Education Changes for Effective VVUQ

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Talk Outline

- Recommendations on education changes
  - Section 7.4 of the report
- Success and challenges of doctoral interdisciplinary cluster
  - Predictive Science & Engineering Design (PS&ED) cluster at Northwestern University

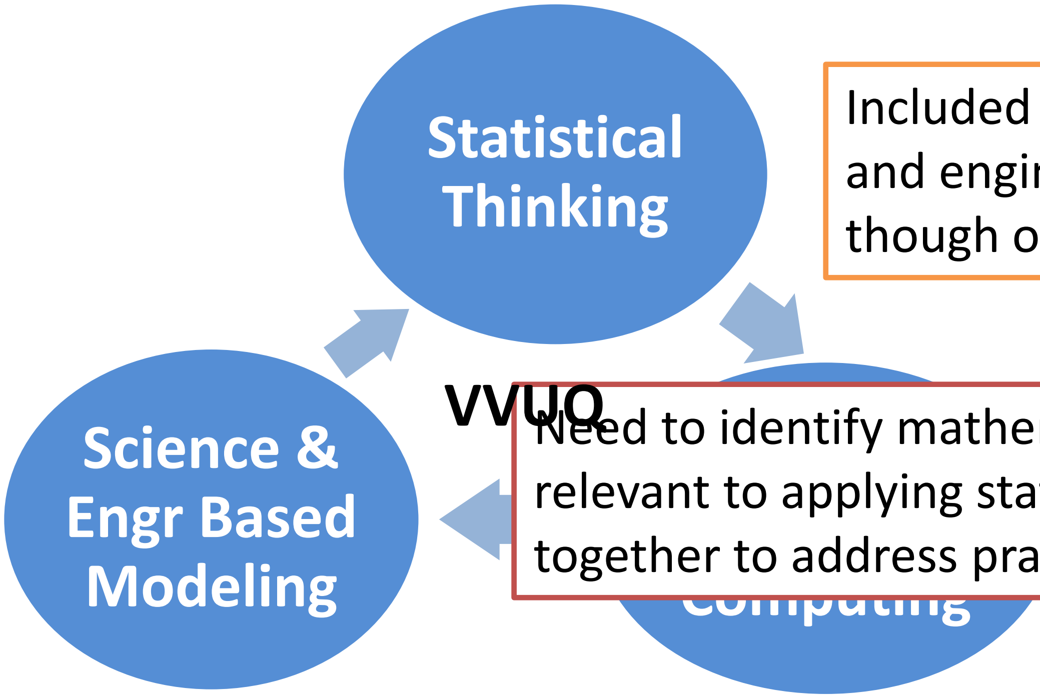
Who do We Target?

- Educate those who use them
  - From different disciplines (scientists, engineers, policy makers)
- Prepare next generation of researchers
  - Engineers of 2020 ("improving our ability to predict risk and adapt systems"; "to create solutions that minimize the risk of complete failure")

Status of VVUQ Education

- Topics in VVUQ are growing at research conferences.
- Select topics are covered in a few (usually graduate) engineering, statistics, and CS courses.
- Not yet a standard part of the education
  - Modeling without a critical assessment of assumption and uncertainty
  - Safety factor is commonly used in design
  - Statistics courses mainly deal with data analysis

Three Components in VVUQ



Included in some science and engineering programs though often not required

Need to identify mathematical tools relevant to applying statistics and science together to address practical problems

Not normally included in

Need to understand how uncertainty can be introduced into deterministic physical laws, and how evidence should be weighted to make model-based decisions

Modern VVUQ Curriculum

- Foundation to reason about risks and uncertainty
- Foster an appreciation of the role that modeling and simulation could play in addressing complex problems
- Provide assessment of exposure, hazard, and risk and strategies for mitigating them.
- Address effective communication of uncertainty and risk to decision makers, stakeholders and UQ experts.

Recommendations 1 & 2

- An effective VVUQ education should encourage students to confront and reflect on the ways that knowledge is acquired, used, and updated.

- The elements of statistical thinking, physical-systems modeling, and numerical methods and computing should become standard parts of the respective core curricula for scientists, engineers, and statisticians.

VVUQ Curriculum

Engineering and science program

- VVUQ integrated into existing courses (uncertainty associated with natural phenomena and engineering systems, followed by statistical thinking)
- Taught and practiced in engineering design courses
- Teach students to regularly confront uncertainty

Probability and statistics program

- Require training in modeling and computational science.

Program in management sciences

- Educate future policy maker to assessing the quality and reliability of the information and make rational decisions

Recommendation 3

- Support for interdisciplinary programs in predictive science, including VVUQ, should be made available for the education of highly qualified personnel in VVUQ methods.

    Interdisciplinary programs incorporating VVUQ are merging as a result of investment by granting bodies.

    - PSAAP centers
    - Institute for Computational and Engineering Sciences (UT Austin)
    - Interdisciplinary PhD in Predictive Science and Engineering (U of Michigan)
    - Predictive Science & Engineering Design Cluster at Northwestern.

