Computational Materials Science

EDUCATIONAL RESOURCES

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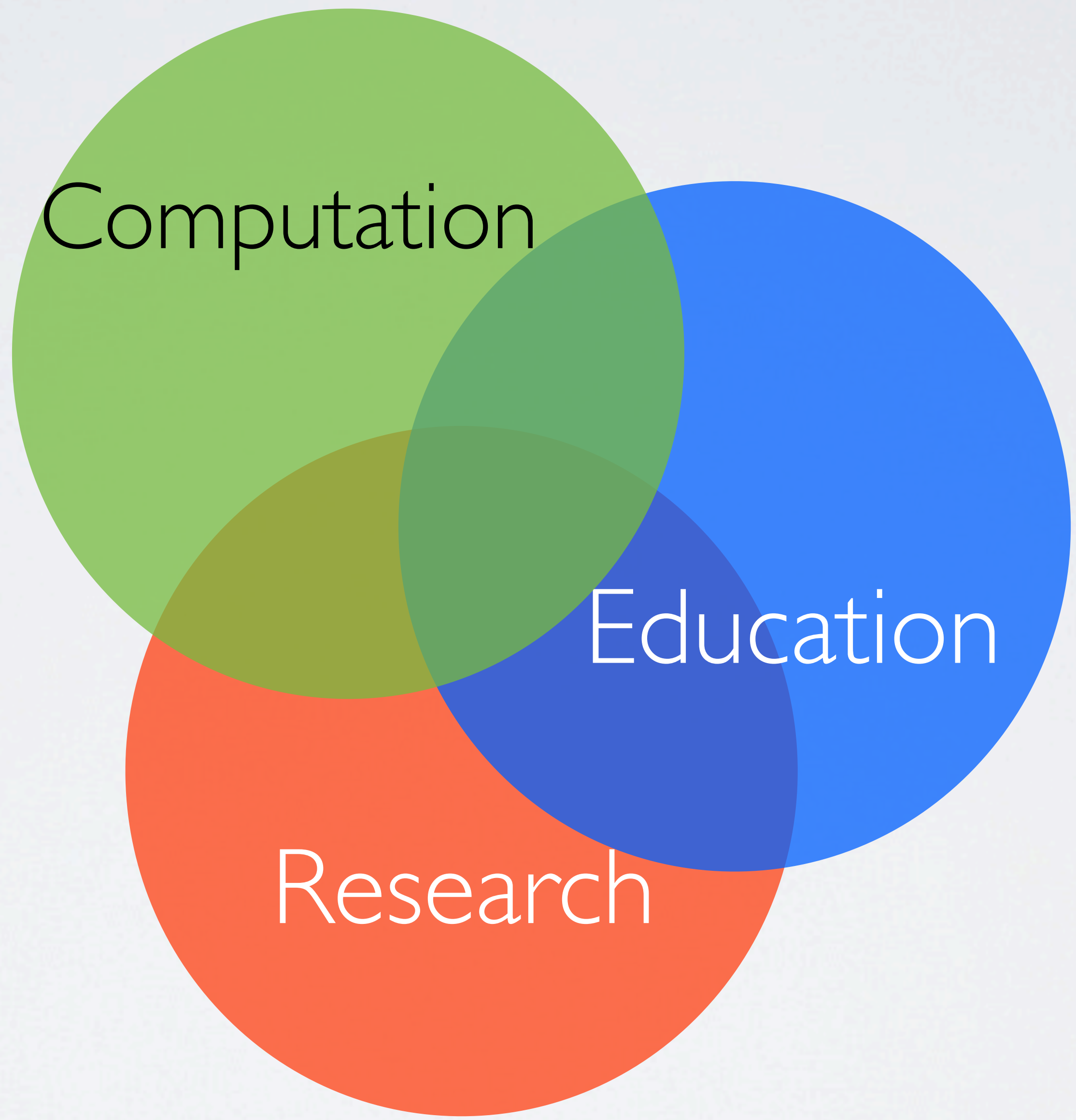
