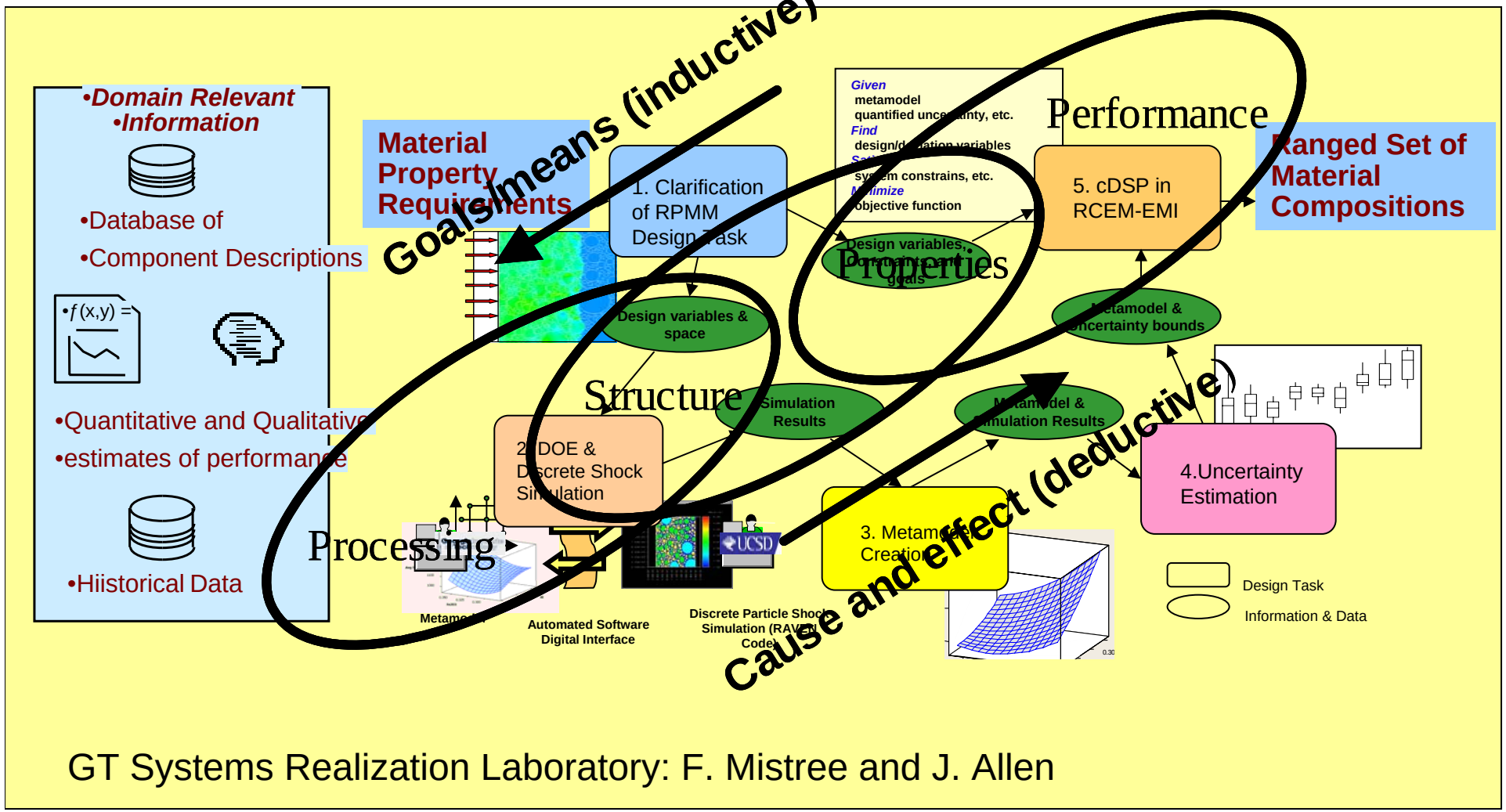
Olson et al. (1990): Design Project for High Performance Alloy Steel



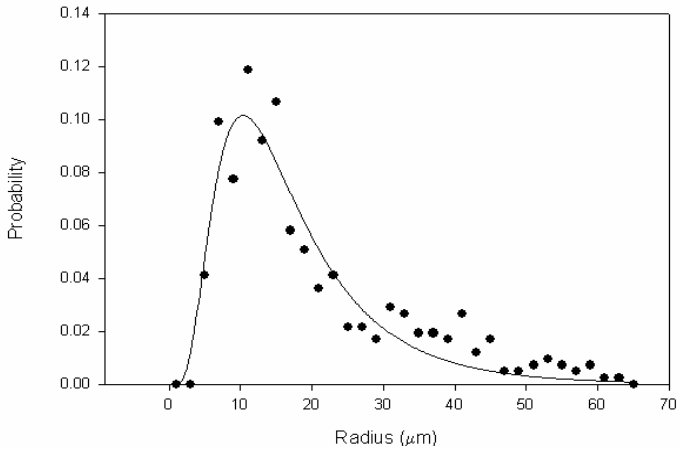
Reproduced from G.B. Olson, **Science**, 29 Aug., 1997, Vol. 277

Simulation-Based Design of Materials
Robust Concept Exploration

Incorporates reciprocity and hierarchy through decision-modeling interfaces



GT Systems Realization Laboratory: F. Mistree and J. Allen



Mapping Concepts

PP

SP

PS

Performance Requirements

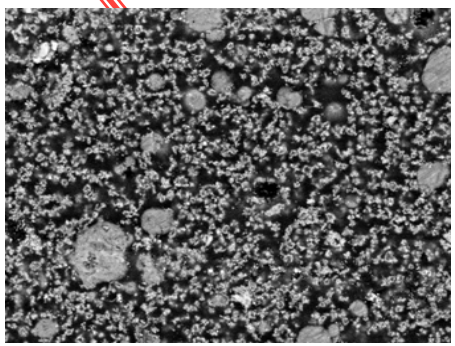
Properties, overlay on A', T, t, R_i

Microstructure Attributes, A', T, t, R_i
* dist functions
* explicit

Properties, overlay on A, T, t, R_i

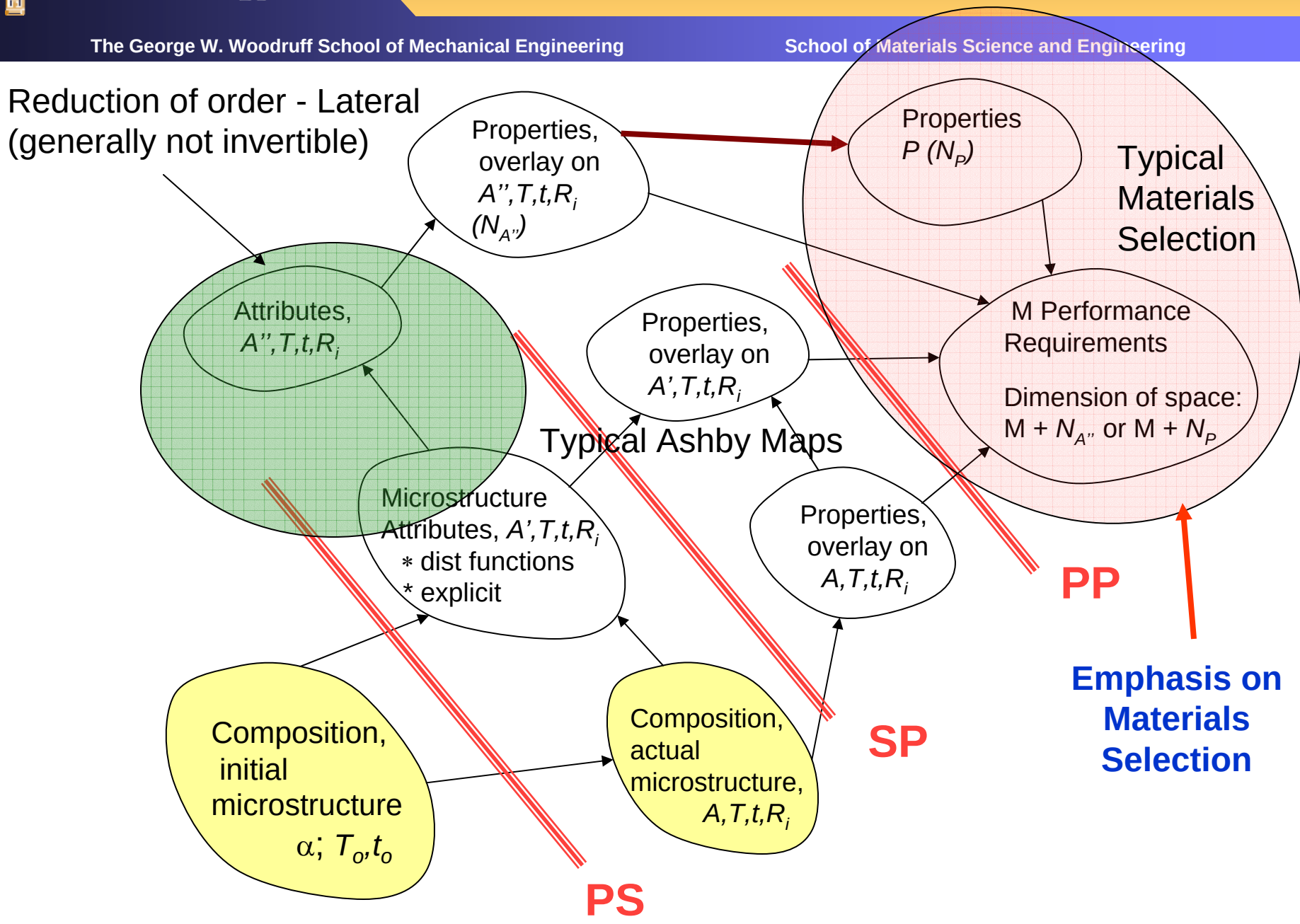
Composition, actual microstructure, A, T, t, R_i

Composition, initial microstructure α; T_o, t_o

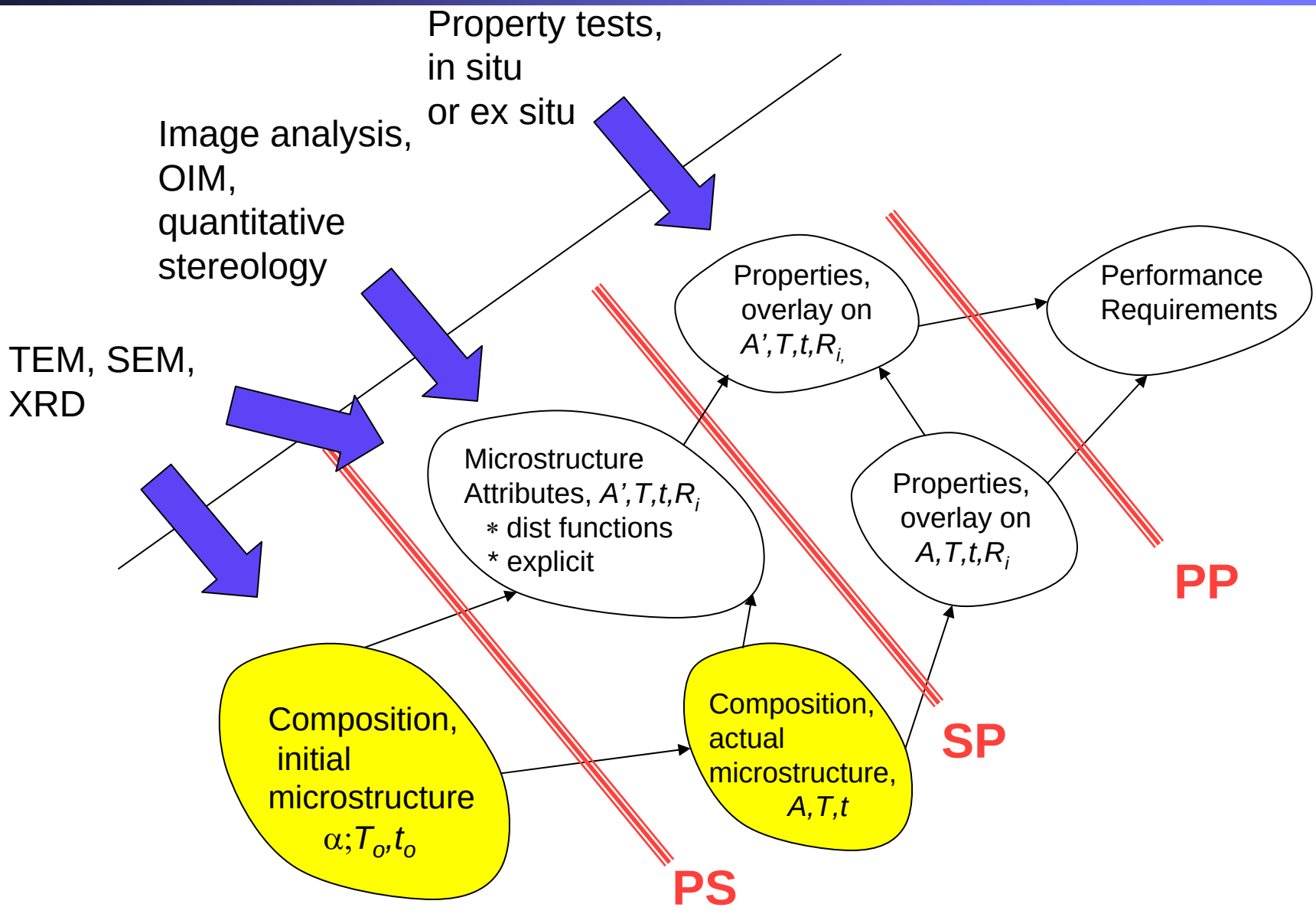


T – temperature
A – microstructure attributes
t – time
R_i – forcing functions

Contrast with Materials Selection



Calibration, Validation

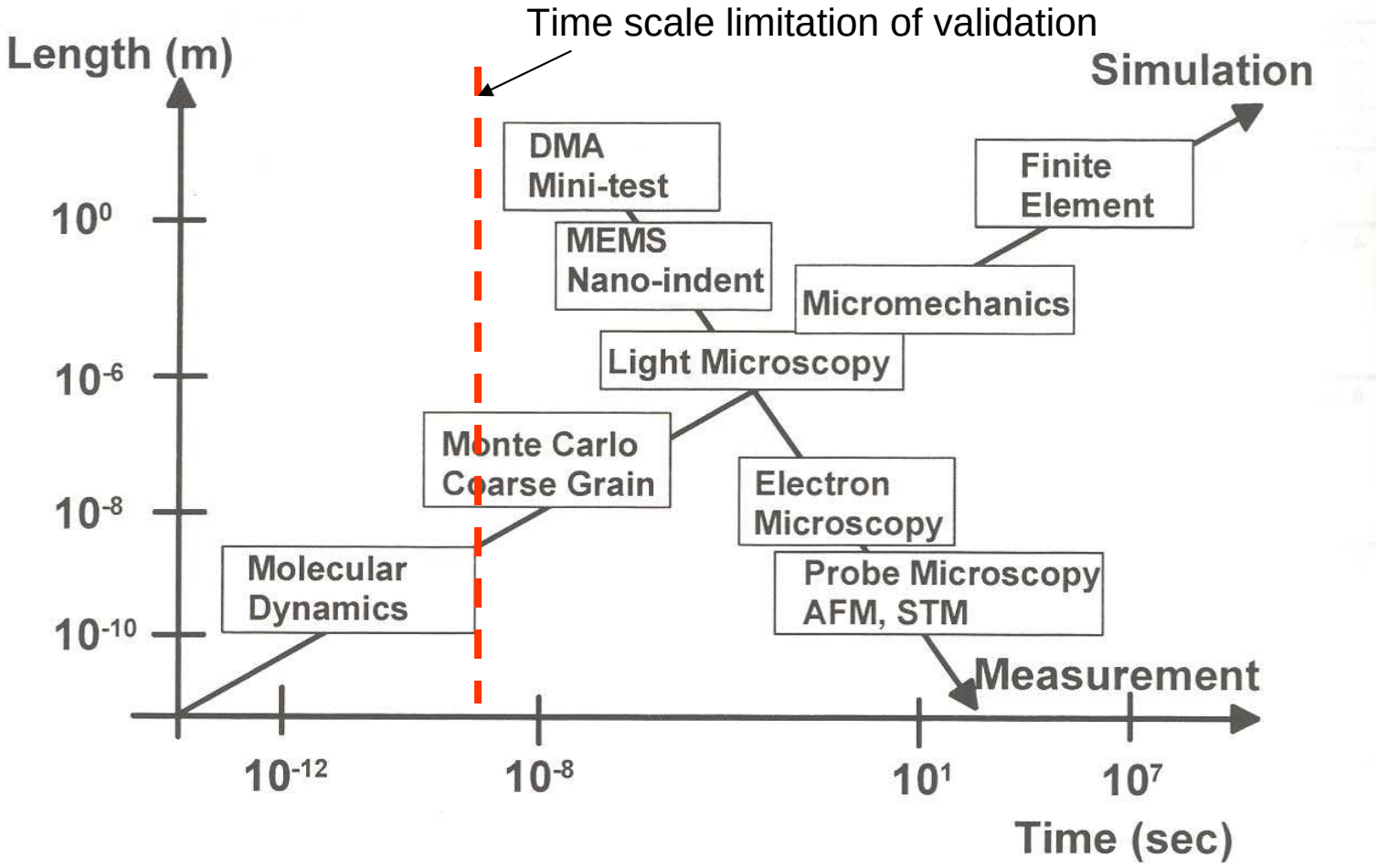


Significant Challenges: Modeling

- Distributions of extreme values of microstructure - important for properties related to fracture and fatigue, for example, not just mean field averages
- Nonlinear, path dependent behavior - limits extent of parametric study and parallelization of continuum analyses; engenders dependence upon initial conditions and limits rigorous inverse problem solutions
- Inverse problems - limited by dynamic to thermodynamic transitions, non-uniqueness in reduction of DOF, coupling of multiple attributes in establishing properties
- Wide range of suboptimal solutions based on specified objective functions are common
- Microstructure representation – how much information should be stored and in what form(s)?
- Process capabilities, thermodynamics and kinetics (history) places bounds on accessible or feasible microstructures
- Uncertainty (natural variability, measurement, model idealization)
- Archiving – archived data structures for later re-interpretation

The Model Validation Challenge

Gates, T.S. and Hinkley, J.A., Computational Materials: Modeling and Simulation of Nanostructured Materials and Systems, NASA/TM-2003-212163, 2003.