Predictive Science & Engineering Design (PS&ED)

Graduate Interdisciplinary Clusters in the Sciences and Engineering at Northwestern University

Established in 2008

Director

Wei Chen

(Professor, Mechanical Engineering)

Co-Directors

Greg Olson (Professor, Materials Science & Engineering)

Wing Kam Liu (Professor, Mechanical Engineering)

http://psed.tech.northwestern.edu/

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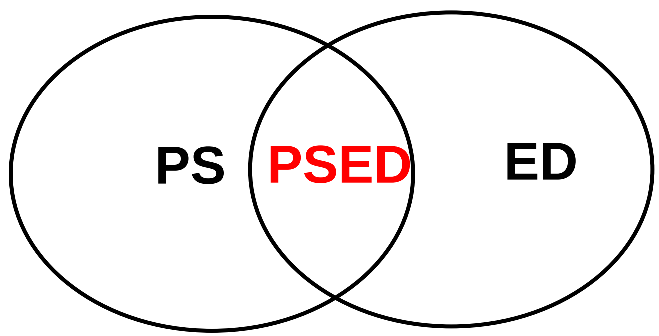
PS&ED Program Objectives

- Discover, develop, and teach the common principles and techniques underlying PS&ED
- Engage faculty in collaborative, interdisciplinary research to pursue new funding opportunities
- Provide an alternative intellectual community with "dual citizenship"
- Enhance the technical depth of NU design initiatives

Predictive Science & Engineering Design Cluster

- Predictive Science (PS) - the application of verified and validated computational simulations to predict the response of complex systems, particularly in cases where routine experimental tests are not feasible.
- Engineering Design (ED) - the process of devising a system, component or process to meet desired needs.



- Certificate Requirements: 3 core courses + 2 electives
  - Modeling, Simulation, and Computing
  - Computational Design
  - PS&ED 510 Seminar

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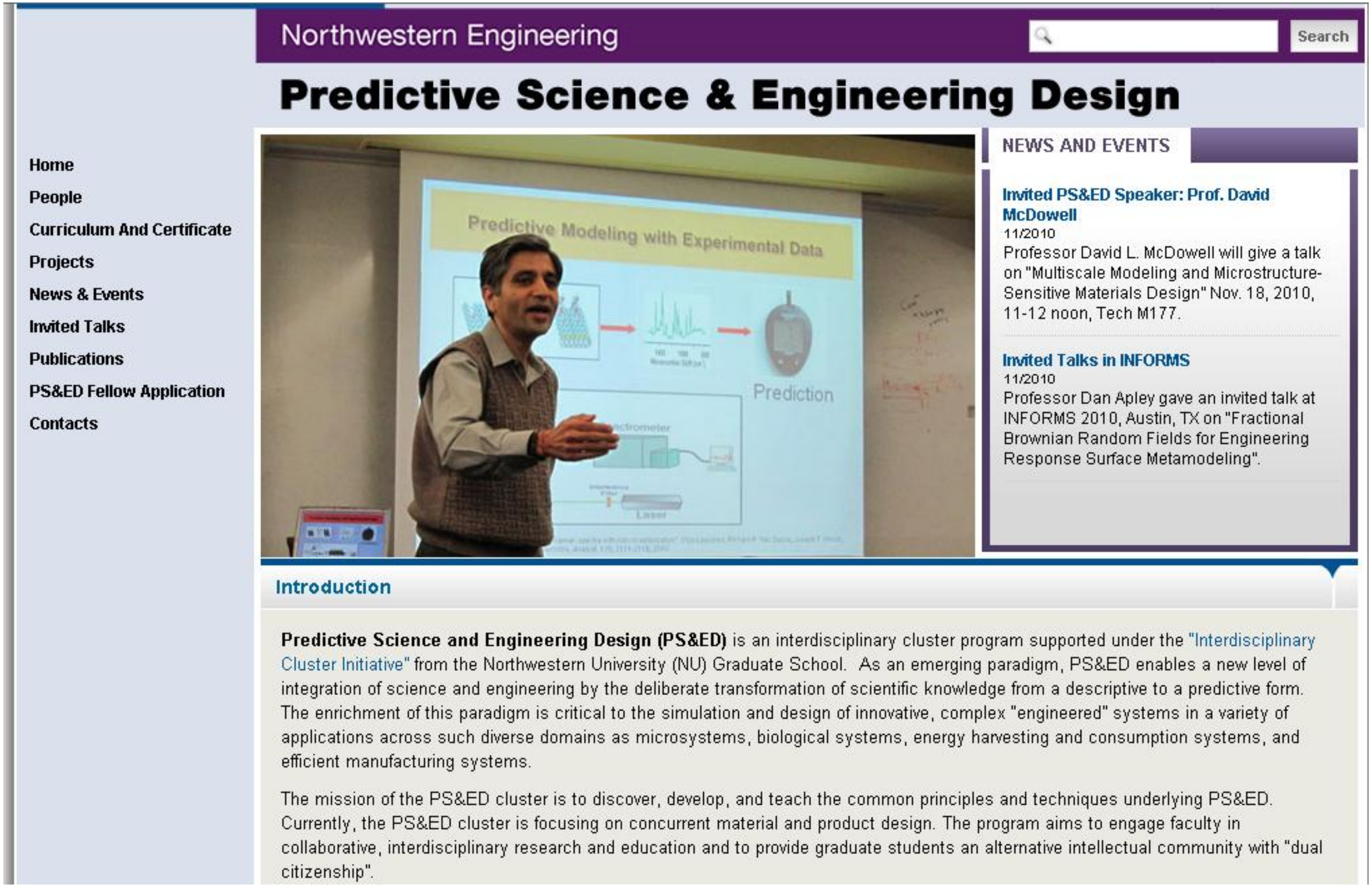
PS&ED Website