University of Florida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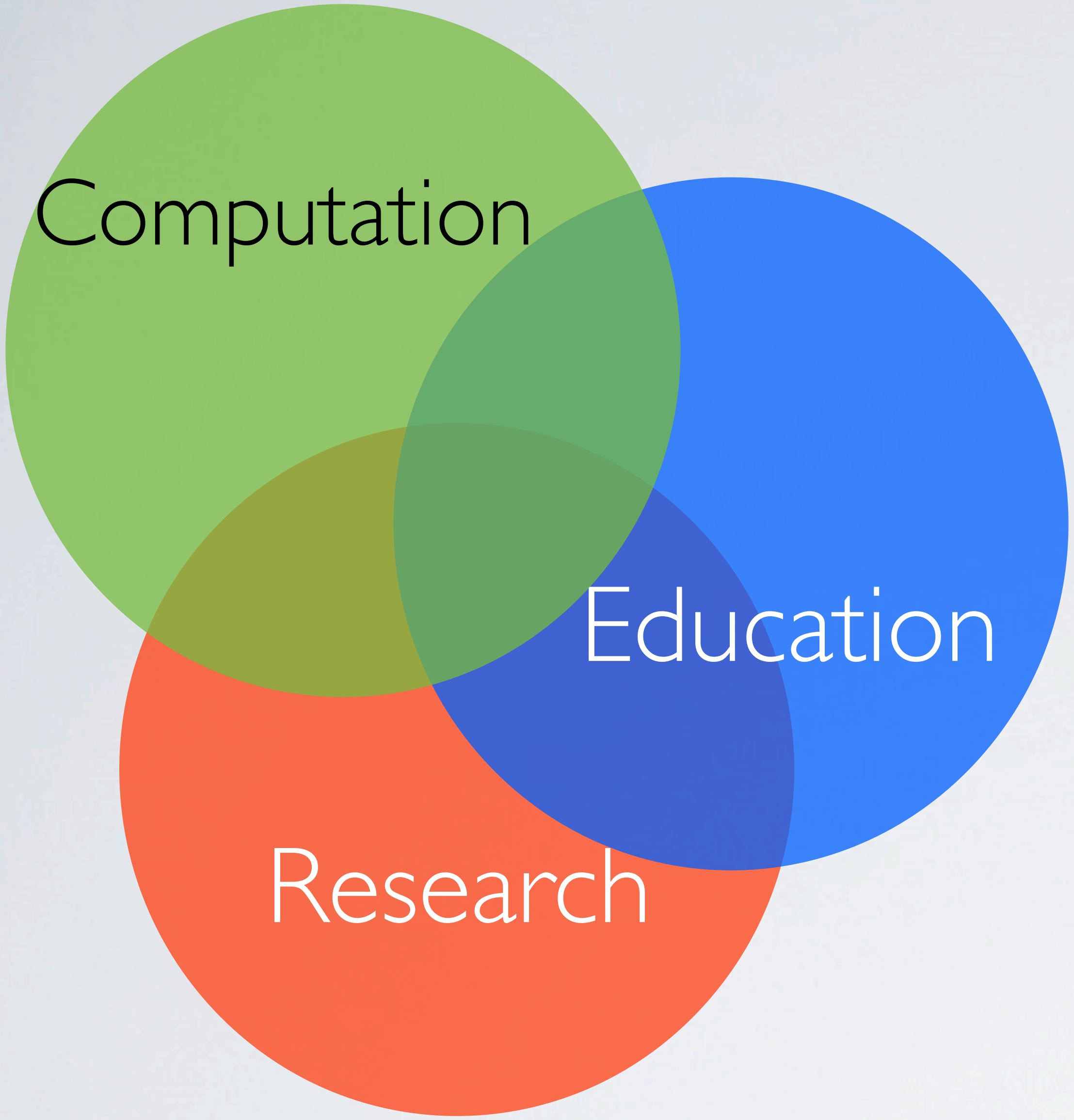
Education
Research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