Example

AFOSR MURI on DESIGN OF MULTIFUNCTIONAL ENERGETIC STRUCTURAL MATERIALS

EXAMPLE OF DISTRIBUTED, COLLABORATIVE, SYSTEMS-BASED MATERIALS DESIGN

(in third year of five year program)

http://www.afosrmuri.gatech.edu/

Multifunctional Material Requirements

One of the key driving forces for development of systems-based design of materials is the need for materials to meet multiple, application-specific performance objectives.

- By definition, a multifunctional material is one for which performance dictates multiple property requirements.
- Single property domain with multiple, often conflicting, requirements:

  example → strength, ductility

- Multiple property domains:

  example – gas turbine engine blade materials

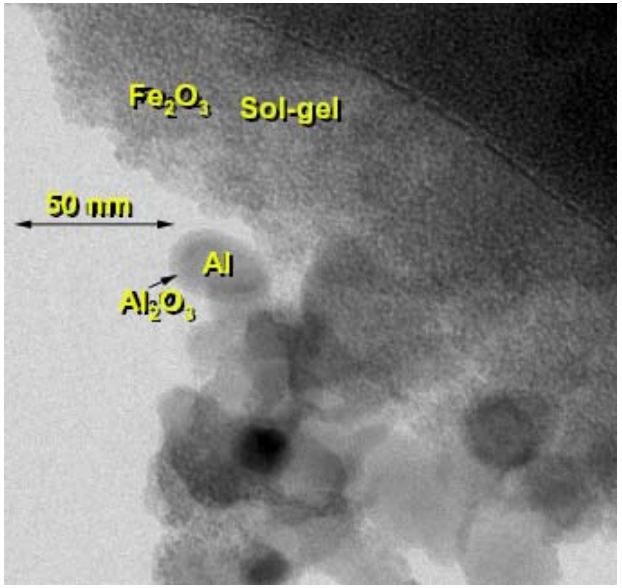
  - conductivity (thermal)
  - oxidation resistance (thermo-chemical)
  - elastic stiffness (mechanical)
  - High temperature creep and fatigue resistance (thermo-mechanical)

→ Need multi-objective, not single objective, design approach

Reactive/Energetic Materials Systems

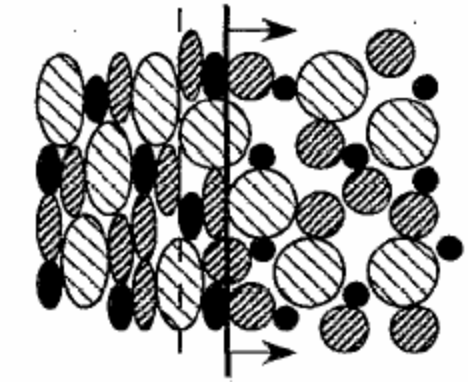
Initial system:

$Fe_2O_3 + 2Al = Fe + Al_2O_3 + \Delta H_R = -282\ kJ/mol$

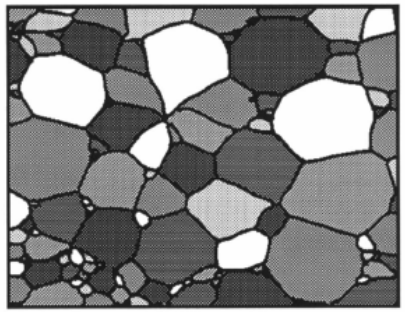


- Variation of Microstructures
  - Void collapse
  - Mass and momentum exchange
  - Dislocation generation

shock front



before



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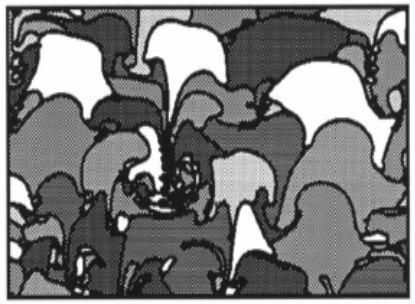
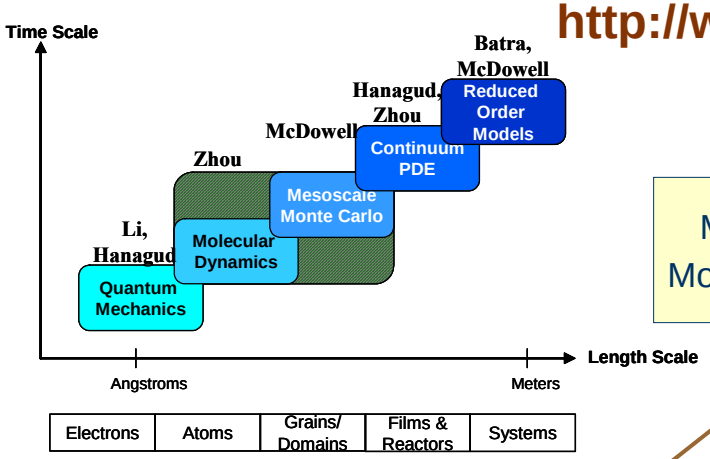


http://www.afosrmuri.gatech.edu/

AFOSR MURI – Research Overview

The George W. Woodruff School of Mechanical Engineering — School of Materials Science and Engineering

http://www.afosrmuri.gatech.edu/



Multiscale Modeling:
- *First-Principles,* MD, Meso scales and continuum scale models.
- Constitutive Equations, dual branches of Failure criteria
- Bridging scales to continuum

Material Tests and Model Validation Tests

Critical experiments to validate constitutive equations, strength, toughness, reaction Initiation, and Reaction propagation on MESM

Universities

- Synthesis of MESM
- Binder + Gas phase materials
- Reinforcement
- Fracture characteristics and Improvement of fracture toughness

Design of MESM and applications

Basic research relevant to applications, demonstration of an application

AFRL & LLNL

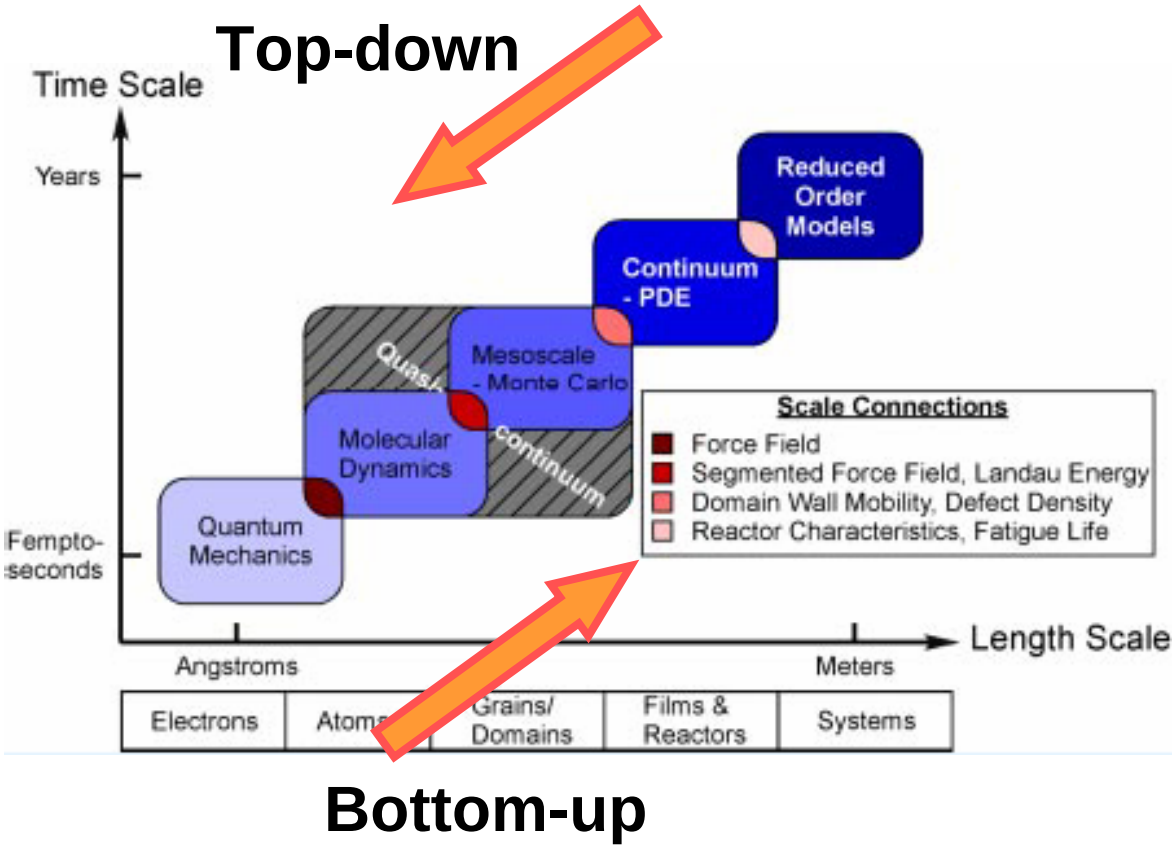
Predictive Equations, Procedures for Munitions Designs, & Procedure of use of dual functioned ESMs

Tests of applications

Analysis of Recovered Penetrators

PI: S. Hanagud

Multiscale Modeling



- Integrate time and length scales
- Ab initio/first-principles
- Molecular dynamics
- Continuum mechanics:
  - *Description of micro-structure: mixture with voids and defects*
  - *Model of microscale responses*
  - *Macroscale response: appropriate ensemble of microscale responses*

Multiscale Modeling for Materials Design

Top down

- Iterative higher/lower scale solution strategies
- “Handshaking”, passing parameters and qualitative nature of results
- Informed higher scale representations

- Domain decomposition
- Equivalence criteria of discrete and continuum solutions
- Matching rates of reaction, dissipation
- Informed constitutive relations

Bottom up

Need an **information model** that

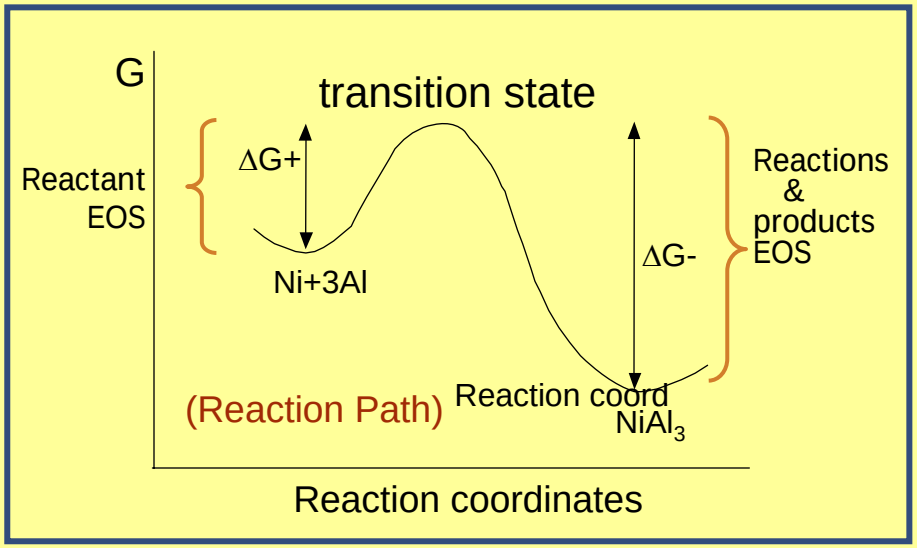
- Captures information at different length scales
- Translates information across time scales
- Incorporates mathematical relations and empirical data
- Facilitates traversing *Top down* and *Bottom up* on length scale

First principles calculations of transition states and EOS

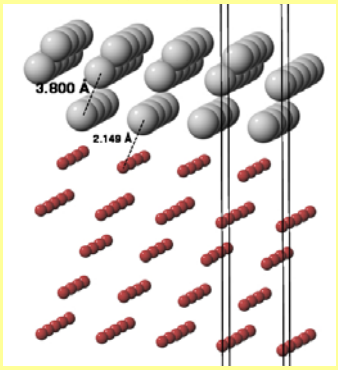
The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

Xia Lu and Sathya Hanagud

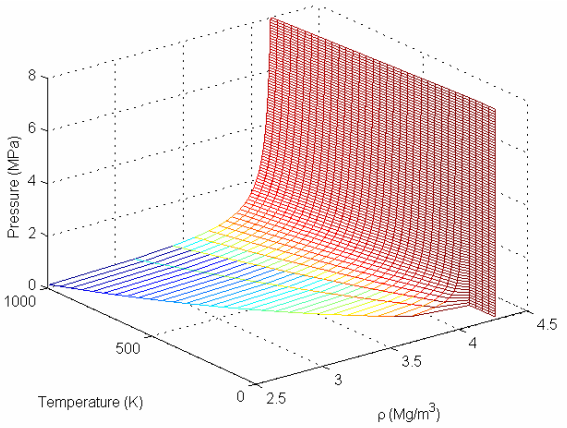


(111) Al

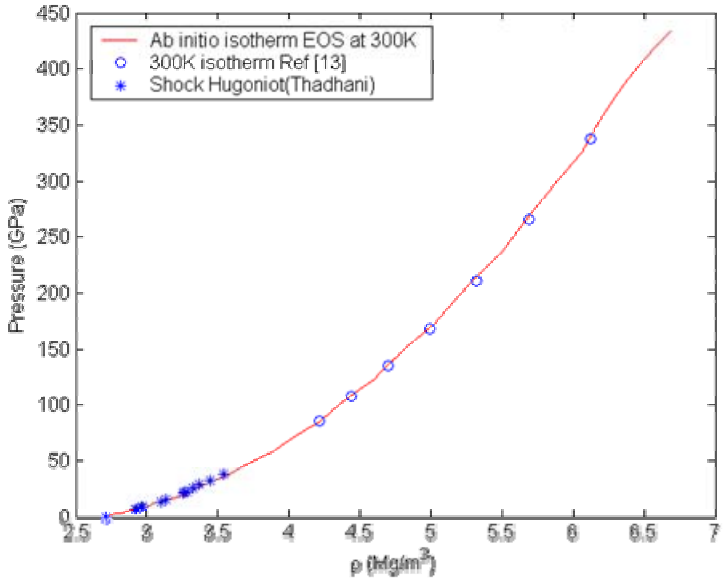


(111) Ni

Transition states for Chemical reactions



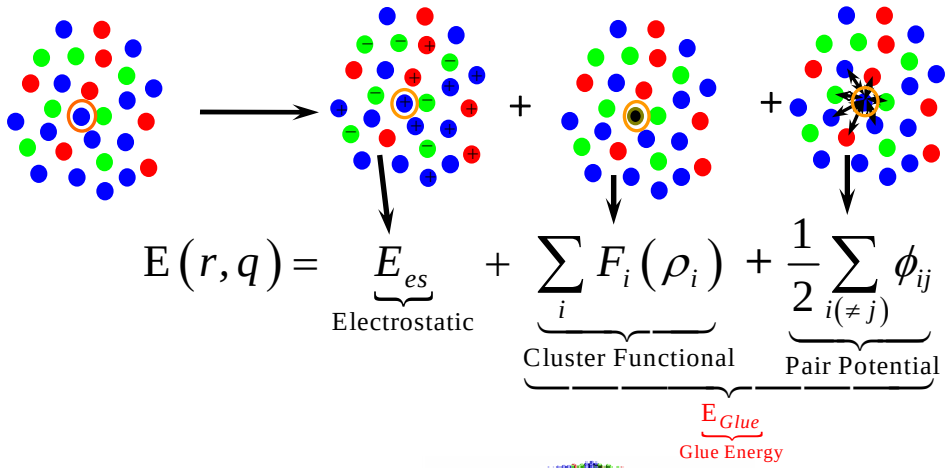
First principles EOS

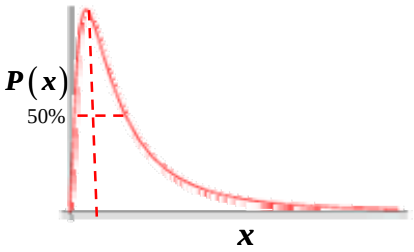


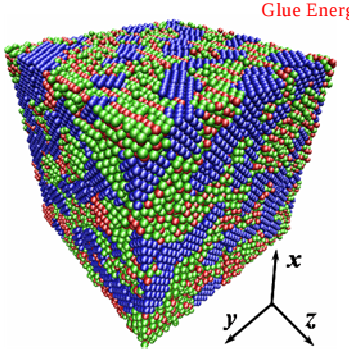
MD Calculations and Analyses

The George W. Woodruff School of Mechanical Engineering
School of Materials Science and Engineering