Northwestern Engineering

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Predictive Science & Engineering Design

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- Contacts

NEWS AND EVENTS

Invited PS&ED Speaker: Prof. David McDowell
11/2010
Professor David L. McDowell will give a talk on "Multiscale Modeling and Microstructure-Sensitive Materials Design" Nov. 18, 2010, 11-12 noon, Tech M177.

Invited Talks in INFORMS
11/2010
Professor Dan Apley gave an invited talk at INFORMS 2010, Austin, TX on "Fractional Brownian Random Fields for Engineering Response Surface Metamodeling".

Introduction

Predictive Science and Engineering Design (PS&ED) is an interdisciplinary cluster program supported under the "Interdisciplinary Cluster Initiative" from the Northwestern University (NU) Graduate School. As an emerging paradigm, PS&ED enables a new level of integration of science and engineering by the deliberate transformation of scientific knowledge from a descriptive to a predictive form. The enrichment of this paradigm is critical to the simulation and design of innovative, complex "engineered" systems in a variety of applications across such diverse domains as microsystems, biological systems, energy harvesting and consumption systems, and efficient manufacturing systems.

The mission of the PS&ED cluster is to discover, develop, and teach the common principles and techniques underlying PS&ED. Currently, the PS&ED cluster is focusing on concurrent material and product design. The program aims to engage faculty in collaborative, interdisciplinary research and education and to provide graduate students an alternative intellectual community with "dual citizenship".

http://psed.tech.northwestern.edu/

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Projects

Home > Projects

The PS&ED cluster fellows were organized into interdisciplinary groups to perform research in complex problems featuring elements from each of their areas of expertise and study. Click the links below to see a poster describing the key components of their year-long team efforts.

2009-2010 Interdisciplinary Projects

1. Concurrent Design of Automotive Shape Memory Alloys and Acuators
   Tengfei Jiang and Aaron Stebner
   Faculty Advisors: Drs. Cate Brinson, David Dunand, Greg Olson
2. Uncertainty Quantification of the Nanodiamond Drug Diamond System
   Michelle Hallikainen and Robert Lam
   Faculty Advisors: Drs. Wei Chen, Dean Ho, Wing Kam Liu, Ann Mckenna
3. Validation and Prediction of Incremental Forming Process
   Paul Arendt and Rajiv Malhotra
   Faculty Advisors: Drs. Dan Apley, Ted Belytschko, Jian Cao, Wei Chen
4. Material and Structure Design for Dynamic Energy Dissipation
   Ravi S. Bellur Ramaswamy, George Fraley, and Steve Greene
   Faculty Advisors: Drs. Wei Chen, Horacio Espinosa, Wing Kam Liu, Greg Olson

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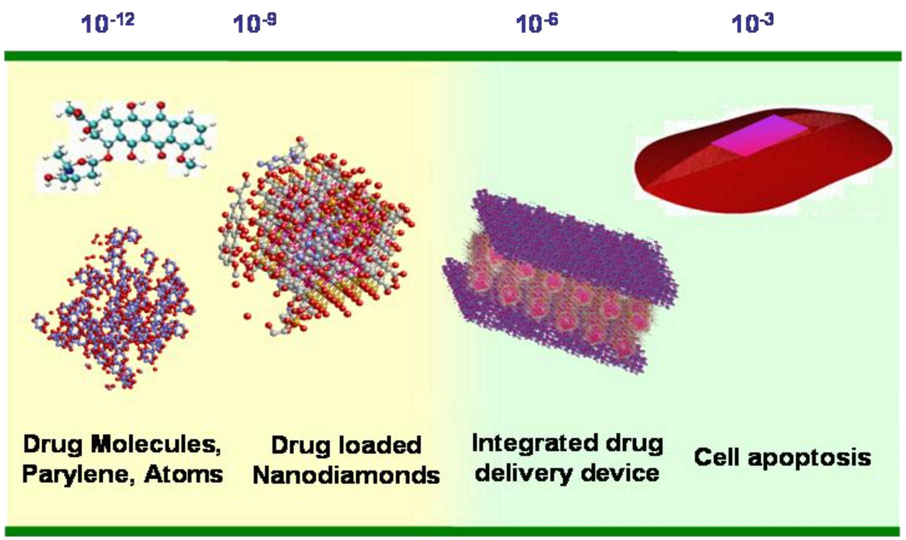
Current PS&ED Cluster Design Focus