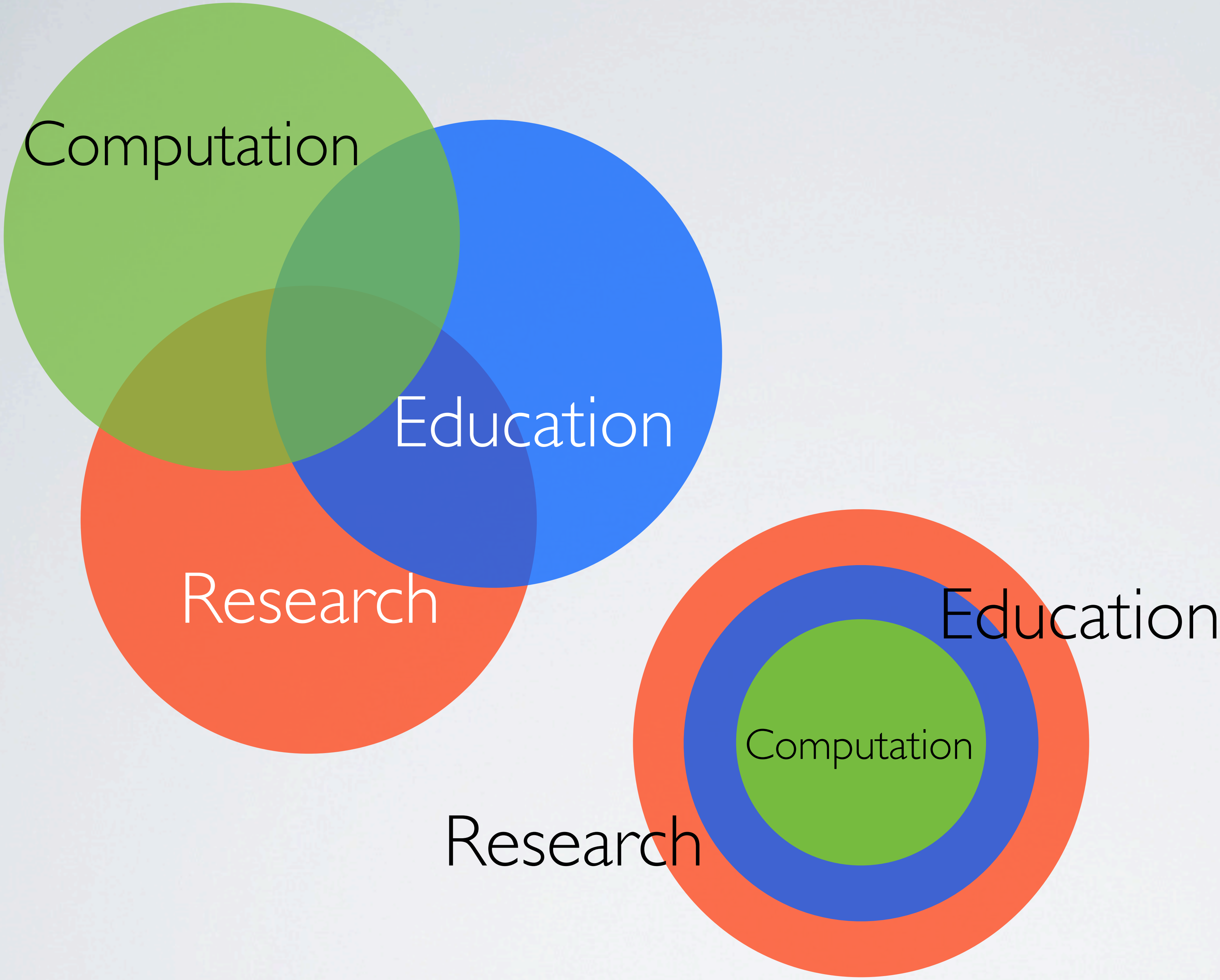
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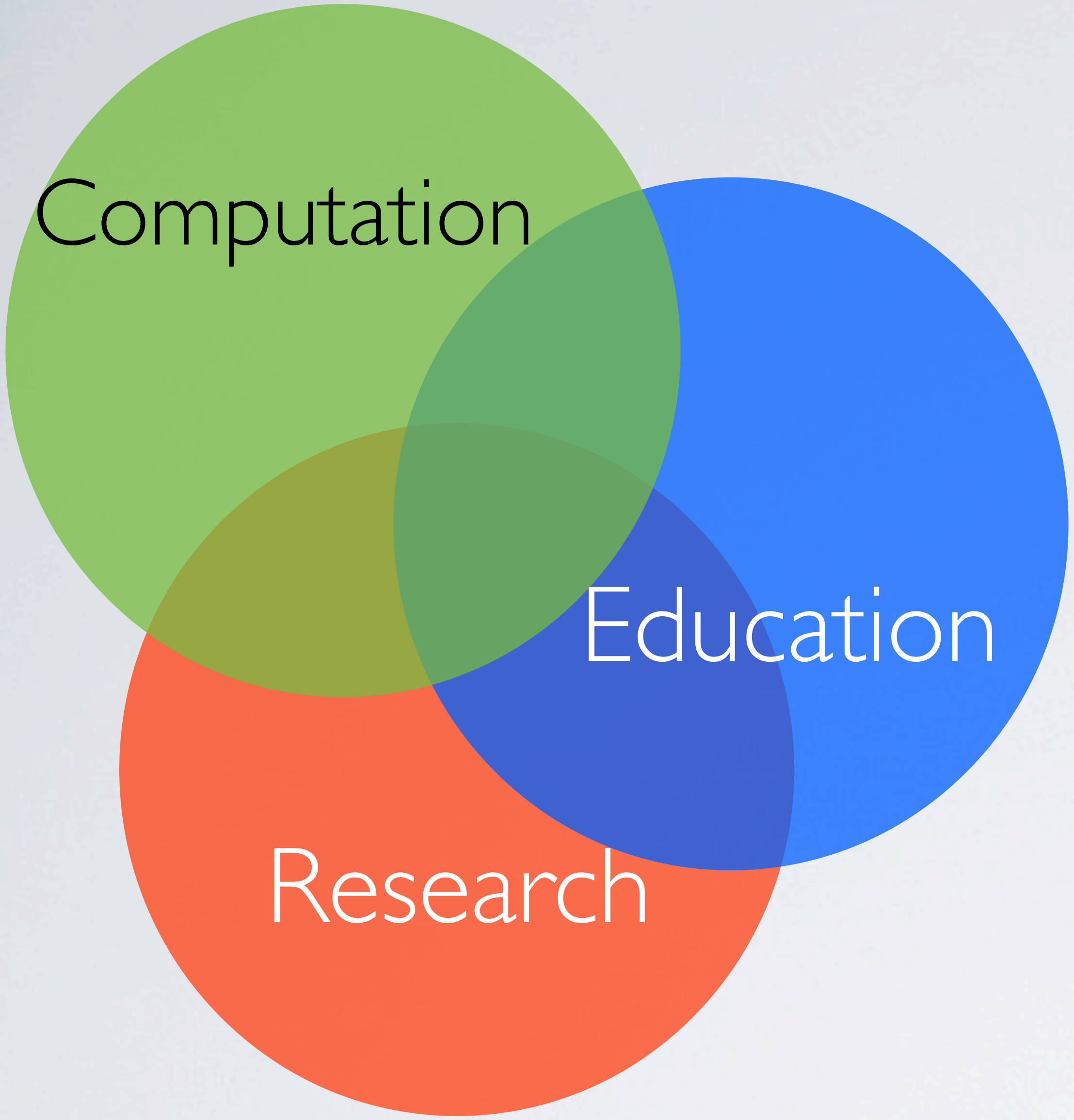
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