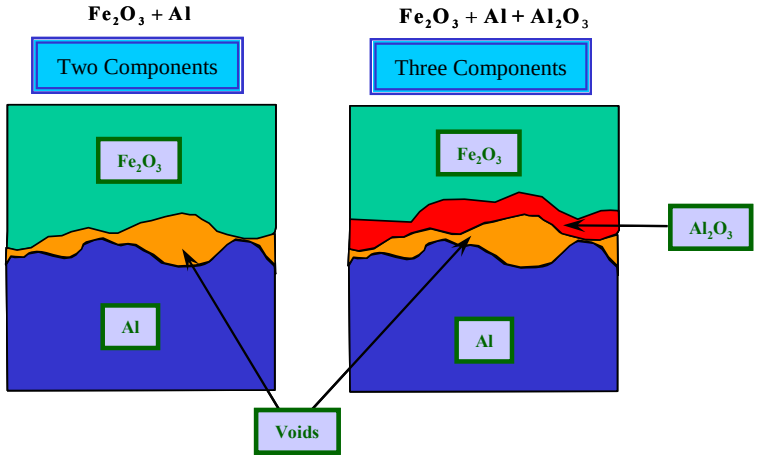
Vikas Tomar and Min Zhou

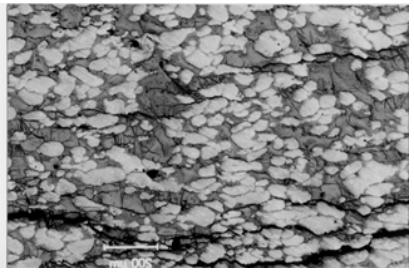






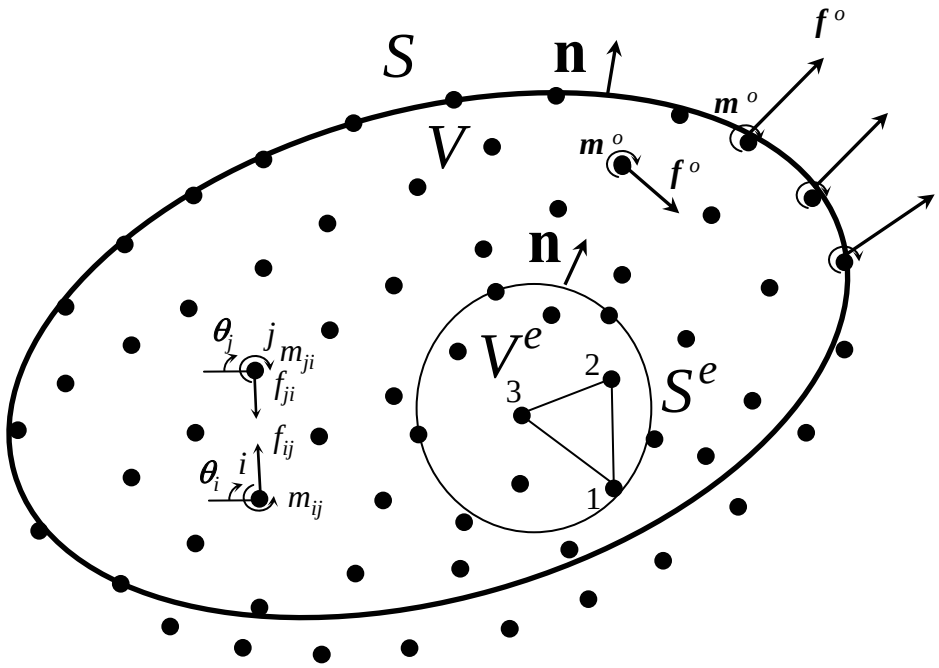
$Al + Fe_2O_3$





Equivalent Continuum (EC)

Zhou & McDowell, Phil Mag, 2002



MD System

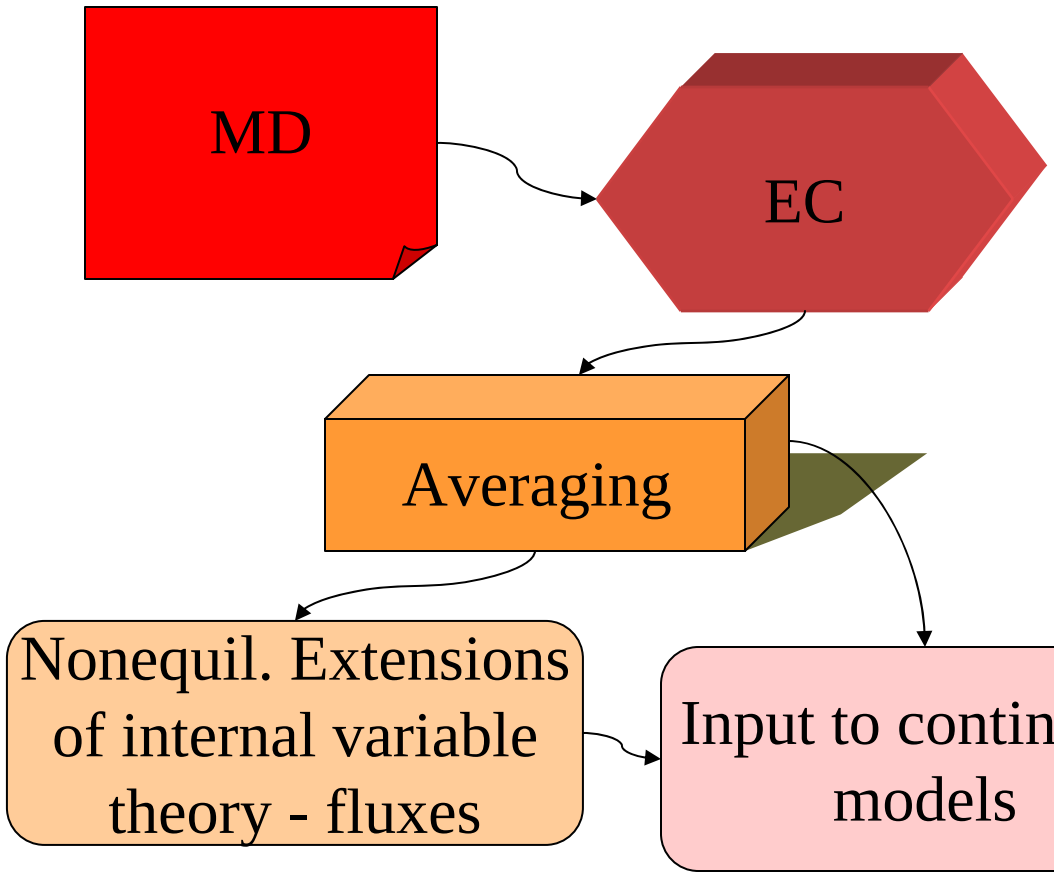
$$E = \frac{1}{2}\sum_{\substack{i,j \\ i \neq j}} \Phi(r_{ij}, \theta_{ij}), \quad m_i, \quad \mathbf{u}_i, \quad \theta_i$$

$$\begin{cases} \boldsymbol{f}_{ij} = \dfrac{1}{2}\dfrac{\partial \Phi(r_{ij}, \theta_{ij})}{\partial r_{ij}}\dfrac{\mathbf{r}_{ij}}{r_{ij}}, & \boldsymbol{f}_{ij} = -\boldsymbol{f}_{ji} \\ \boldsymbol{m}_{ij} = \dfrac{1}{2}\dfrac{\partial \Phi(r_{ij}, \theta_{ij})}{\partial \theta_{ij}}. & \boldsymbol{m}_{ij} = -\boldsymbol{m}_{ji} \end{cases}$$

Continuum

$$\boldsymbol{\sigma}, \ \boldsymbol{\mu}, \ \boldsymbol{t}, \ \boldsymbol{m}^S, \ \boldsymbol{b}, \ \boldsymbol{m}^b, \ \mathbf{u}, \ \theta, \ \rho$$

MD to Continuum



MD System

$$E = \frac{1}{2}\sum_{\substack{i,j \\ i \neq j}} \Phi(r_{ij}, \theta_{ij}), \quad m_i, \quad \mathbf{u}_i, \quad \theta_i$$

$$\begin{cases} \boldsymbol{f}_{ij} = \dfrac{1}{2}\dfrac{\partial \Phi(r_{ij}, \theta_{ij})}{\partial r_{ij}}\dfrac{\mathbf{r}_{ij}}{r_{ij}}, & \boldsymbol{f}_{ij} = -\boldsymbol{f}_{ji} \\ \boldsymbol{m}_{ij} = \dfrac{1}{2}\dfrac{\partial \Phi(r_{ij}, \theta_{ij})}{\partial \theta_{ij}}. & \boldsymbol{m}_{ij} = -\boldsymbol{m}_{ji} \end{cases}$$

Continuum

$$\boldsymbol{\sigma}, \ \boldsymbol{\mu}, \ \boldsymbol{t}, \ \boldsymbol{m}^S, \ \boldsymbol{b}, \ \boldsymbol{m}^b, \ \mathbf{u}, \ \theta, \ \rho$$

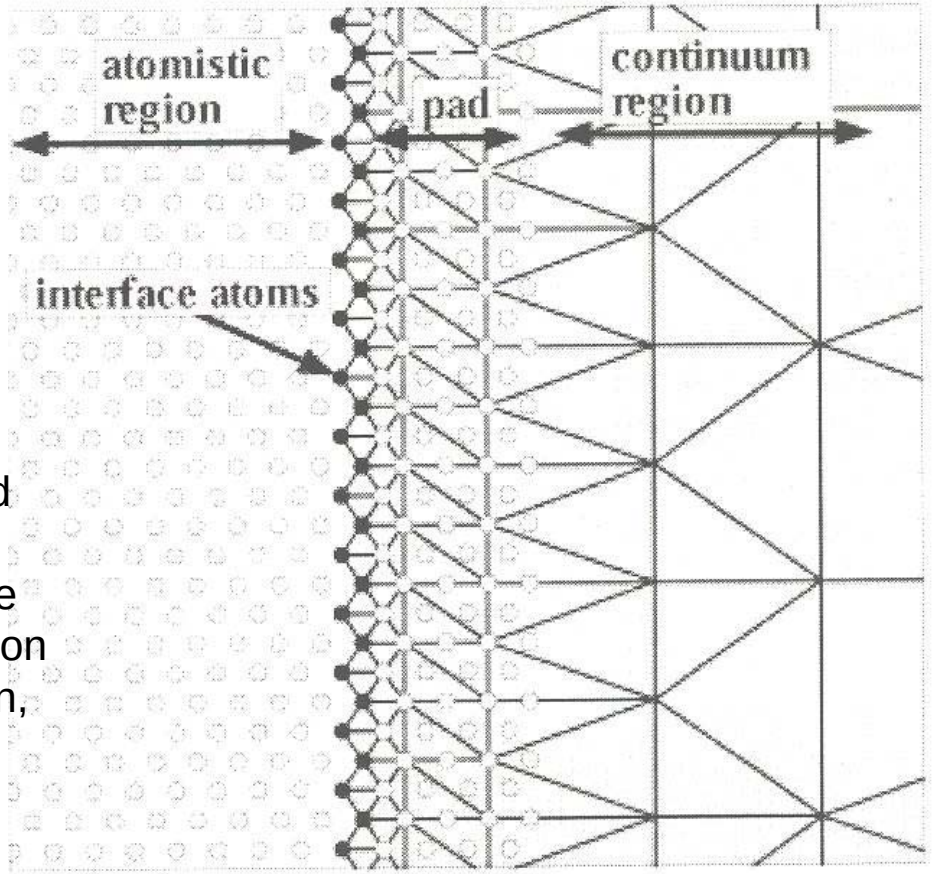
Methods for Domain Decomposition

Generic transition region from atomistics to continuum

No “unified” theory exists for the Transition.

Generic transition:

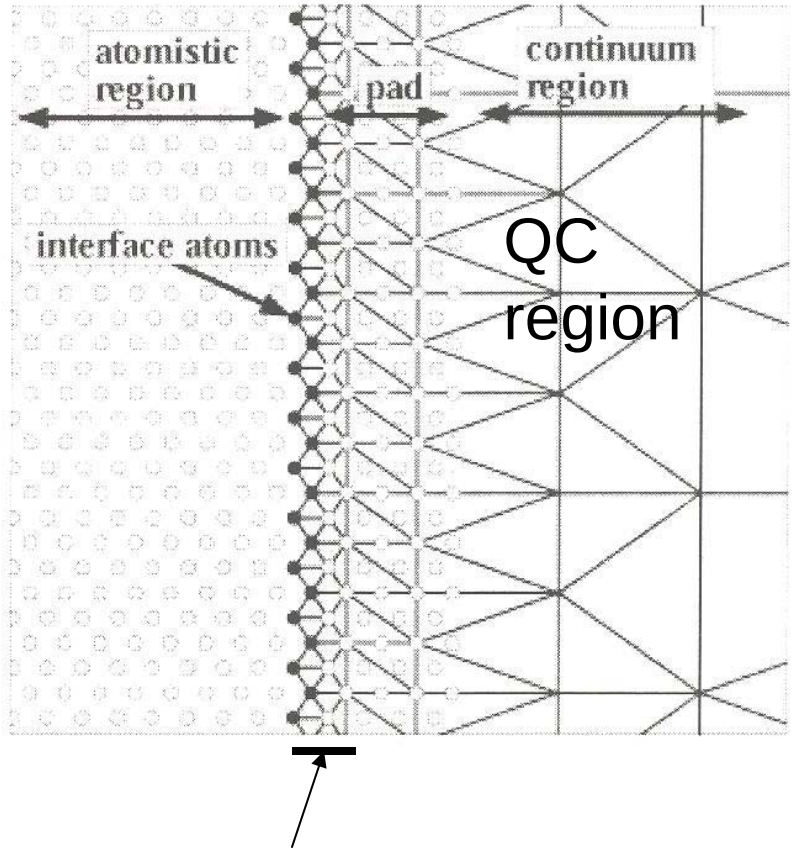
- Atomistic: every atom is explicitly represented
- Interface: one-to-one correspondence between atoms in atomistic region and nodes in FE mesh
- Beyond interface, mesh becomes more sparse as it spans into continuum region
- Atoms overlap FE mesh in “pad” region, necessitated by nonlocal nature of interatomic interactions; without it, aphysical surface energy would be introduced at atomistic/FE interface.



Quasicontinuum Method

Tadmor, E.B., Ortiz, M., Phillips, R., Phil. Mag. A73(6):1529-1563, 1996.
Shenoy, V.B., Miller, R., Tadmor, E., Rodney, D, Phillips, R. and Ortiz, M., J. Mech. Phys. Solids, 47:611-642, 1998.

- No classical continuum model – only distinction between "local" and "nonlocal" representative atoms
- "nonlocal" representative atoms are representative of atomistic regions in other methods
- "local" representative atoms are analogous to continuum FE nodes
- Energy of elements that touch interface atoms is weighted differently in total potential energy
- Energy of elements in continuum or "local" region is computed using atomistic potentials for a given deformation gradient for an infinite crystal (Cauchy-Born approximation is made that uniform macroscopic leads to uniform elastic deformation – effectively removes atomic DOF, but severely limits admissible atomic motion; cannot describe motion of point or line defects)



Hierarchical Modeling

Quasicontinuum Method

• Tadmor, E.B., Ortiz, M., Phillips, R., Phil. Mag. A73(6):1529-1563, 1996.
• Shenoy, V.B., Miller, R., Tadmor, E., Rodney, D, Phillips, R. and Ortiz, M., J. Mech. Phys. Solids, 47:611-642, 1998.