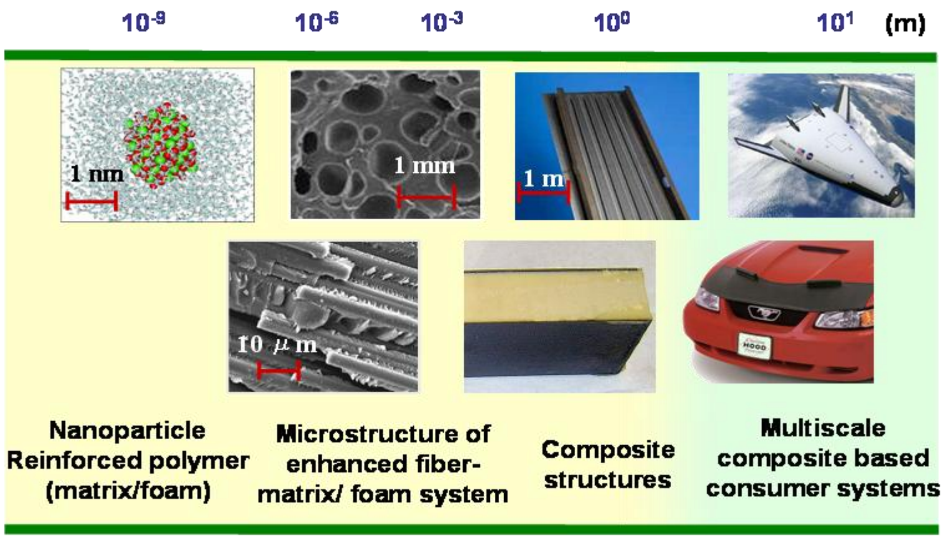
Hierarchical Materials and Product Design

Concurrent optimization of hierarchical materials and product designs across multiple scales, accounting for the multiscale nature of physical behavior and manufacturing restrictions.

Bio-Multiscale System for Drug Delivery



Micro-Nano-Composites Structure



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Dynamic Energy Dissipation for Earthquake Protection, PSED Cluster 2009-2010

Graduate Student Fellows:
GEORGE FRALEY
STEVEN GREENE

Faculty Advisors:
WEI CHEN, WING KAM LIU
GREG OLSON

Academic Disciplines:
MECHANICAL ENGINEERING, CIVIL ENGINEERING
MATERIALS SCIENCE & ENGINEERING

June 03, 2010

RESEARCH OBJECTIVE

Integrate contemporary materials and structure analysis & design principles to create products with better functionality as ***passive energy dissipation*** devices. Through exploring the codependent physics in the material (nano, micro) and continuum (meso, macro) domains, automated design techniques utilize experimental data, structural concepts, and atomistic and continuum simulations to consider mutual design issues across disparate scales in length and time. The end mission of the project is to use the integrated design approach to unlock new devices for earthquake protection, with a specific focus on historic buildings.

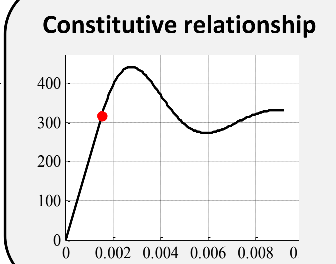
composition

processing

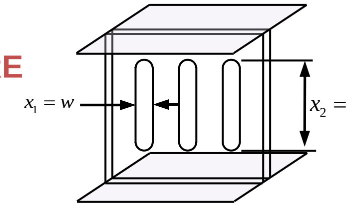
microstructure

maximize driving force of austenite precipitation

MATERIAL DOMAIN



STRUCTURE DOMAIN



maximize energy dissipation

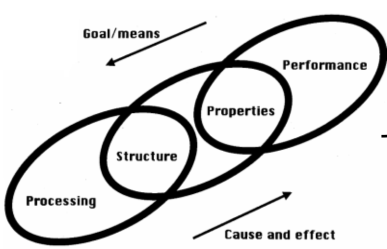
compatible components

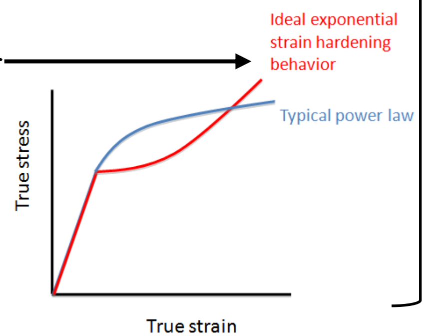
geometry

sizing

BENCHMARK PROBLEM

- Preliminary material and structural design of slit steel damper
- Optimal combination of material & geometry sought
- Dissipation occurs through metal yielding
- Material/structure integration through constitutive relationship