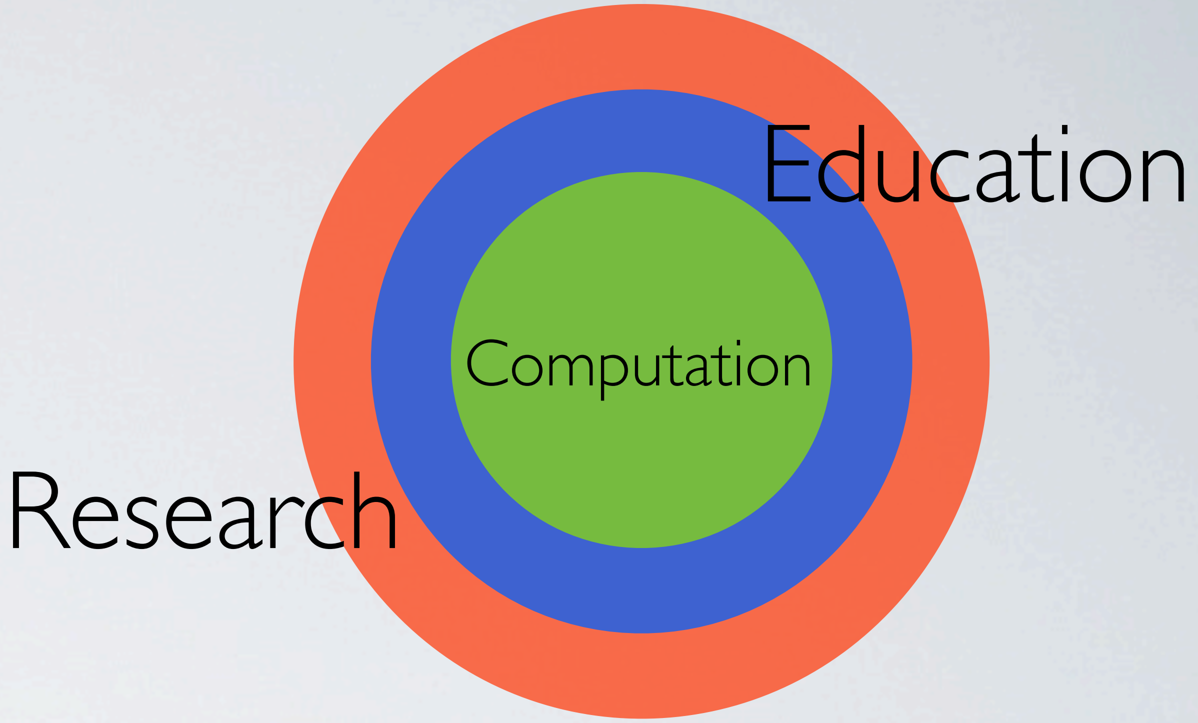
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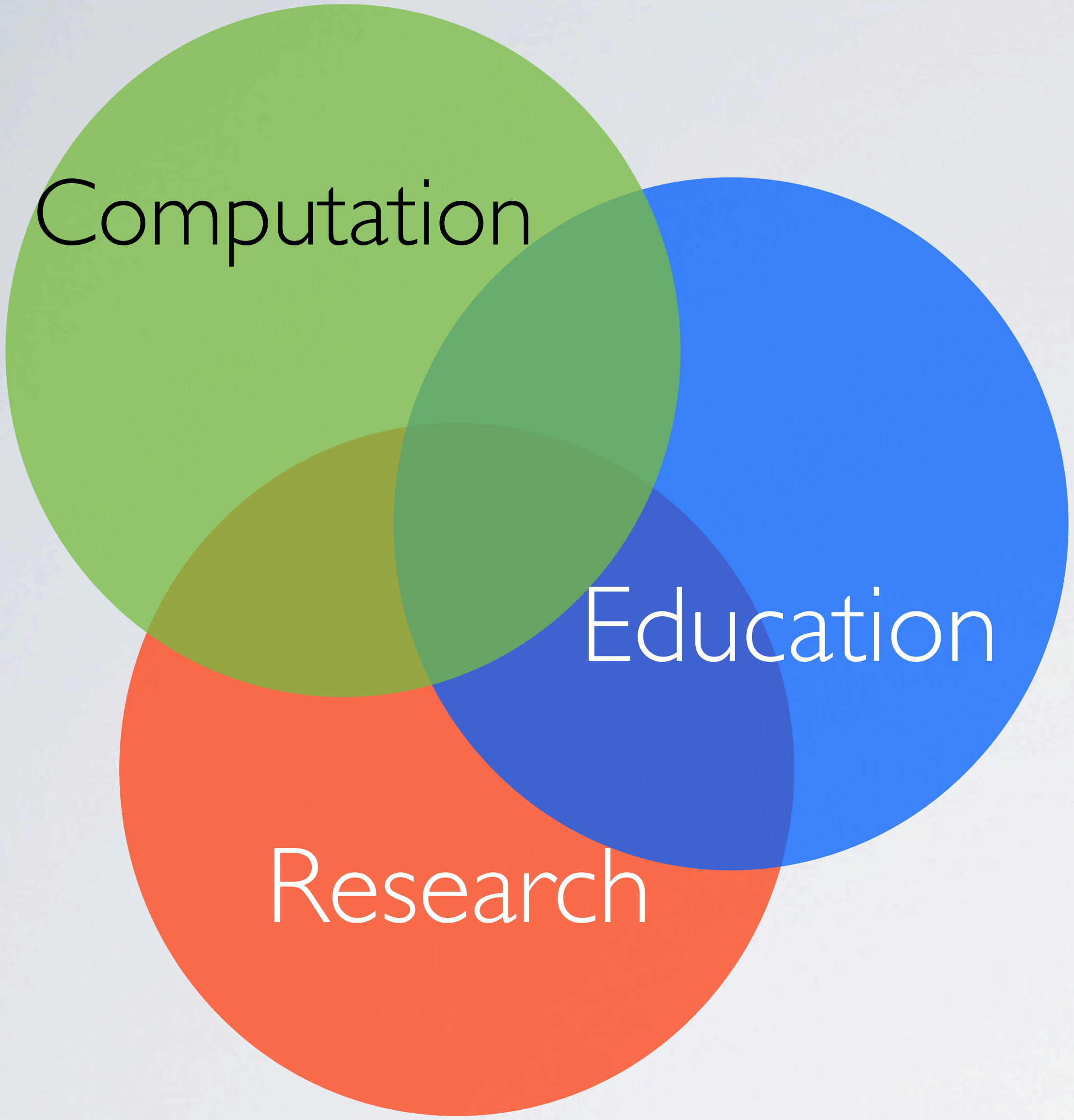