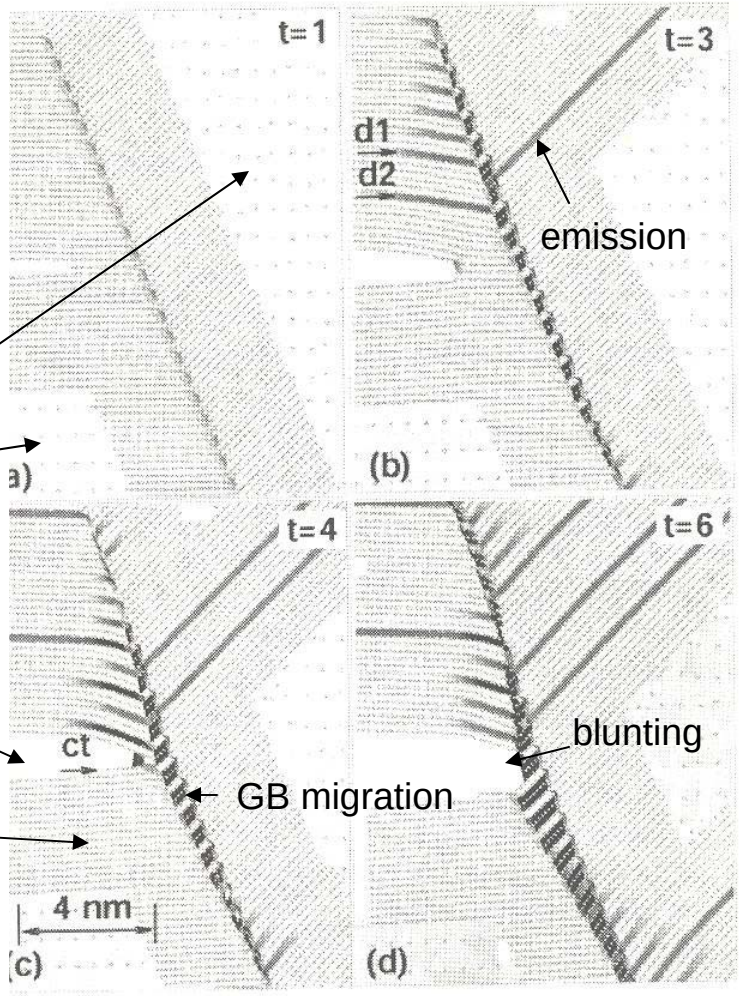
Molecular statics simulations

QC

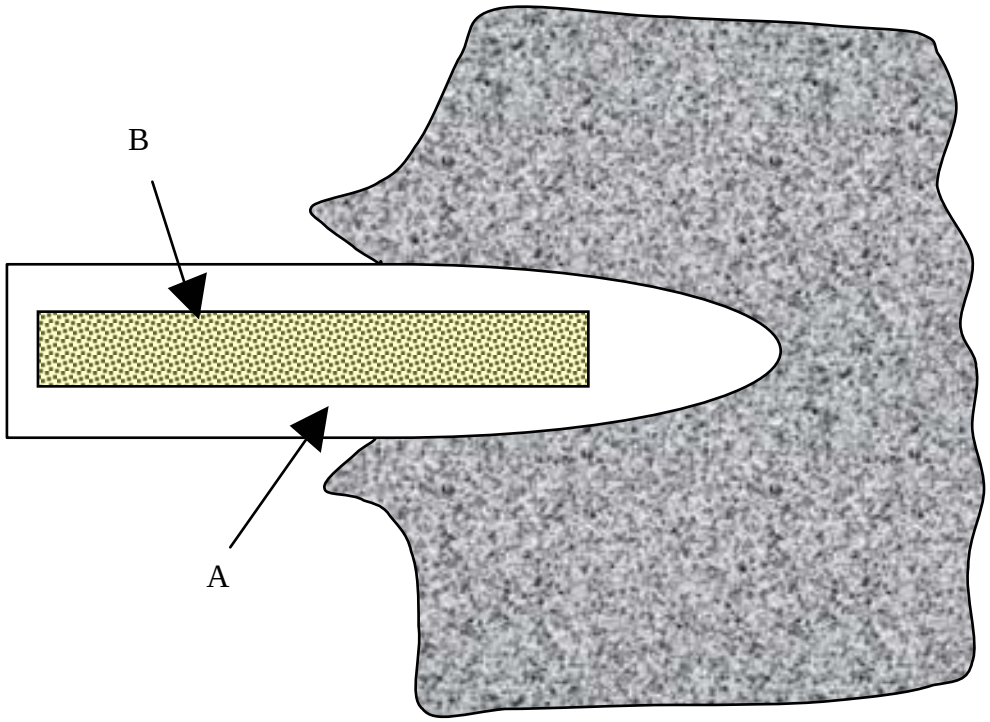
crack

atomistic

Crack impinging on GB



Top-Down Modeling Strategy



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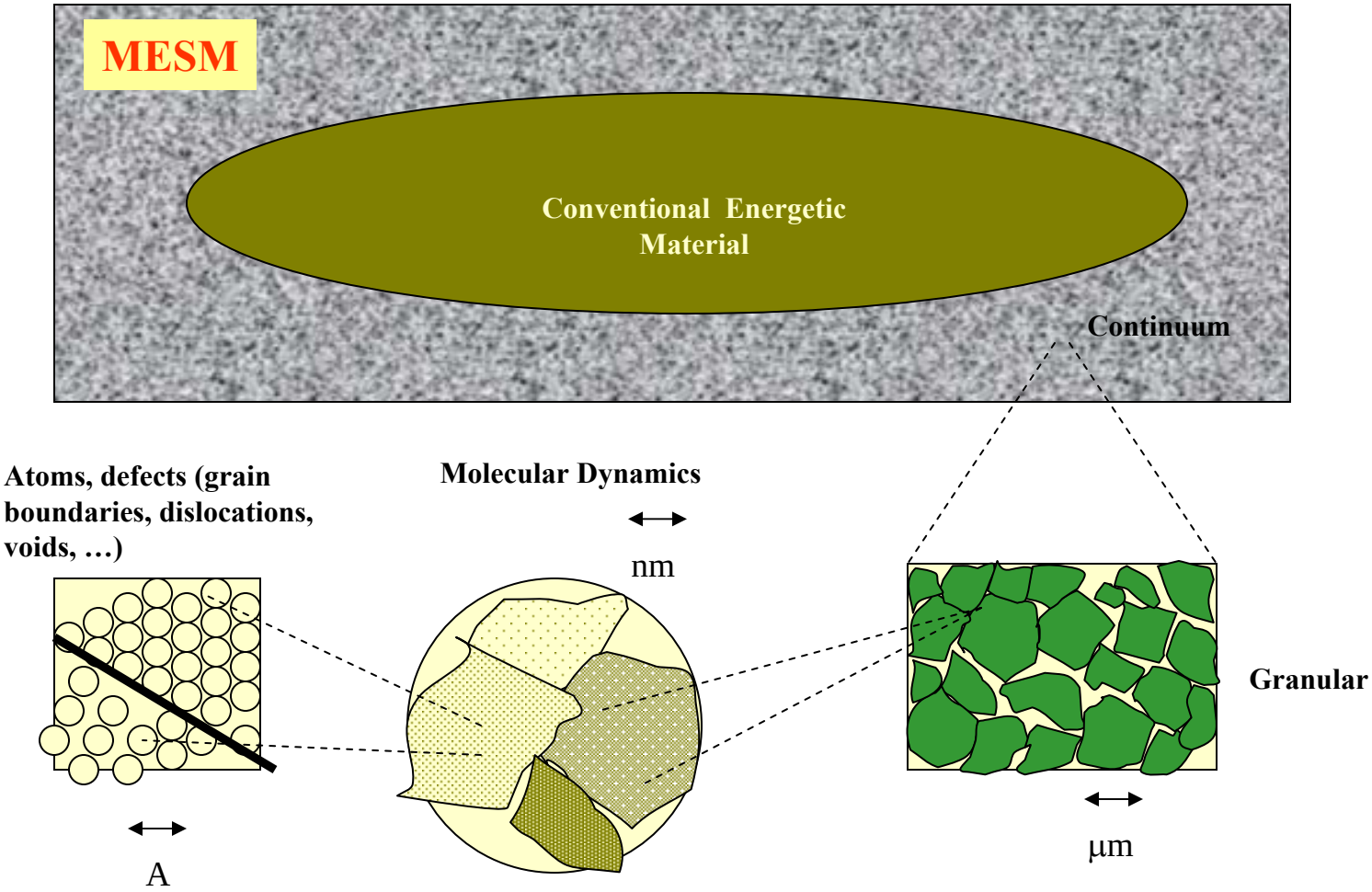
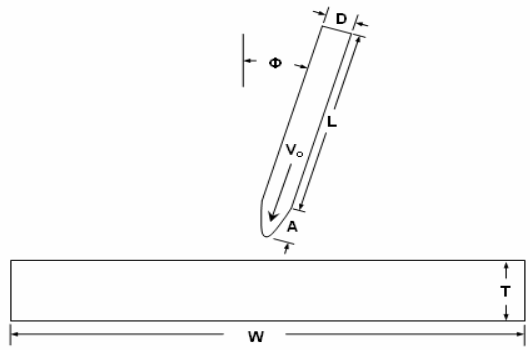
Multifunctional Energetic Structural Material

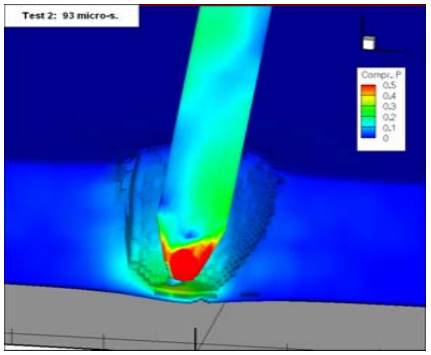


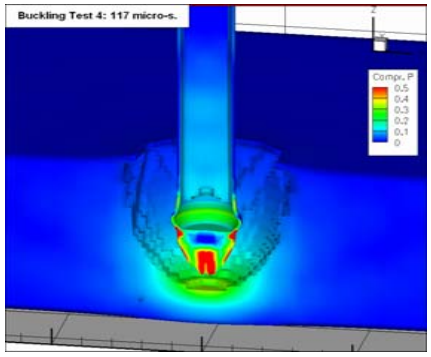
http://www.afosrmuri.gatech.edu/

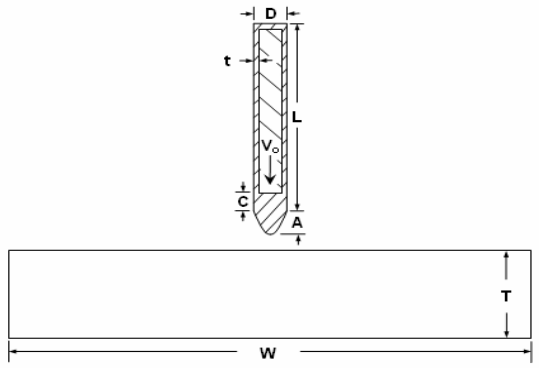
Full Scale Projectile Calculations

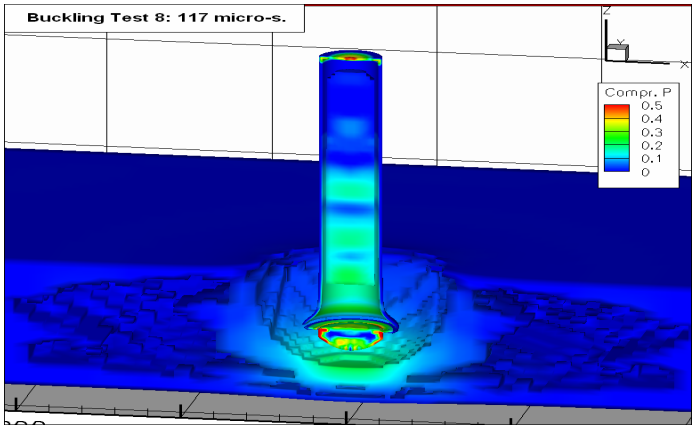
Batra et al., VT









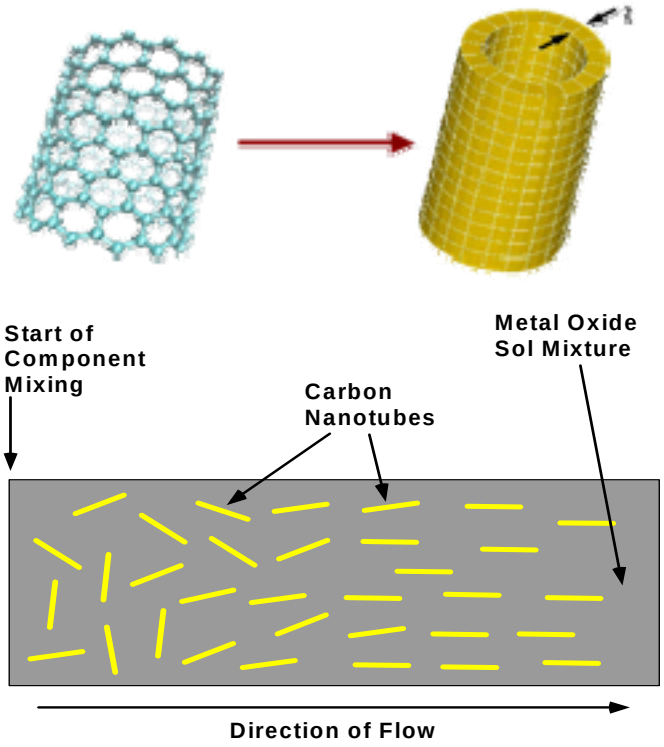


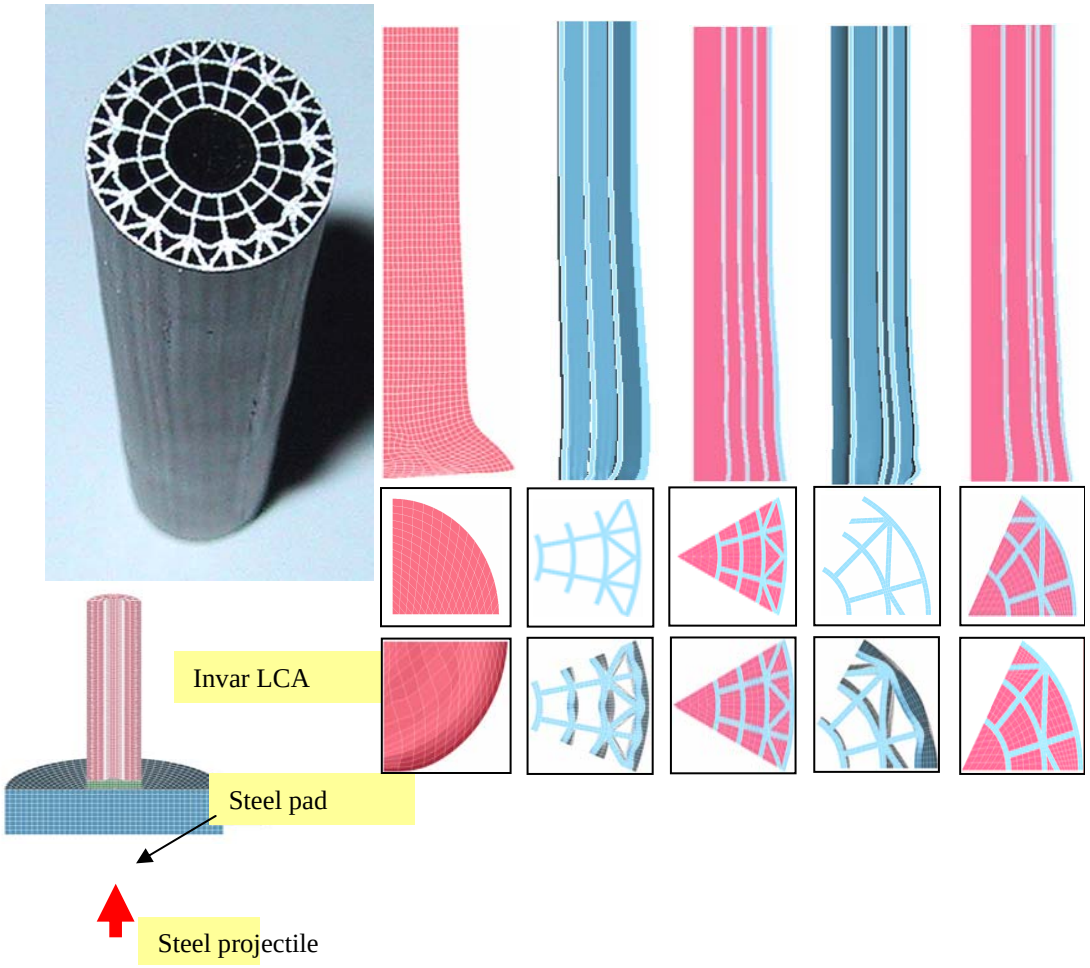
Reinforcement Concepts for Strength

The George W. Woodruff School of Mechanical Engineering
School of Materials Science and Engineering

Romesh Batra and Students

Aijun Wang, Ryan Austin, Dave McDowell, Joe Cochran and Naresh Thadhani



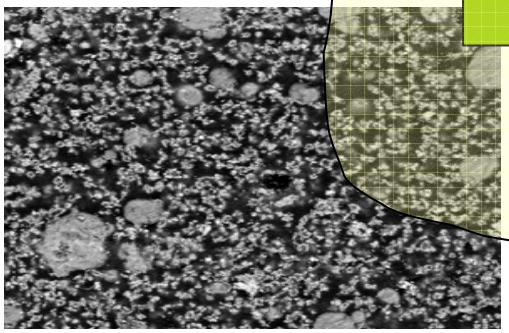


Analysis of Discrete Particle Systems

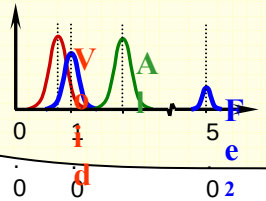
The George W. Woodruff School of Mechanical Engineering
School of Materials Science and Engineering