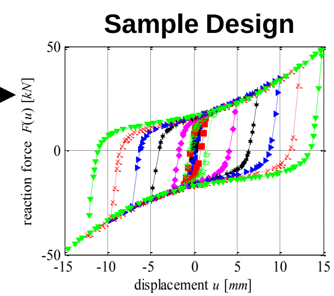


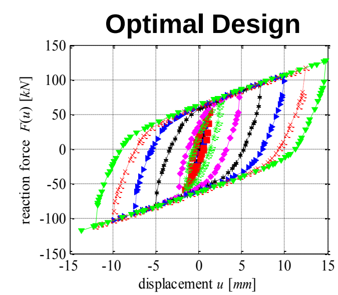


Class of secondary hardened Martensitic steel is considered to exploit transformation plasticity.

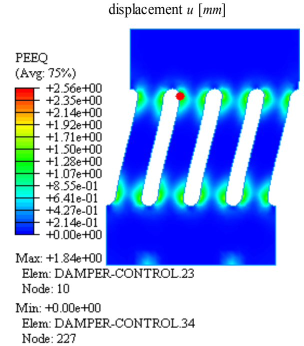
Materials design provides optimal constitutive relationship for energy dissipation

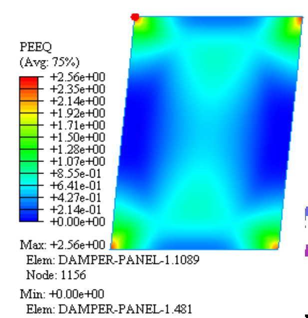
Structural design produces solid shear panel, confirmed by literature, due to highest plastic strain from mobilized shear deformation





Cyclic loading hysteresis loop





Equivalent plastic strain field

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Metal-Polymer Laminate Composite: Modeling and Design, PSED Cluster 2010-2011

Graduate Student Fellows:
Jiayi Yan, Ying Li, Yang Li

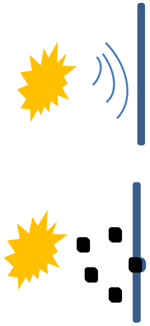
Faculty Advisors:
WEI CHEN, WING KAM LIU
GREG OLSON, CATE BRINSON

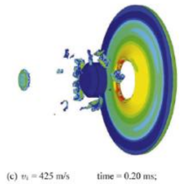
Academic Disciplines:
MECHANICAL ENGINEERING
MATERIALS SCIENCE & ENGINEERING

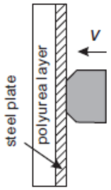
Mar 19 , 2011

RESEARCH OBJECTIVE

The rapid development of industry in recent decades greatly raises the demand of high-performance structural materials to survive severe mechanical loadings. Our objective is to provide some insight to materials behavior of Metal Polymer laminates composites, and come up with novel designs. With impact resistance improved and other advantages maintained, such designed materials will have a board spectrum of applications, including aircrafts, automobiles, armors, electronic devices and helmets.

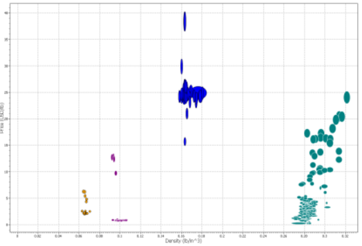






MATERIAL SELECTION

The properties of composites significantly depend on their constitutive components. To obtain some insight from existing MPLCs, we need to relate their general properties to materials selection. Based on the desirable performance, we will make a list of primary and secondary properties taken into account with comprehensive consideration. We will follow the ideas from Ashby and use CES EduPack.

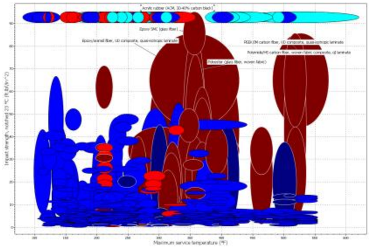


Metal
Al alloy
Mg alloy
Steel
Ti alloy
…

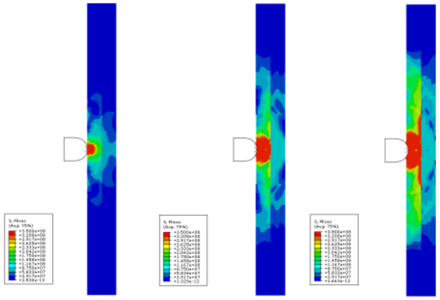
Tensile strength
Ductility
Density
Cost
Modulus