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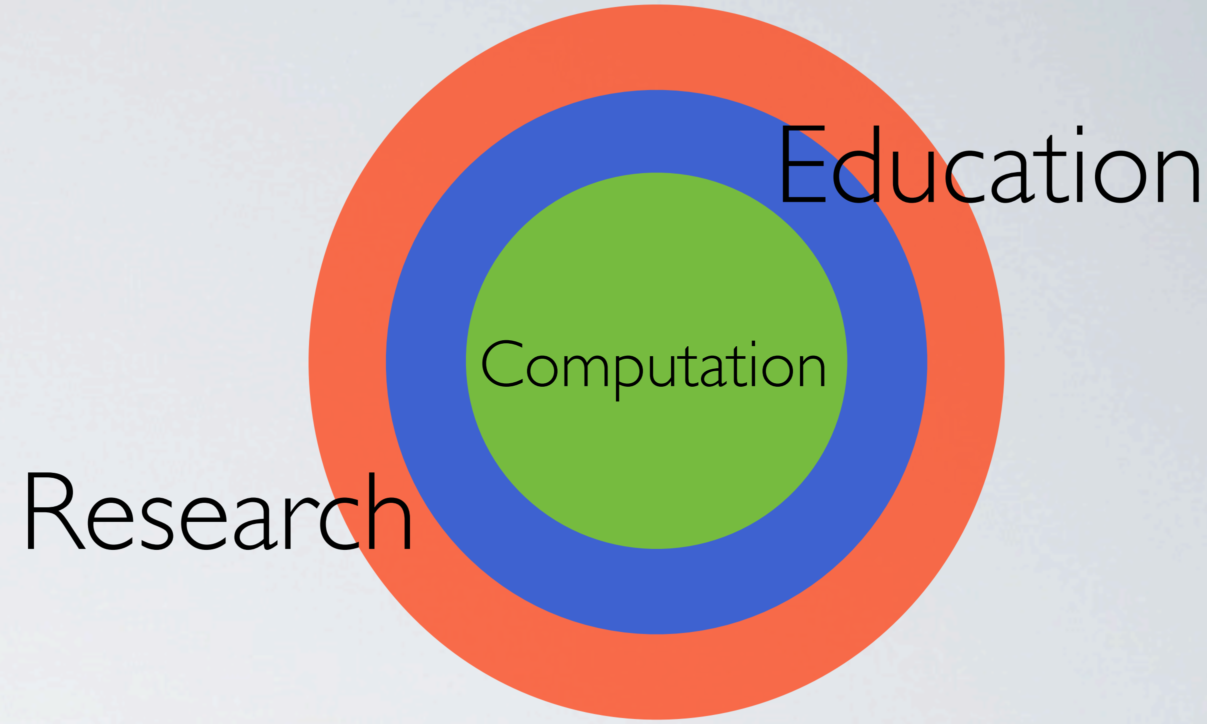
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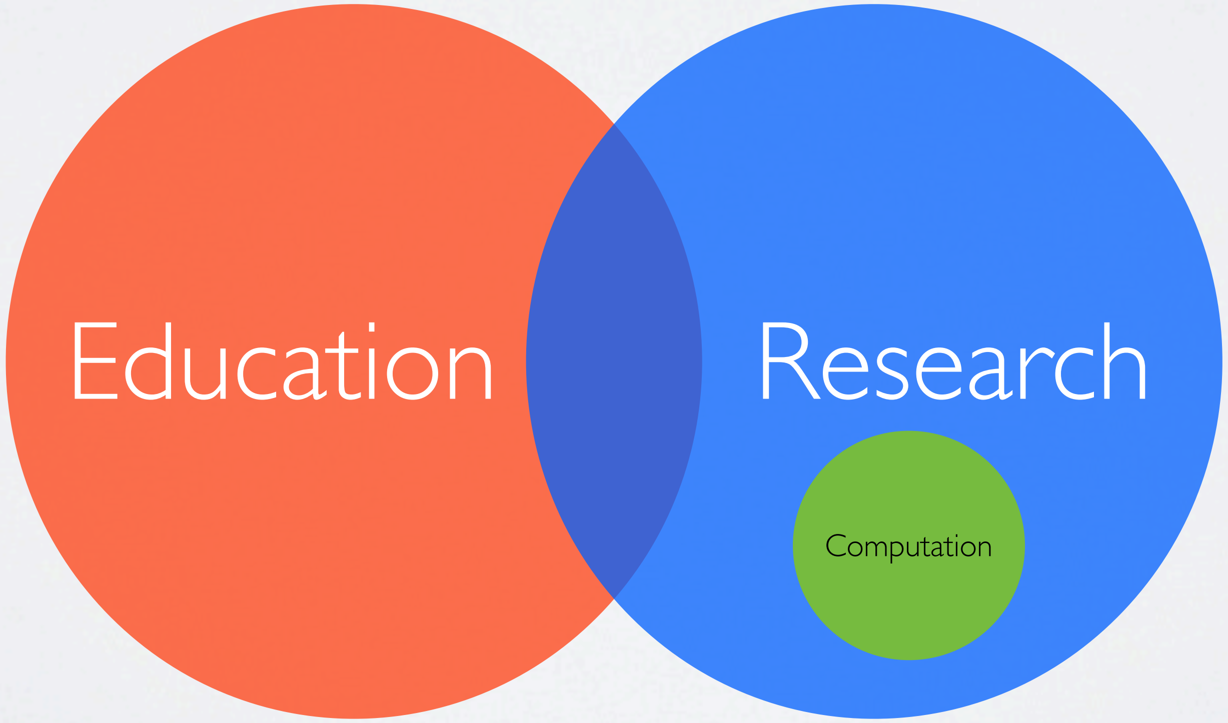