Ryan Austin and Dave McDowell

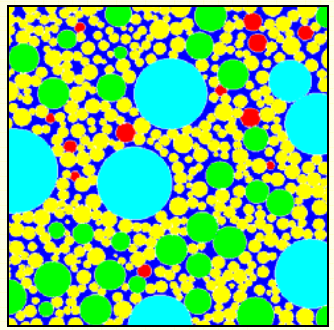
Actual Microstructure



Microstructural Descriptors

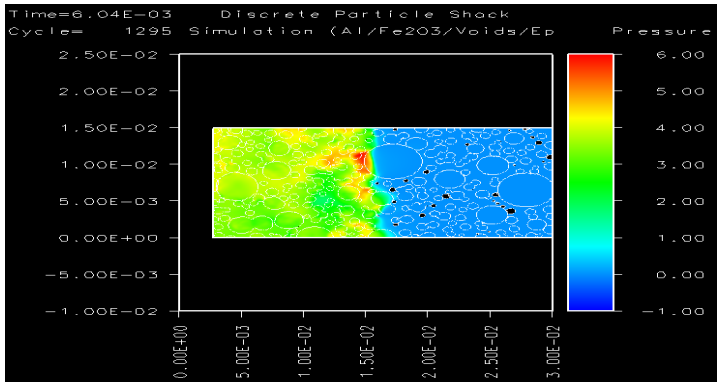


RAVEN



Simulated Microstructures

Element Meshing



With D. Benson, UCSD

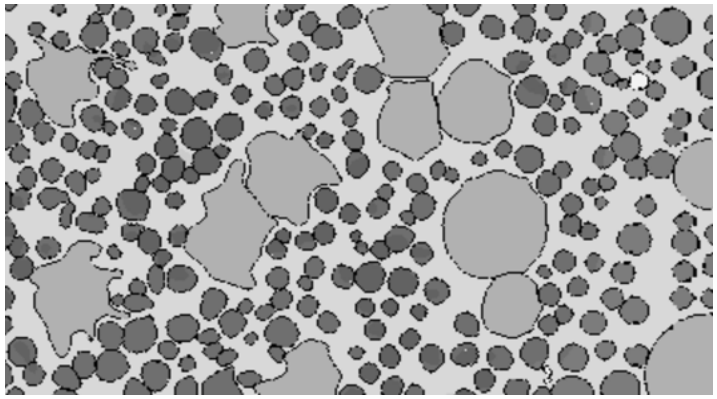
Explicit Hydrocode Simulations of Shock Wave Propagation

Parametric Studies and Design of Microstructures

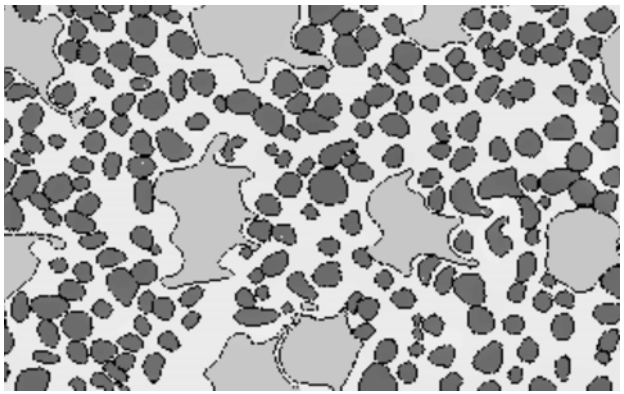
AFOSR MURI on Multifunctional Energetic Structural Materials

Thermomechanical Responses

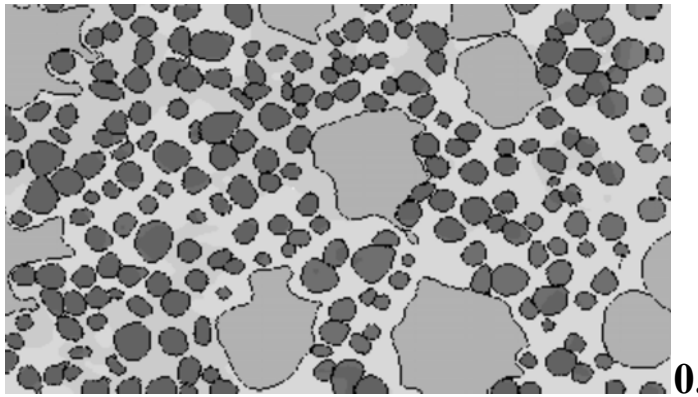
- Post-shock morphology (20% epoxy wt.)



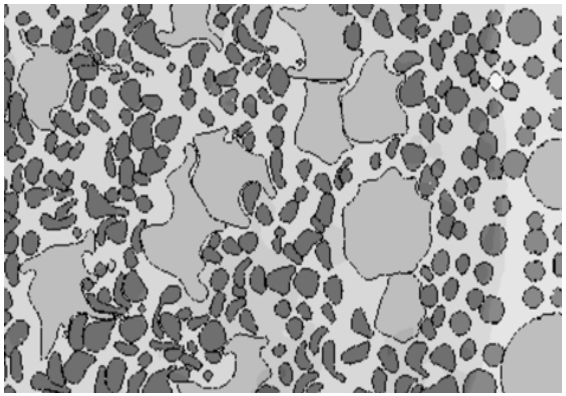
0.5 km/s



0.75 km/s



0.625 km/s



1.0 km/s

Non-Equilibrium Mixture Theory of Reactive Particle Systems

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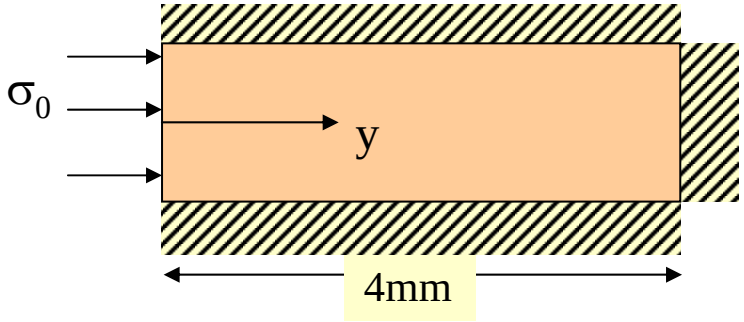
School of Materials Science and Engineering



Initial Stoichiometric mixture

reactants

c_{Al}=0.2545

c_{Fe2O3}=0.7455

products

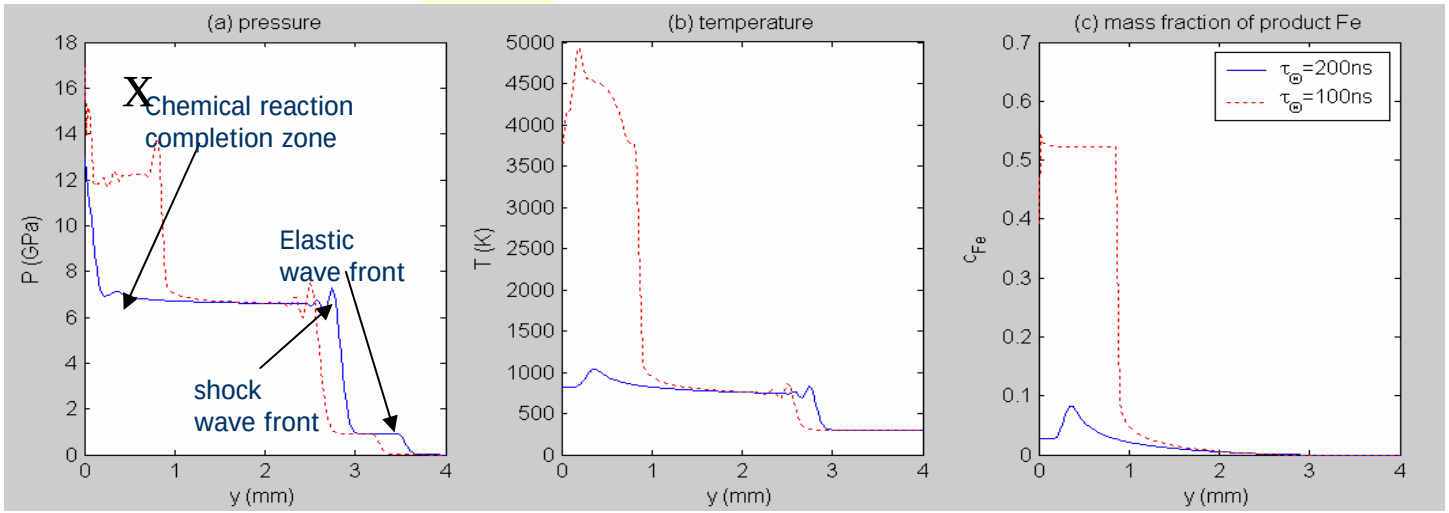
c_{Fe}=0

c_{Al2O3}=0

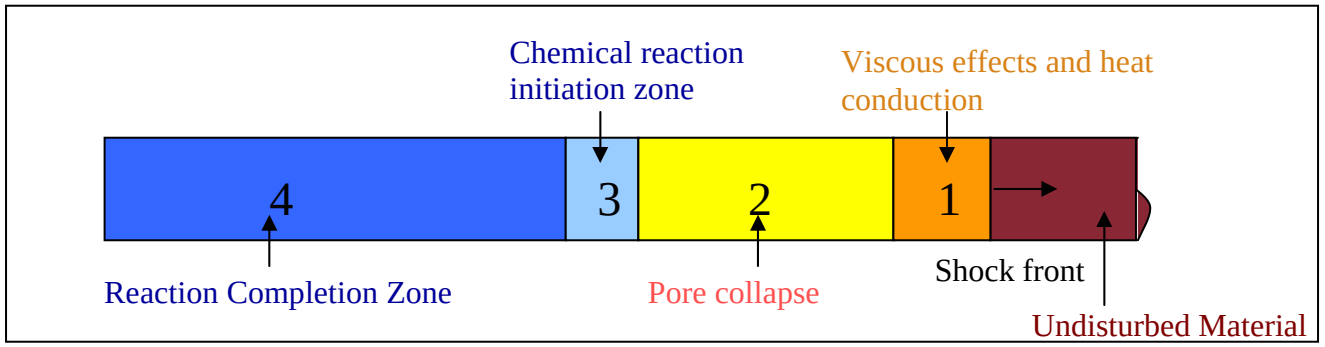
Initial porosity

α_0=1.5

$Fe_2O_3 + 2Al \rightarrow 2Fe + Al_2O_3$



Vindhya Narayanan, Xia Lu and Sathya Hanagud



MURI – MESM Test Problems

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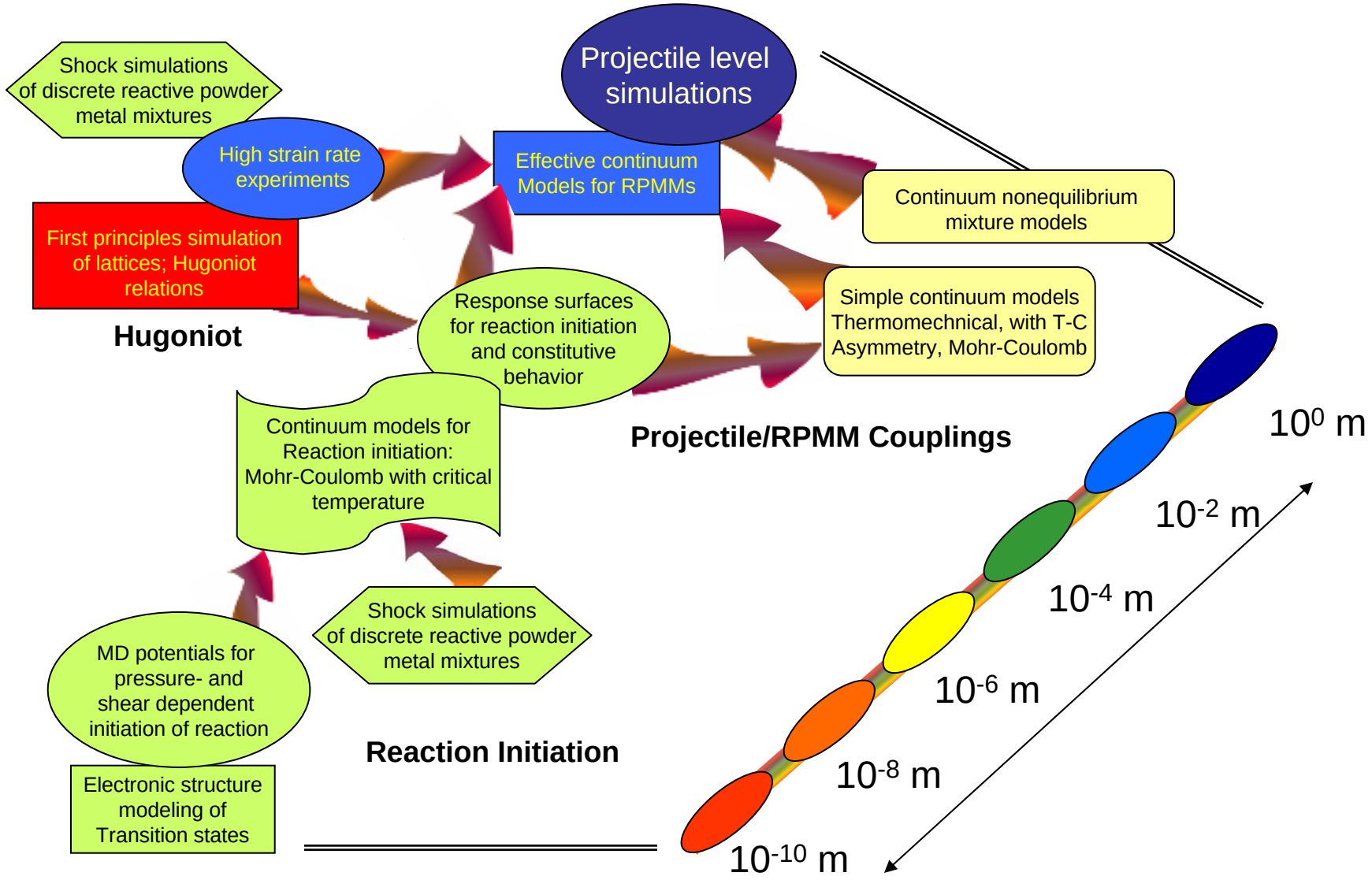
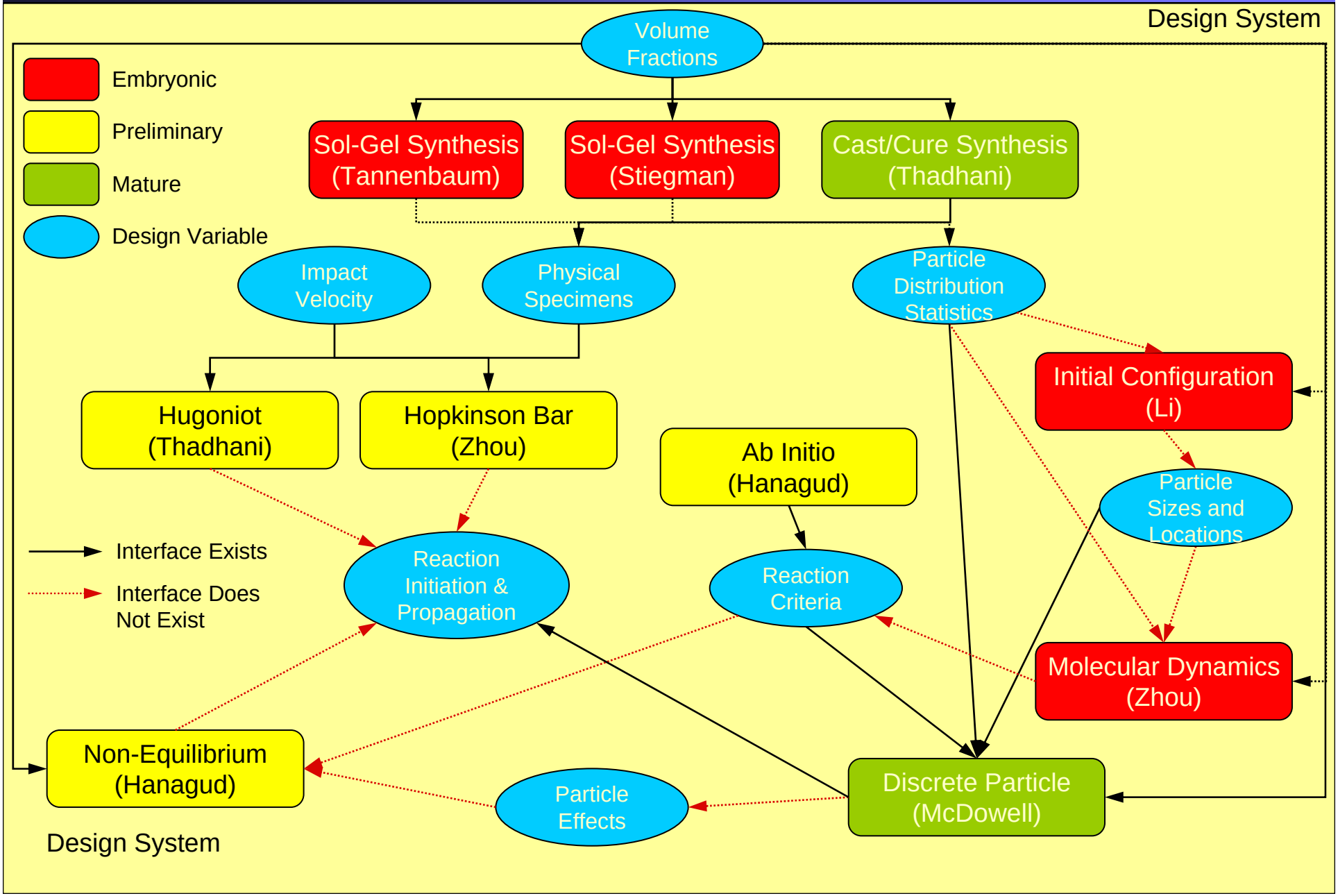


http://www.afosrmuri.gatech.edu/

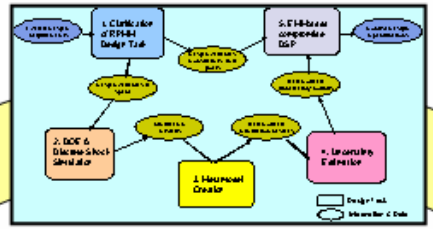
Reaction Criteria Sub-Problem (Design in Progress)