Polymer
Polyurea
PC
…

Tensile strength
Ductility
Density
Cost
Modulus



FINITE ELEMENT SIMULATION



Stress wave propagation under round-nosed projectile

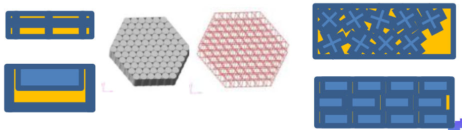
FUNCTION-ORIENTED OPTIMIZATION

Divide the structure into functional layers

- Shielding layer
- Supporting layer
- Anti-trauma layer

↓

Concept design of each layer



↓

Adjust ratio of each functional layer

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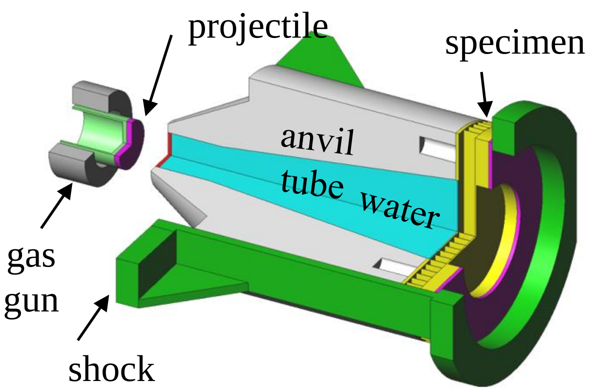
Blast Resistant
Fiber Reinforced Plastic (FRP) Sandwich

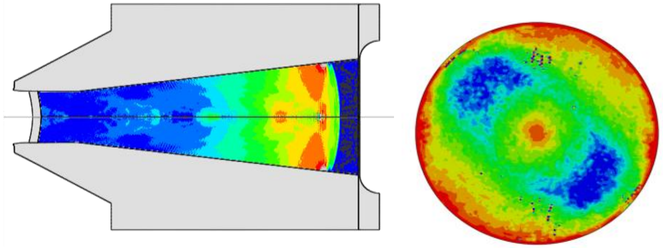
X (known inputs)

Flyer plate thickness and velocity, and **time**

Experiment Setup

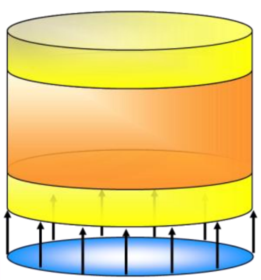


FE Model



Specimen Damage Maps

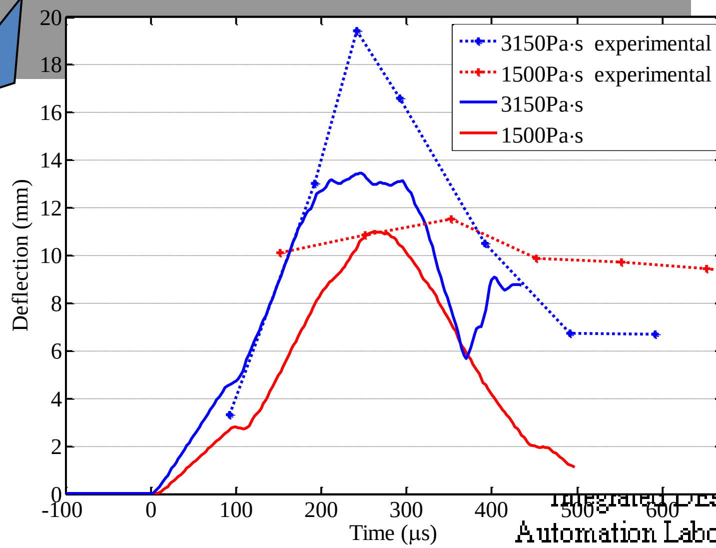
Assume well calibrated model



Displacement

$$u^m = y^m(x,\theta)$$

$$u^e = y^e(x)$$



Collaboration with Prof. H. Espinosa

Figures provided by Ravi Bellur Ramaswamy

Multi-level Validation of a Nanodiamond Drug Delivery System, PSED Cluster

Graduate Student Fellows:
ROBERT LAM
MICHELLE SCHWALBE

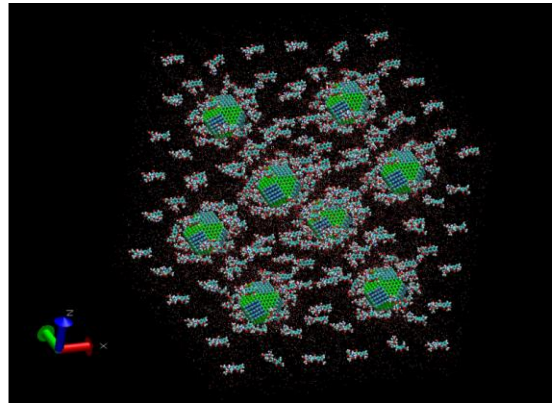
Faculty Advisors:
WEI-CHEN, DEAN HO, WING KAM LIU