Education
Research
Computation

Integration of Computational MSE in Education

- Role of Computational MSE in the graduate curriculum at the University of FLorida
  - Implementation, Execution, Resources
- Role of Computational MSE in the undergraduate curriculum at the University of Florida
  - Implementation, Execution, Resources
- Strategies for integrating computational tools in curriculum

Education at The graduate Level

EMA 6803 Classical Methods in Computational MSE
EMA 6804 Quantum Computational Materials Science
EMA 6938 Atomistic Methods in Computational Materials Science
EMA 6938 Applied Crystallography and Powder Diffraction
EMA 6938 Materials Design
Research Seminars
Training Through Research

Graduate Students

DIVERSITY OF BACKGROUNDS

- Cultural
  - International (primary India, China, and Korean) and Domestic
- Institutional
  - Research Intensive and Liberal Arts
- Educational
  - Engineering-related fields (primarily materials, chemical, and mechanical)
  - Science-related fields (primarily physics and chemistry)
  - Other (computer science, industrial, etc.)
- Experience
  - Wide variety of programming experience
  - Rare to find computational MSE experience

ATOMISTIC METHODS

IMPLEMENTATION

- Focus
  - Molecular Dynamics
  - Molecular Statics
- Centerpiece: Writing and verifying own MD code from scratch
- Basics of Atomistic Simulation
  - Simulation Methodologies
  - Interatomic potentials
  - Materials properties
- Also featured
  - Monte Carlo
  - Kinetic Monte Carlo
  - Parallel Computing
- All work on free-standing 4-node cluster

Quantum Methods

IMPLEMENTATION

- Basics of quantum chemistry
    - Force fields
    - Semi-empirical Hückel theory and related methods
    - Fundamentals of Hartree-Fock theory
    - Inclusion of correlation: including MP2, MP4, CCT
- Density functional theory
    - Kohn-Sham equations
    - LDA and GGA
    - Pseudopotentials
    - DFT-MD
    - Time Dependent DFT
- Multi-scale methods
    - Force fields + QM
    - DFT + QM
- Students become familiar with standard packages
    - Gaussian
    - VASP

Atomistic and Quantum Methods

SEQUENCING

- Two classes are independent
- Students often have research experiences before class
- Students in computational MSE research group generally take both classes
- Some students may take only one course
  - Choice according to research topic
  - Curiosity
  - Mechanical and Chemical engineering students

Materials Design overview

The central point in this course is to introduce students to the principles, tools and applications of materials design. Concepts relating to the formulation of property-performance relations, systems approach and optimization, microstructural engineering, and design theory will be discussed

Topics Covered:

Principles of Design

Systems Concept and Approach

Materials Selection

Statistical Analysis & Design of Experiments

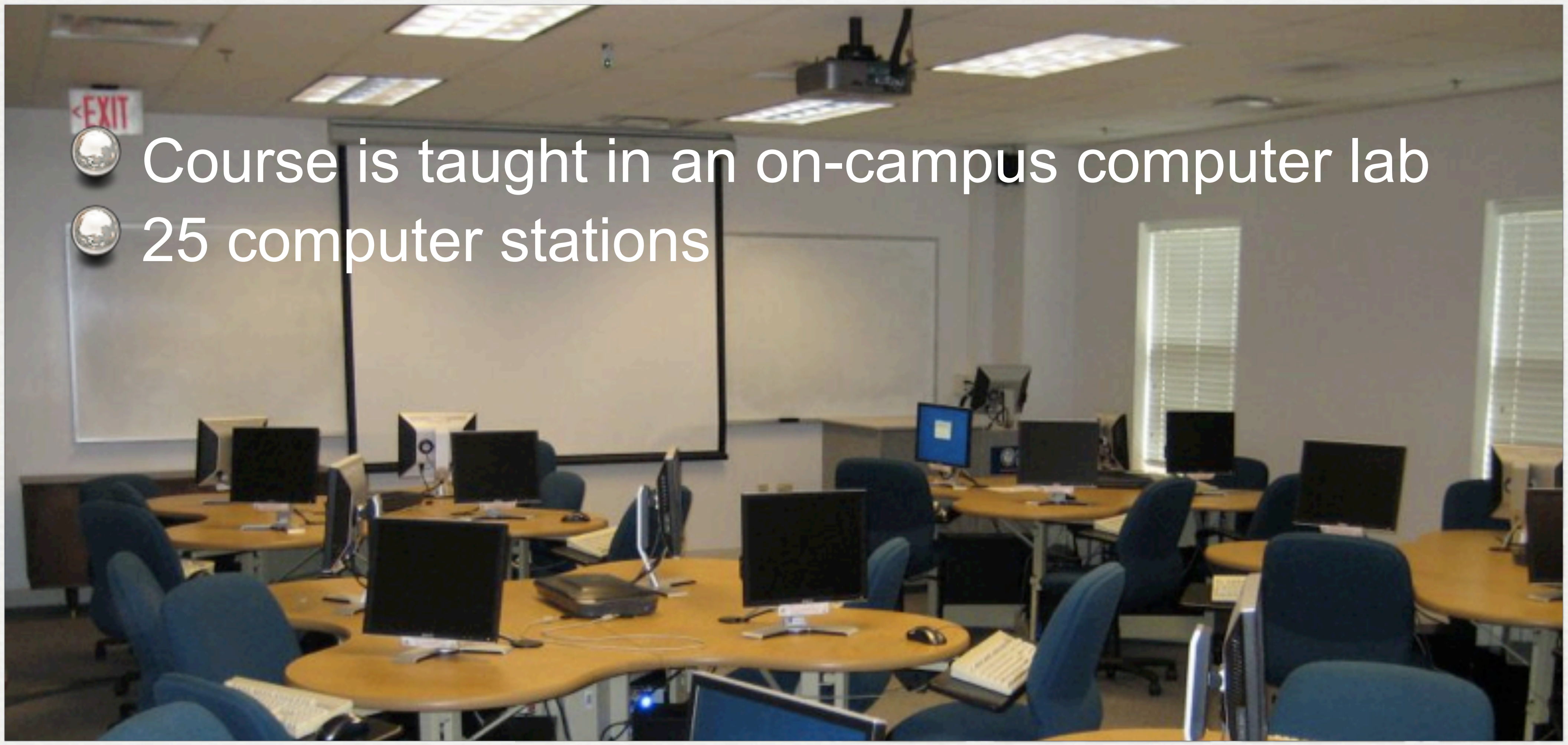
Computational Thermodynamics

Optimization

Process-Structure Relationships

Structure-Property Relationships

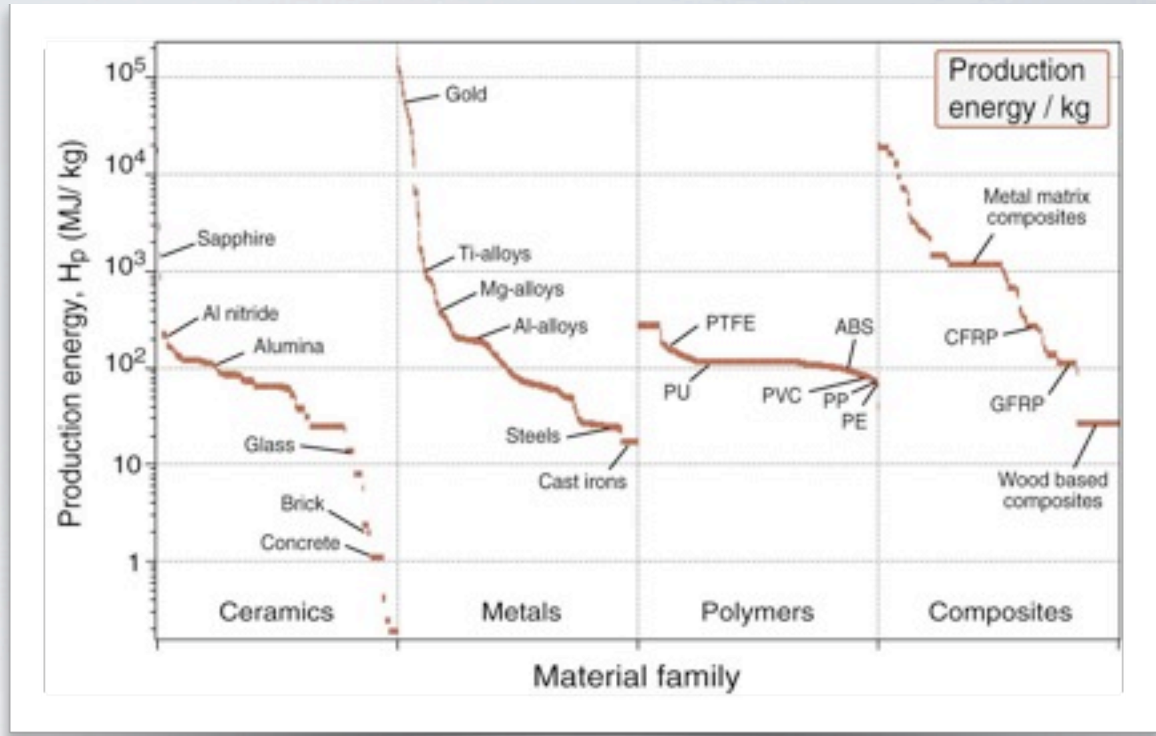
MATERIALS DESIGN IMPLEMENTATION