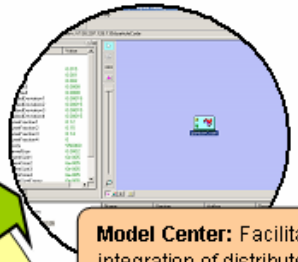


Virtual Materials Design Studio

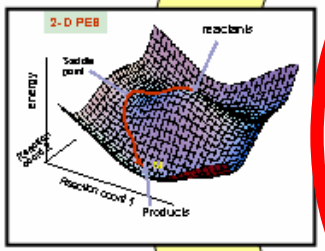
MURI Web Board: Facilitates collaboration among distributed stakeholders, project management, online discussions, and information archive (*http://www.afosrmuri.gatech.edu/phpBB2/index.php*)

Robust MESM Design

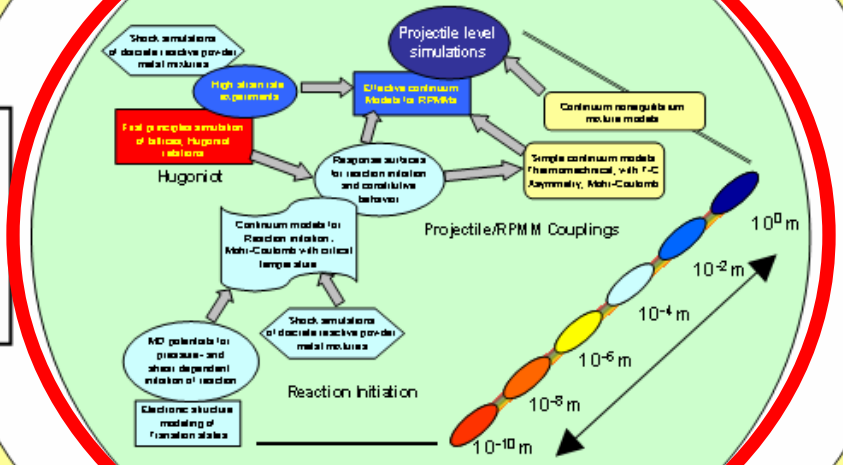


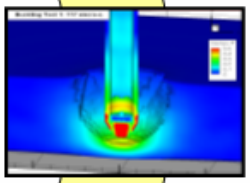


Model Center: Facilitates integration of distributed computing resources

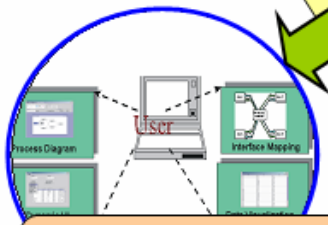


Chemical Reaction Initiation

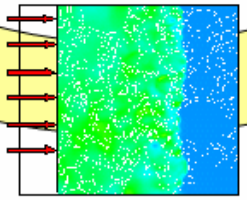




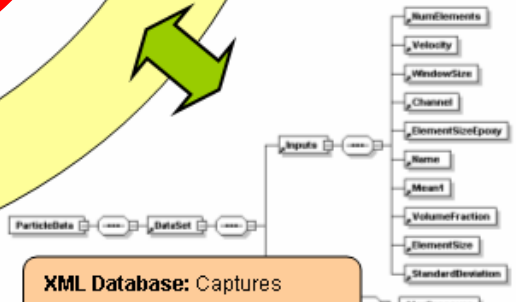
Projectile Level Simulation



X-DPR (eXtensible Distributed Product Realization): An open computer infrastructure, developed to allow integrated utilization of distributed resources (e.g., software codes and data).



Particle Shock Simulation

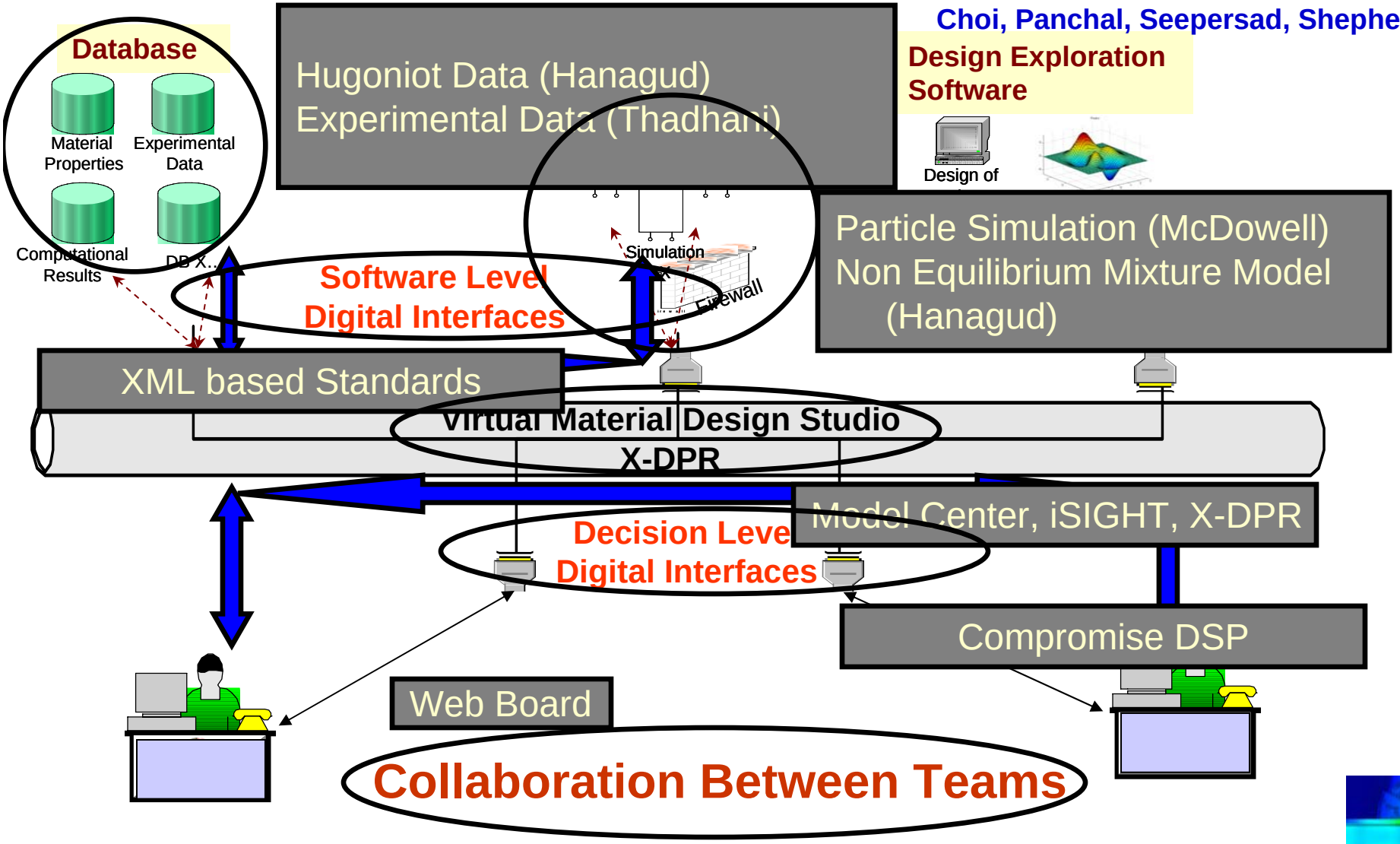


XML Database: Captures materials data, serves as a standard for inputs and outputs

Virtual Materials Design Studio

The George W. Woodruff School of Mechanical Engineering

Farrokh Mistree, Janet Allen
and Dave McDowell
Choi, Panchal, Seepersad, Shepherd



Type IV Robust Materials Design in Virtual Materials Design Studio

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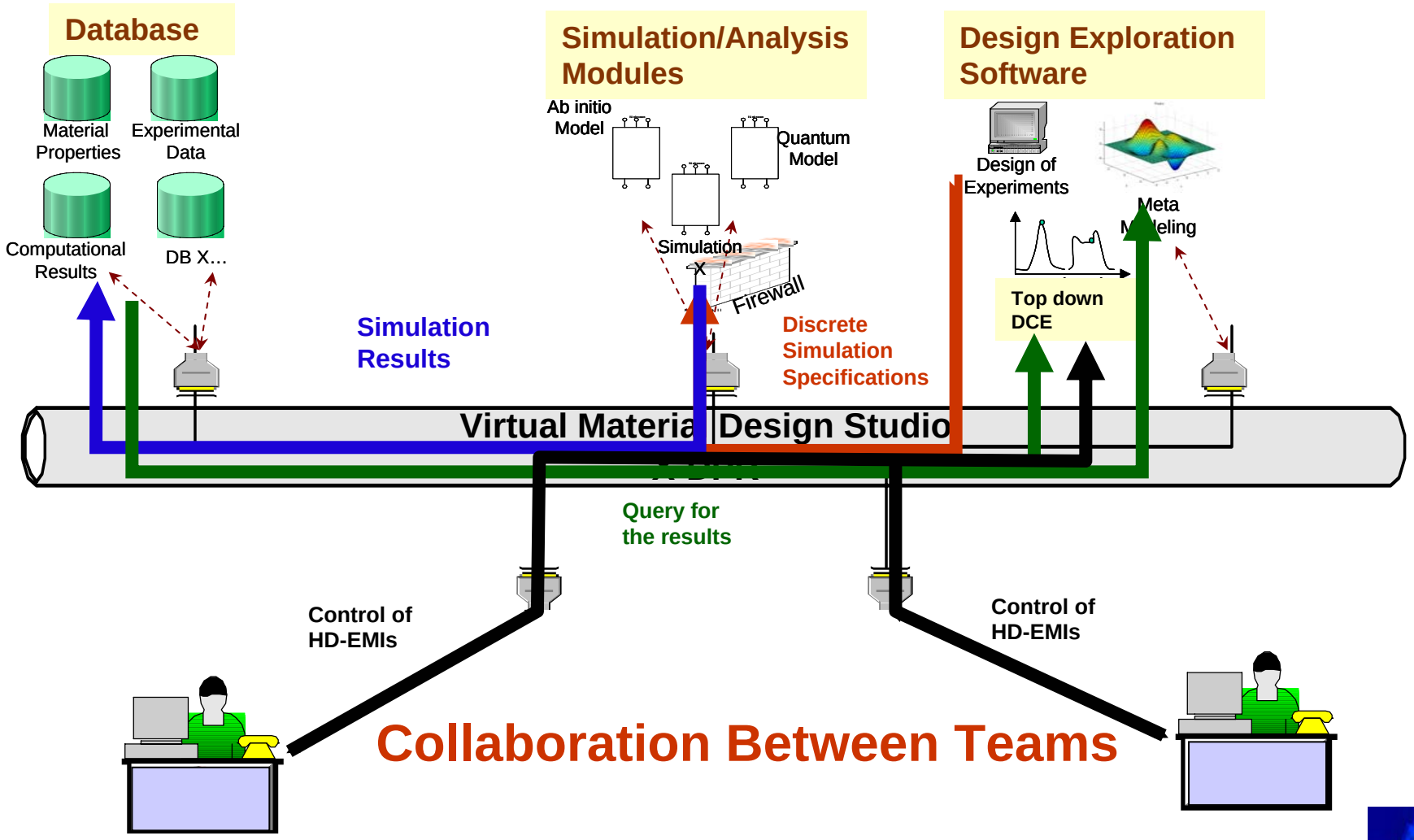
School of Materials Science and Engineering



Farrokh Mistree, Janet Allen and Dave McDowell

AFOSR MURI on Multifunctional Energetic Structural Materials

Multi-objective Decision Support

The Compromise Decision Support Problem

Traditional Single-Objective Optimization…

- What is it?
  - Mathematical model that facilitates the improvement of a feasible alternative through modification
  - Hybrid model based on mathematical programming and goal programming
- Why use it?
  - Provides structure and support for modeling decisions that involve seeking compromise among multiple conflicting goals or objectives

Given
n, number of decision variables
p, number of equality constraints
q, number of inequality constraints
$f(\boldsymbol{x})$, an objective function
$g_i(\boldsymbol{x})$, constraint functions

Find $\boldsymbol{x}$

Subject to
$g(\boldsymbol{x})=0 \quad i=1,\ldots,p$
$g_i(\boldsymbol{x})\leq 0 \quad i=p+1,\ldots,p+q$

Optimize
$f(\boldsymbol{x})$

Constraints from Math Programming

Single Objective

Goals and Deviation Variables from

Multiple Objectives

Goal Programming

Multi-Objective Decision Support: Compromise DSP…

Given
n, number of decision variables
p, number of equality constraints
q, number of inequality constraints
m, number of system goals
$g_i(\boldsymbol{x})$, constraint functions

Find
$\boldsymbol{x}$ (system variables)
d_i^-, d_i^+ (deviation variables)

Satisfy

System constraints:
$g(\boldsymbol{x})=0 \quad i=1,\ldots,p$
$g(\boldsymbol{x})\leq 0 \quad i=p+1,\ldots,p+q$

System goals:
$A_i(\boldsymbol{x})/G_i + d_i^- - d_i^+ = 1$

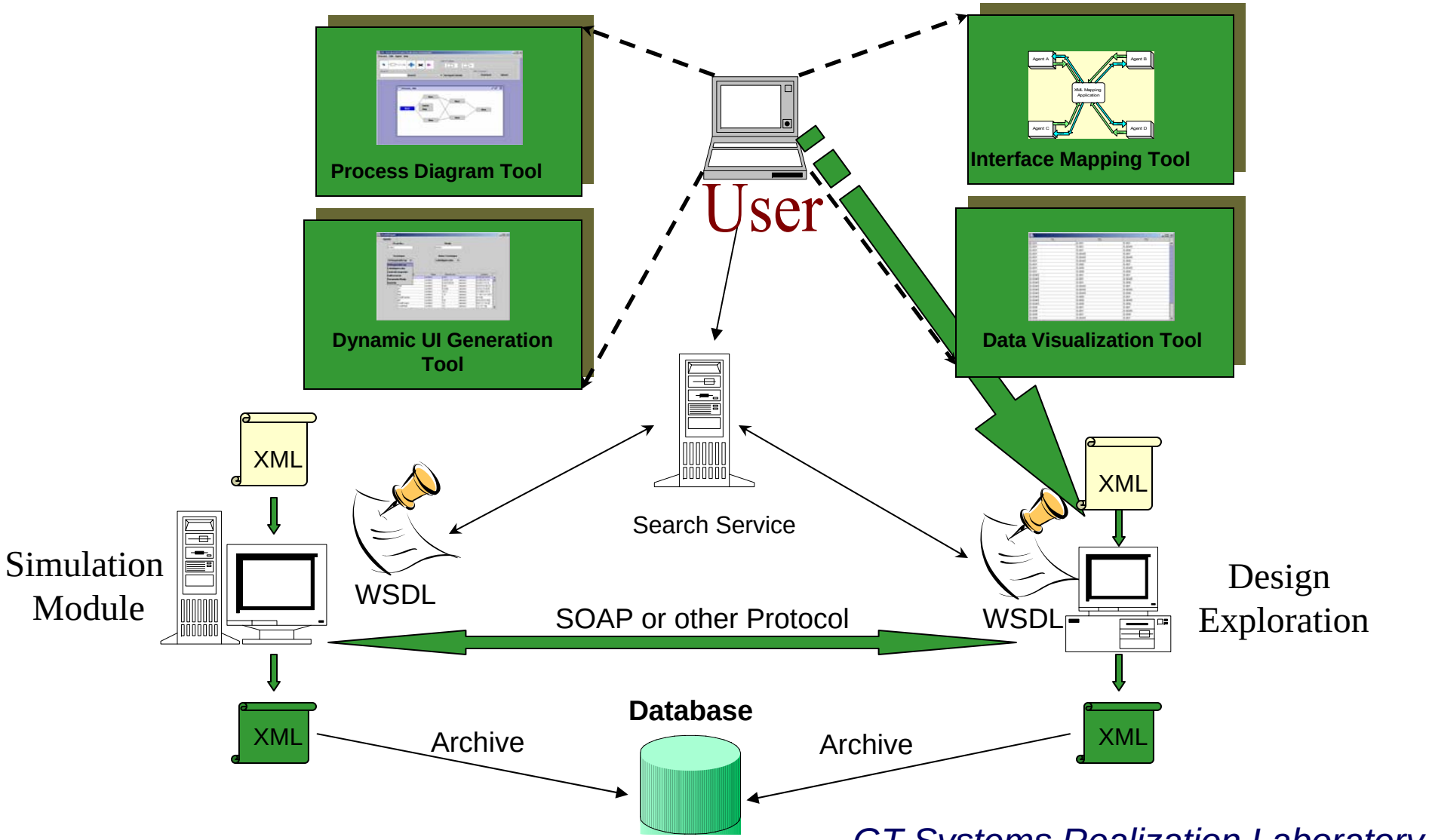
Bounds:
$X_i^{min} \leq X_i \leq X_i^{max}$
$d_i^-, d_i^+ \geq 0$ and $d_i^- \cdot d_i^+ = 0$

Minimize
$Z = [f_1(d_i^-, d_i^+), \ldots, f_k(d_i^-, d_i^+)]$ *preemptive*
$Z = \Sigma W_i (d_i^- + d_i^+)$ *Archimedean*