Academic Disciplines:
MECHANICAL ENGINEERING
BIOMEDICAL ENGINEERING

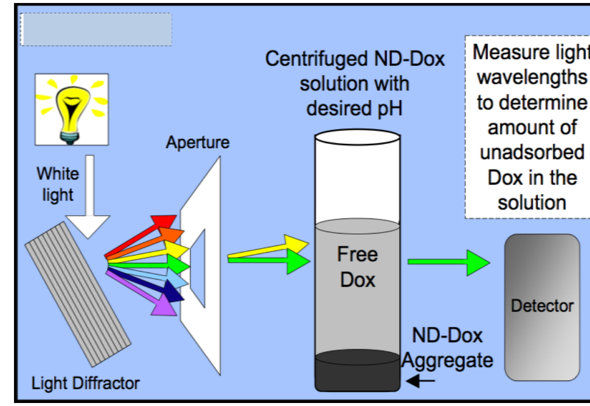
RESEARCH OBJECTIVE

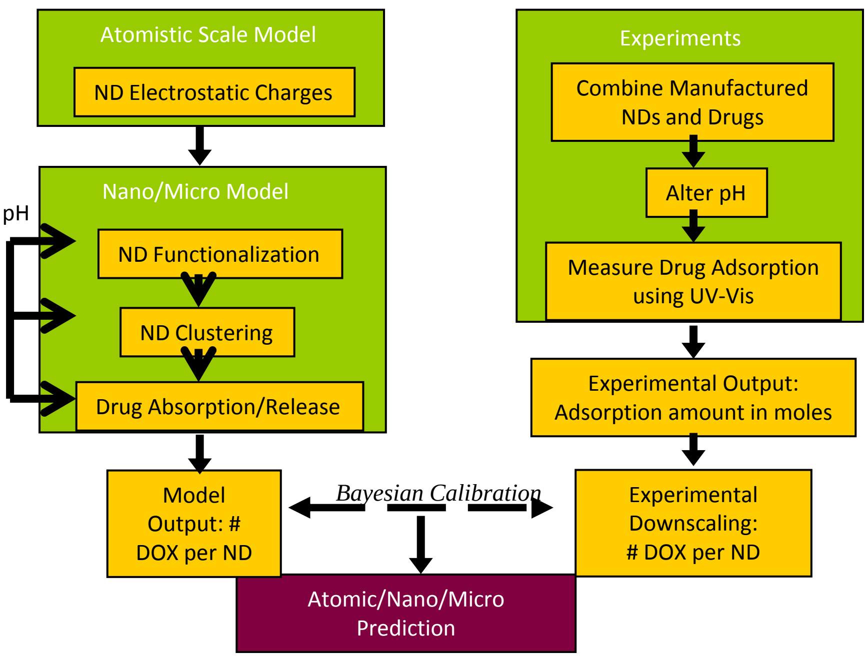
Collaborative effort to combine simulations and experiments at different physical scales in order to construct a predictive model for carbon nanoparticle (nanodiamond)-drug interactions. Bayesian calibration is required in order to bridge the differences between atomic/nanoscale simulations and micro-/mesocale experiments. Drug (doxorubicin) adsorption is simulated with varying amounts of carboxyl functional groups on the surface. Centrifugation pull-down and UV-Vis spectroscopy measurements confirm the amount of adsorbed drug onto nanoparticles in response to pH

SIMULATIONS

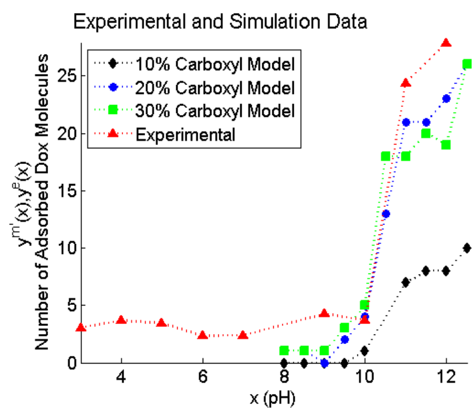


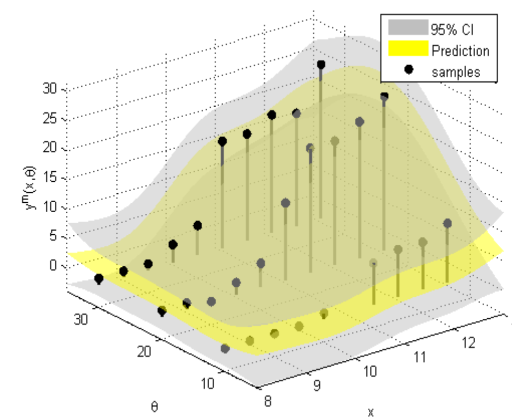
EXPERIMENTAL VALIDATION





COMPARISON AND FUTURE WORK





Resultant metamodels created from simulation and experimental data can be utilized to predict future nanodiamond-drug interactions, eliminating the need for costly comprehensive experiments and simulations.