X-DPR Framework

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

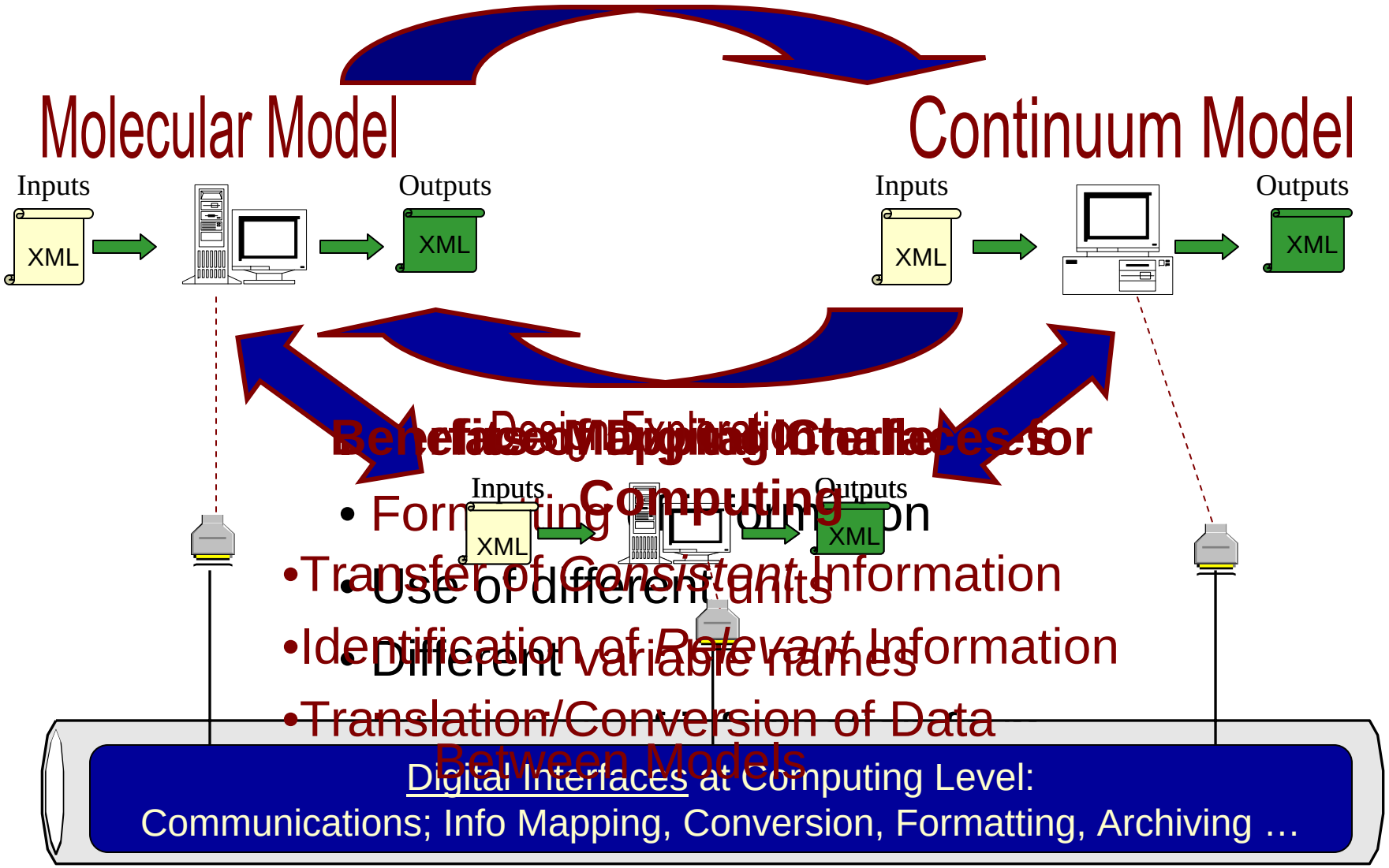


GT Systems Realization Laboratory

Panchal J. H., 2002, "Towards a Design Support for Distributed Product Realization", *MS Thesis*, G.W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA.

- **Process Level**
  - Information transfer between phases, events, entities, stakeholders
  - Capture, communicate and filter critical information
- **Computing level**
  - Interpret, communicate information and decision templates
  - Software representation of information
  - Communications protocol between software applications

Digital Interfaces at Computing Level



Characterization of Uncertainty

- Natural Uncertainty (system variability)
  - Errors induced by processing, operating conditions, microstructure variation, etc. (noise and control variables)

→ E.g. Y = 2X, where $\Delta X = \pm 0.1$

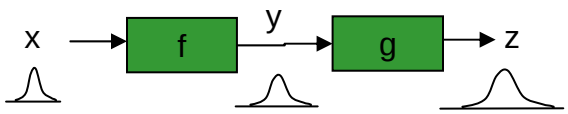
- Model Parameter Uncertainty (parameter uncertainty)
  - Incomplete knowledge of model parameters due to insufficient or inaccurate data

→ E.g. Y = aX, where a = [0.1, 3.0]

- Model Structural Uncertainty (model uncertainty)
  - Uncertain structure of a model due to insufficient knowledge (approximations and simplifications) regarding a system.

→ E.g. Y = 2X or Y = Exp(X)

- Uncertainty Created in a Chain of Events (process uncertainty)
  - Propagation of natural and model uncertainty through a chain of models

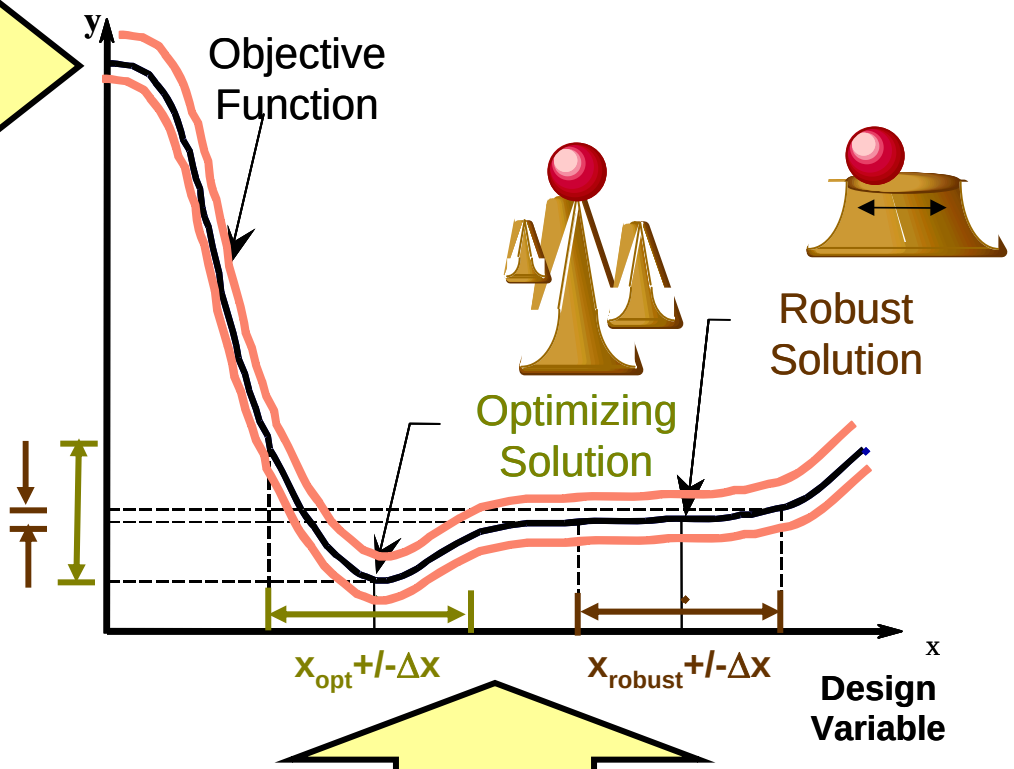


Method: System based Robust Materials Design – Type I, II, and III

Model Variation
Unparameterizable Variability

Type III (RCEM-EMI):
Insensitive to variability of a model

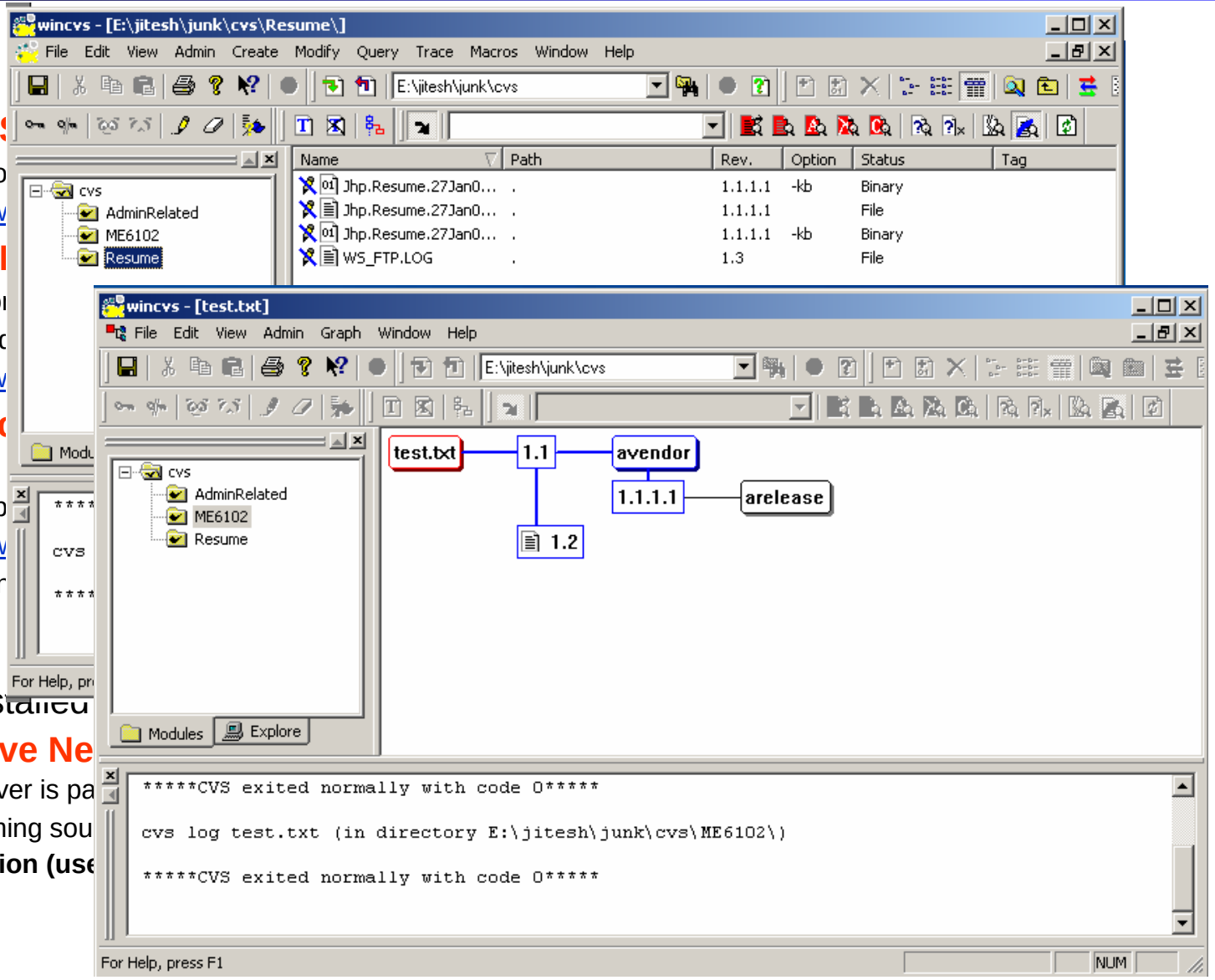
Response Variation
Stress, Stiffness,
Heat Transfer Rate,
Temperature
Others …



Type I and II (RCEM): **Insensitive to uncertainty uncontrollable and controllable variables**

Input Variation
Processing
Operating conditions
Variance in Volume Fraction

- **MURI Web S**
  - Introductio
  - http://www
- **MURI Web I**
  - Informatio
  - File upload
  - http://www
- **C.V.S (Conc**
  - File Vault,
  - Web Enab (http://www
  - Desktop Ir
- ***Bugzilla*** instal
- **Collaborative Ne**
  - Every server is pa
  - Programming sou
  - **Registration (use**



What Needs to be Done…

- **Information management in a multi-team environment**
  - Management of information and task flow
  - Facilitating efficient effective multi-user interaction
- **Development of the collaborative framework**
  - Digital interfaces for information exchange
  - Integration of software applications
  - Enhanced security for sensitive information
  - Lack of possibility of full automation; expert work orders
  - Flexible, adaptive wrappers at computing level
  - Efficient, dynamically reconfigurable, high bandwidth data transfer
  - Protocols for web-based models (readiness index, certification of certainty levels, liability, standard interfaces, etc.)
- **Develop process- and computing- level techniques**
  - Managing and facilitating collaboration among distributed teams
  - Decision level interfaces using compromise DSP, game theory
  - Techniques for managing interaction
- **Data and information capture, archival and reuse**
  - Effective databases
  - Methods for extraction of relevant information

Summing it Up: How Can It Work?

- Confluence of:
  - Computational Materials Science
  - Materials Characterization
  - Mechanics of Materials
  - Information Technology (information flow, wrappers, digital interfaces, web protocols)
  - Decision theory
  - MDO
  - Decision-based → human in loop!
- The "Payoffs":
  - More efficient, concurrent design of material and components to meet specified performance requirements
  - Increased incorporation of physically-based modeling in design system from 10% to 30% would be a huge gain
  - Prioritizing models and computational methods in terms of degree of utility in design
  - Prioritizing mechanics and materials science phenomena to be modeled
  - Conducting feasibility studies to establish probable return on investment of new material systems at corporate or national levels

Center for Computational Materials Design

http://www.ccmd.psu.edu

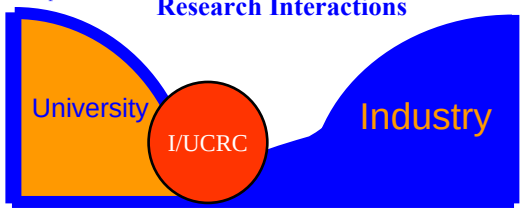
PENNSTATE | Georgia Tech

The George W. Woodruff School of Mechanical Engineering | School of Materials Science and Engineering

NSF Industry/University Cooperative Research Center (I/UCRC)

- **Industry/University Cooperative Research**
  - –Partnership between universities and industry.
  - –Featuring high-quality, industrially relevant fundamental research
  - –Strong industrial support of and collaboration in research.
  - –Direct transfer of university-developed ideas, research results, and technology to U.S. industry to improve its competitive posture in world markets.
- **Innovative education of graduate and undergraduate students**
  - –Next generation of scientists and engineers with a broad, industrially oriented perspective on engineering research and practice.

Research Interactions



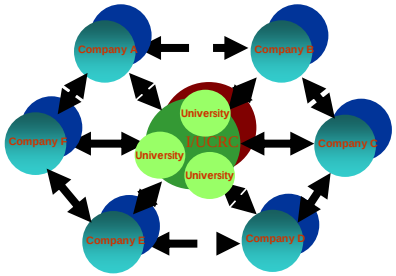
Impact of an I/UCRC

A strong indication of the value of an I/UCRC to industry is the continued participation of industry.

More than 80 I/UCRC Centers involving over 100 universities, 600 faculty, 1000 students, 600 members.

–The total industrial R&D investment attributed to the I/UCRCs in FY 2003 was approximately $100 million.

Follow-on investment by companies demonstrates that they derive benefits from the I/UCRC program of research that they believe merits further development and commercialization.

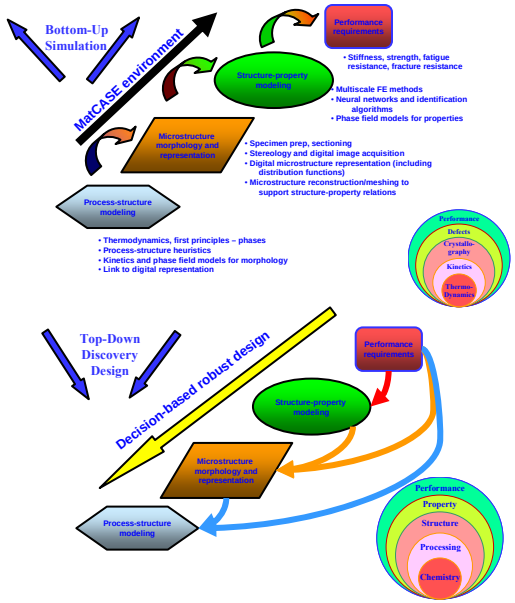


The model allows industries to interact with pre-competitive research

CCMD Mission and Vision

Mission: Educate the next generation of scientists and engineers with a broad, industrially relevant perspective on engineering research and practice

Vision: Be Recognized as the Premier Collaborative Activity in Computational Materials Design among U.S. Universities, Industries and Government Laboratories



Benefits and Payoffs

More efficient, concurrent design of material and components to meet specific performance requirements.

Realization of greater degree of control on materials life cycle management (cradle to grave), including sustainability.

Facilitates feasibility studies to establish probable return on investment of new material systems.

Facilitates prioritization of models and computational methods in terms of degree of utility in design.

Facilitates prioritization of essential materials phenomena and requirements to be modeled in product design/support.

Extended interaction with a large group of students and research fellows for a long period of time.

Philosophy of CCMD: Tools and Methods for Simulation-Based Materials Design

Focus of CCMD is on development of:

–novel simulation tools to support design decisions

–Novel methods for collaborative, decision-based systems design of materials

Tools and methods should be transferable among different materials design problems and classes of materials.

Research Project Themes

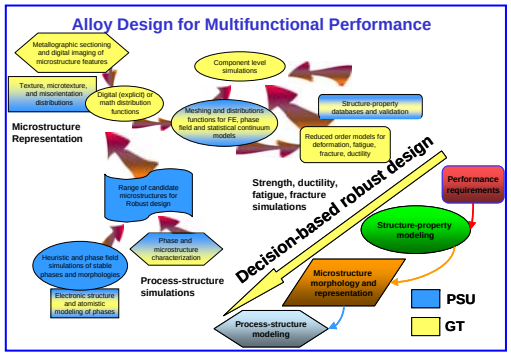
Design of multifunctional structural alloys

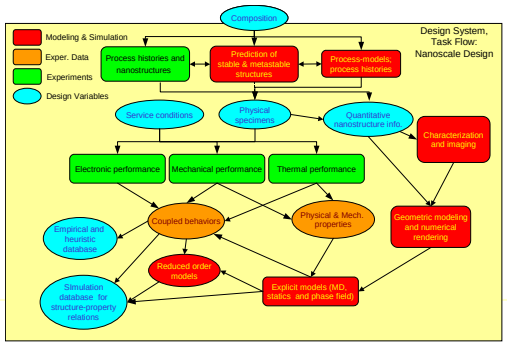
➢Application domains of materials initially include Ni base superalloys, α–β Ti alloys, lightweight casting alloys (Al, Mg), and steels.

Nanoscale to microscale design

➢Application domains in this research theme include nanoscale sensors/actuators (e.g. nanocoils) and thin films and protective surface coatings/treatments

Specific research projects to be solicited and voted by the member advisory board (MAB).

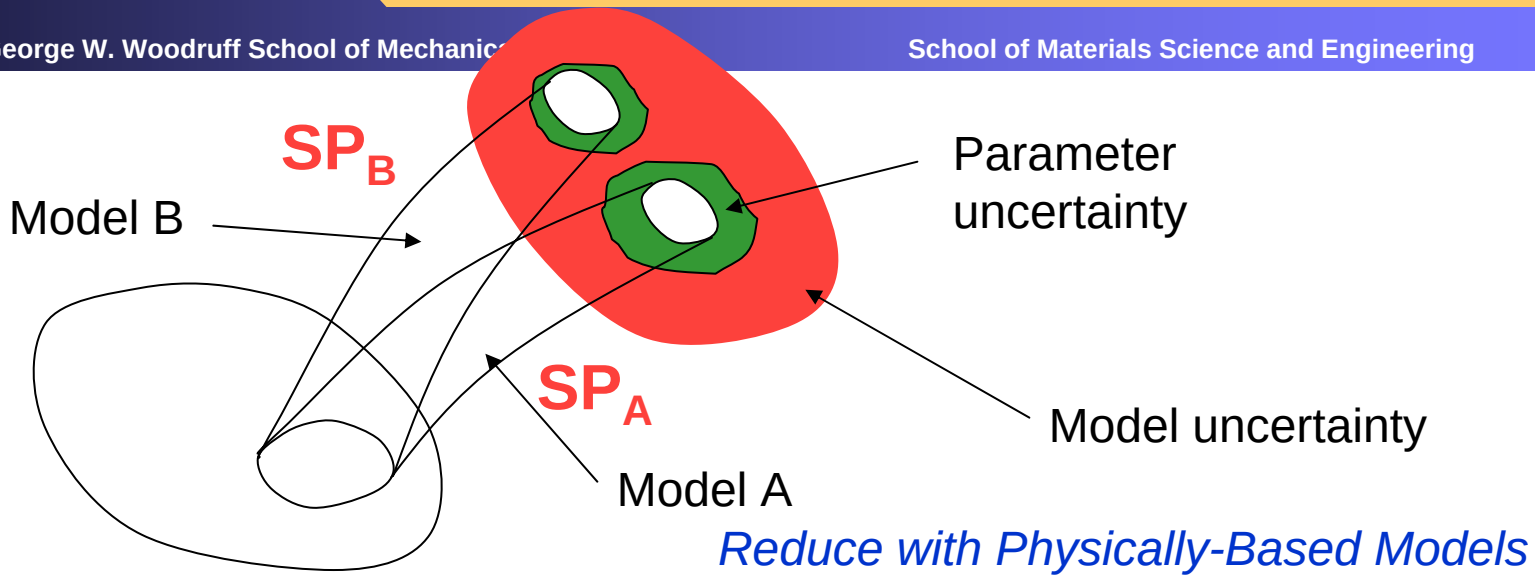




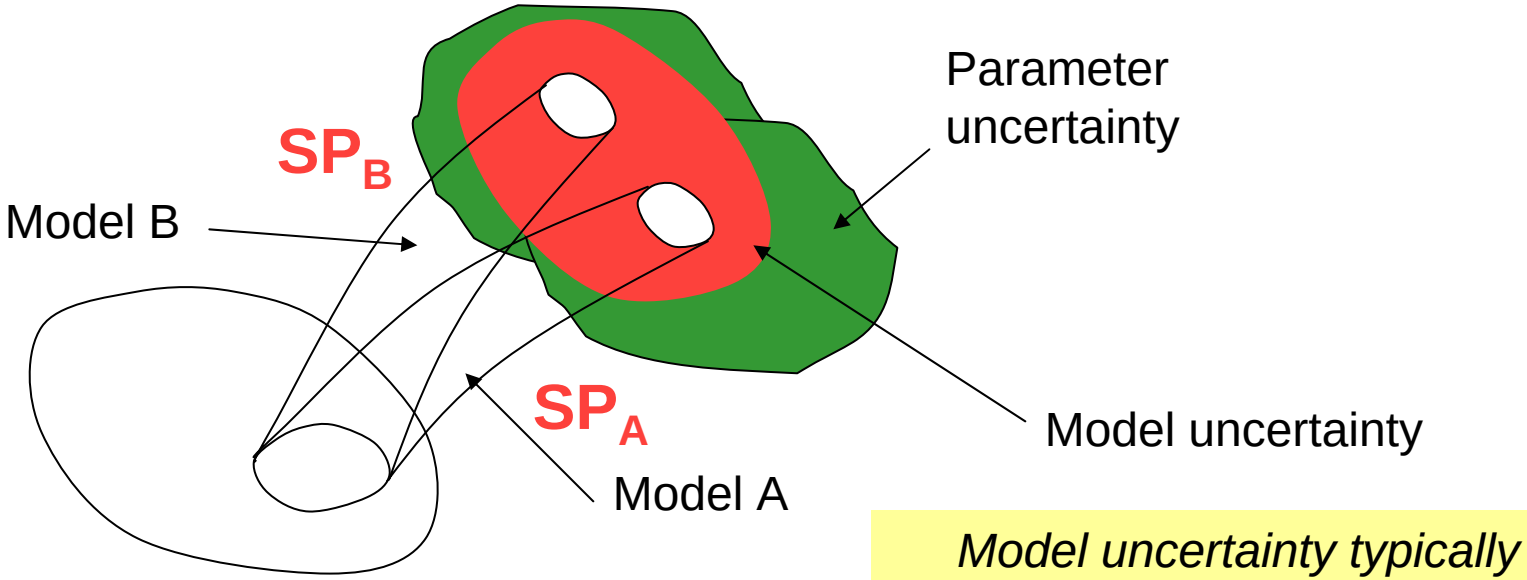
Questions?

Backup Slides

Variability and Uncertainty



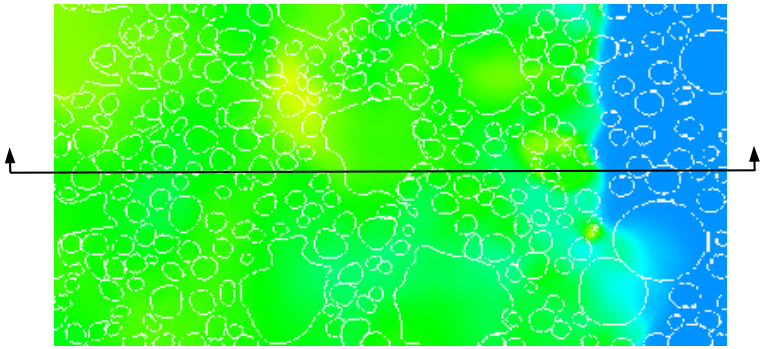
Reduce with Physically-Based Models

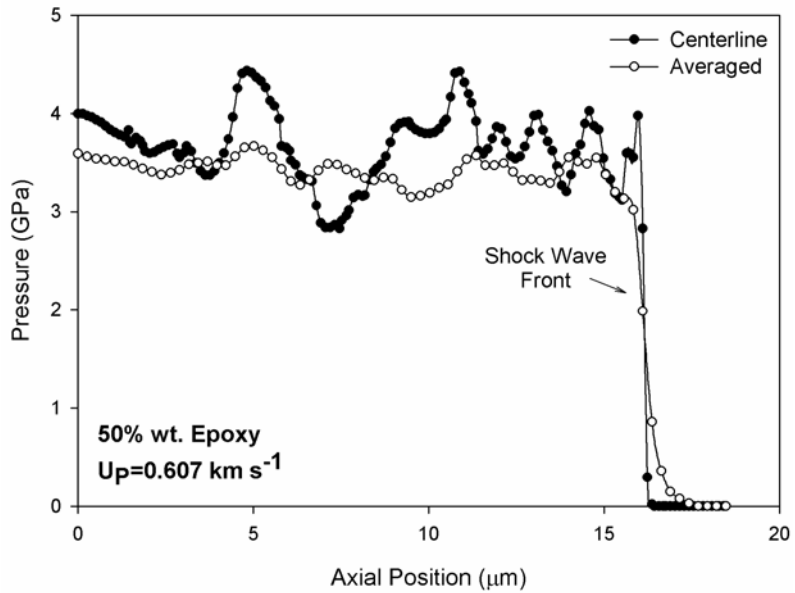


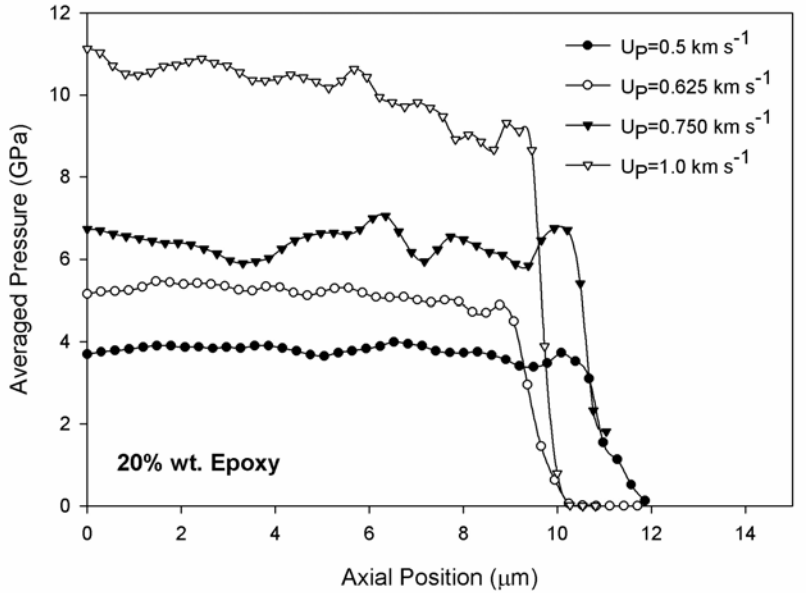
Model uncertainty typically increases as DOF decreases

Thermomechanical Responses

- Spatial Distributions of Pressure
  - Centerline
  - Averaged







Mesoscale Reaction Initiation Criterion

Variables :

$$\theta = \frac{\Delta G}{RT_h^{\,2}}\left(T - T_h\right)$$

$$\xi = \frac{x}{r}; \quad \tau = t\frac{Q}{\rho C_P}\frac{\Delta G}{RT_h}k_0 \exp\left(\frac{-\Delta G}{RT_h}\right)$$

Parameters :

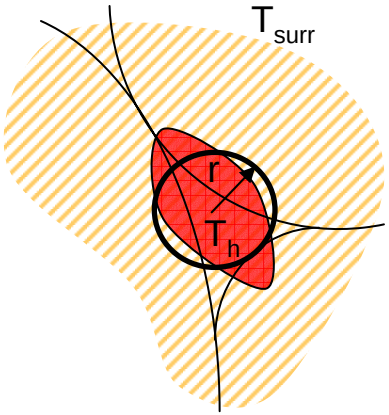
$$\theta_0 = \frac{\Delta G}{RT_h}\left(T_h - T_{surr}\right)$$

$$\delta = \frac{Q}{\kappa}\frac{\Delta G}{RT_h^{\,2}}r^2 k_0 \exp\left(\frac{-\Delta G}{RT_h}\right)$$

T_h = hot spot temperature

T_{surr} = surrounding tempertaure

r = hot spot radius



This allows (1) to be written as ...

$$\frac{\partial\theta}{\partial\tau} = \exp\theta + \frac{1}{\delta}\left(\frac{\partial^2\theta}{\partial\xi^2} + \frac{1}{\xi}\frac{\partial\theta}{\partial\xi}\right)$$

$$\delta = 7.39\left(\ln\theta_0\right)^{0.83}$$

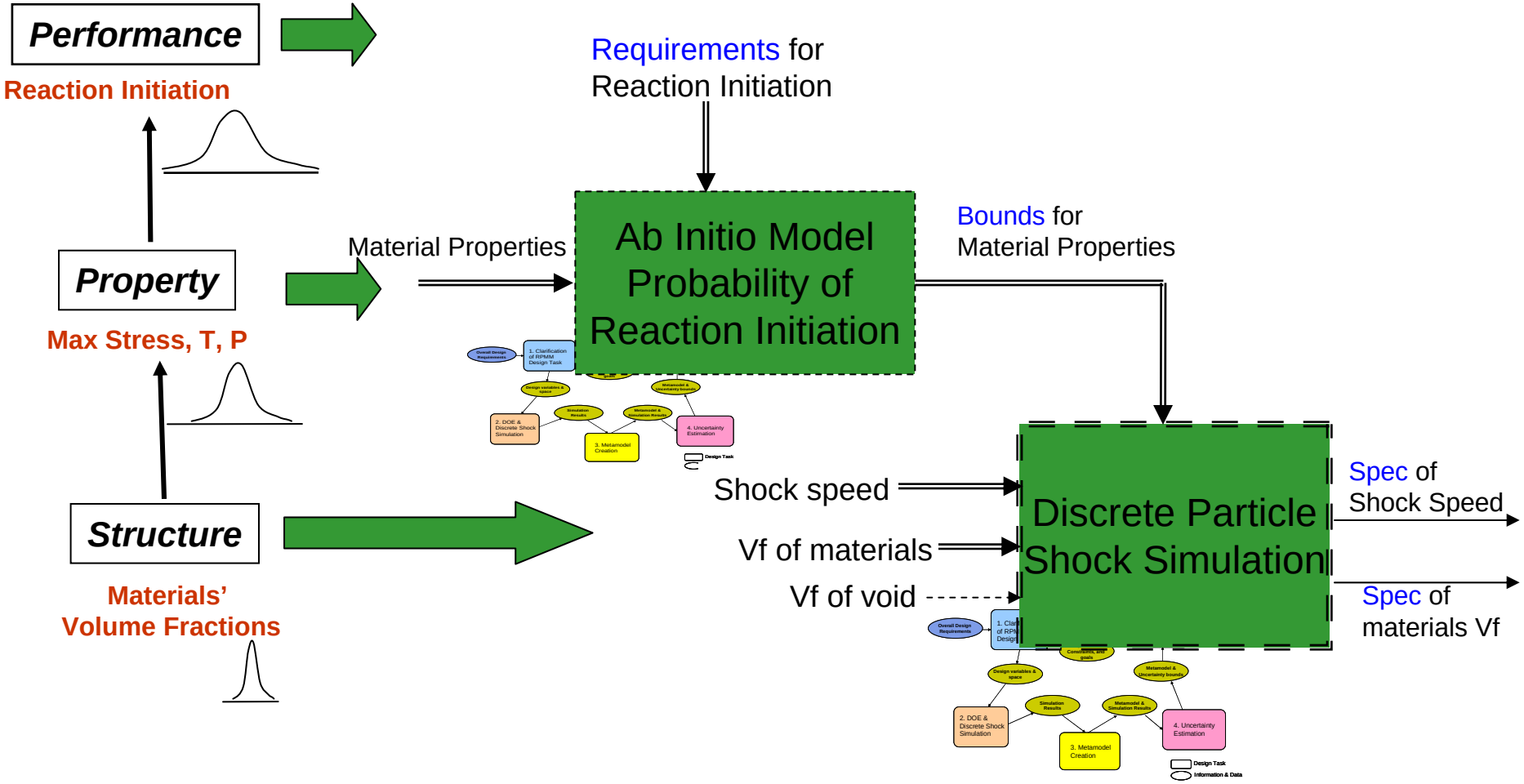
... which may inverted to solve for the critical hot spot radius

U_P (km s^{-1})	Mixture	# Potential Sites	# Activated Sites
1.0	a	10	1
	b	9	1
	c	4	0
0.75	a	0	0
	b	1	0
	c	0	0

Potential site = mixed element with T>900 K

Activated site = potential site meeting reaction criteria

Example: Mitigation of Uncertainty Propagation in MESMs Design



Haejin Choi