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Validation and Prediction of Single Point Incremental Forming (SPIF), PSED Cluster 2009-2010

Graduate Student Fellows:
RAJIV MALHOTRA
PAUL ARENDT

Faculty Advisors:
WEI CHEN, DAN APLEY
JIAN CAO

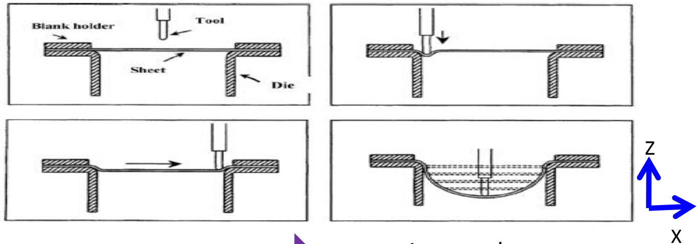
Academic Disciplines:
MECHANICAL ENGINEERING, INDUSTRIAL ENGINEERING AND MANAGEMENT SCIENCES

June 03, 2010

Research Objective

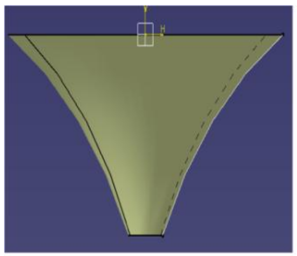
1) Calibrate the fracture model to predict formability in SPIF using FEA
2) Obtain knowledge about uncertainties in simulations and experiments in SPIF
3) Assess the predictive capability of FEA simulations for SPIF

Single Point Incremental Forming (SPIF)



Cheaper, generic tooling →	Less tool cost, greater process flexibility
Reduced tool forces →	Reduced machine size, use in micro-factories
Higher Formability →	Reduced joining processes, greater component strength

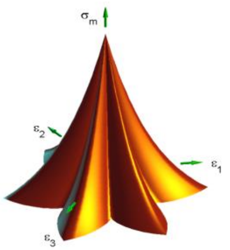
Experiments



Incremental depth (Δz):
Increments by which tool goes down in z direction

Failure:
Controlled by Δz
Tested by forming funnel shapes at different Δz

Fracture Model



Fracture envelope depends on pressure and on shear modes of deformation

Uncertainty Quantification and Prediction

Calibration and Bias-Correction Probabilistic Model Formulation (Kennedy and O'Hagan 2001)

Experimental Prediction

Computer Model
Lack of computer data
Gaussian Process (GP) Model

Experimental Error

$$y^e(x) = y^m(x, \theta) + \delta(x) + \varepsilon$$

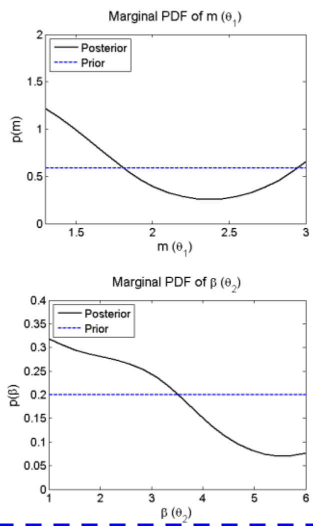
Variable Inputs
Incremental Depth (Δz)

Unknown Parameters
m and β

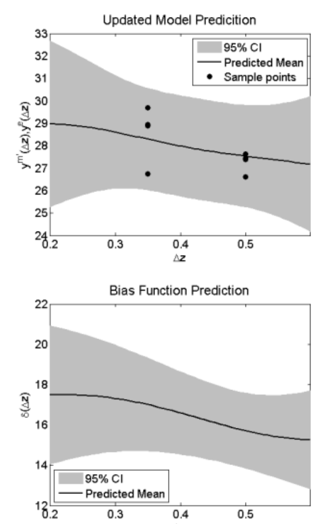
Bias Correction Function
Lack of experimental data
GP Model
Difference between simulation and experiments

	Simulation Inputs	Description
x	Δz	Incremental depth (mm)
θ_1	m	Damage evolution parameter
θ_2	β	Weakening function parameter

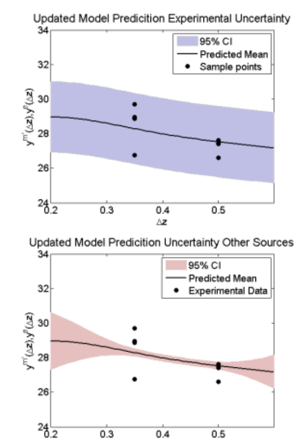
Probability Distribution of Calibration Parameters



Prediction and Uncertainty of Experimental process



Different Sources of Uncertainty



	Simulation Output	Description
$y^m(x, \theta_1, \theta_2)$	$y^m(\Delta z, m, \beta)$	Fracture depth (mm)

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Success and Challenges

– Enable interdisciplinary collaboration on VVUQ study
– Broaden the depth and scope of dissertations
– Integrate theory and practice
– Integrate statistical, computational, design thinkings.

– VVUQ textbook
– VVUQ software
– Balance of modeling vs. VVUQ efforts