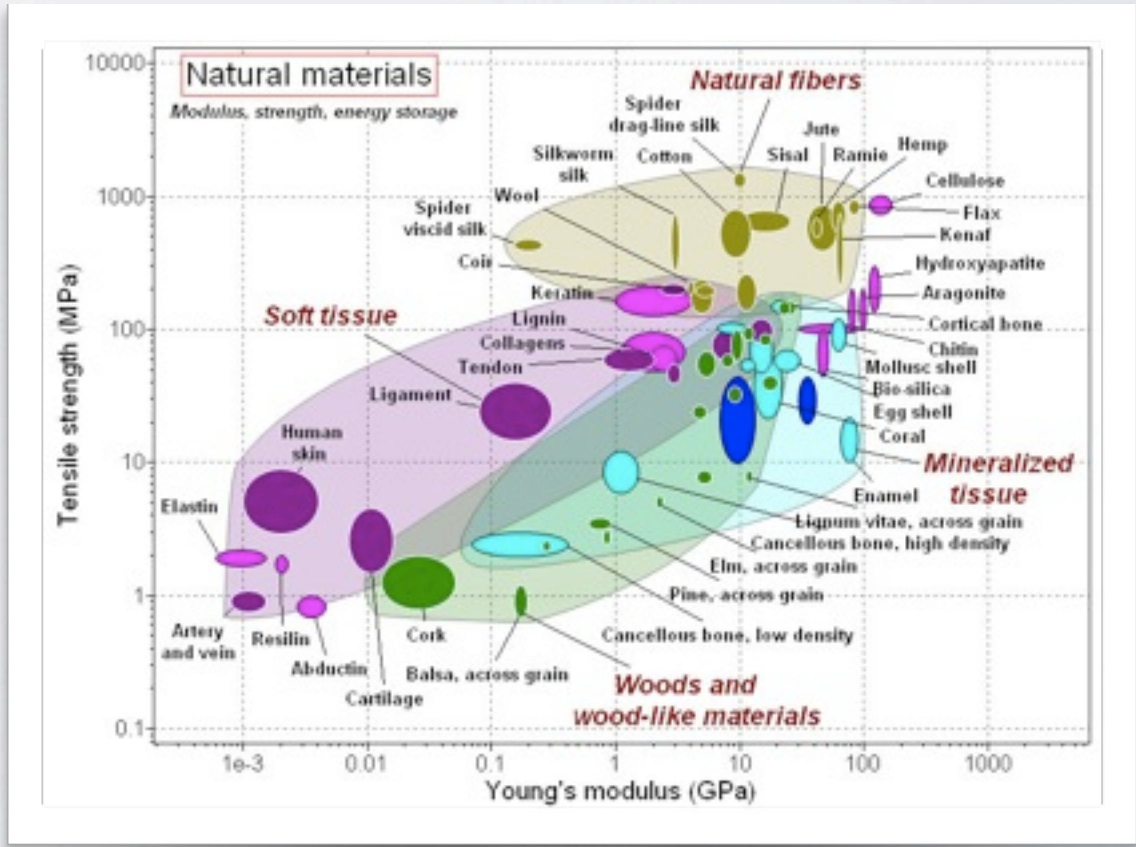
- Course is taught in an on-campus computer lab
- 25 computer stations

MATERIALS DESIGN MATERIALS SELECTION

- Provides a database for materials properties and processes
- Used as a screening method to identify material classes that are optimized for specific applications

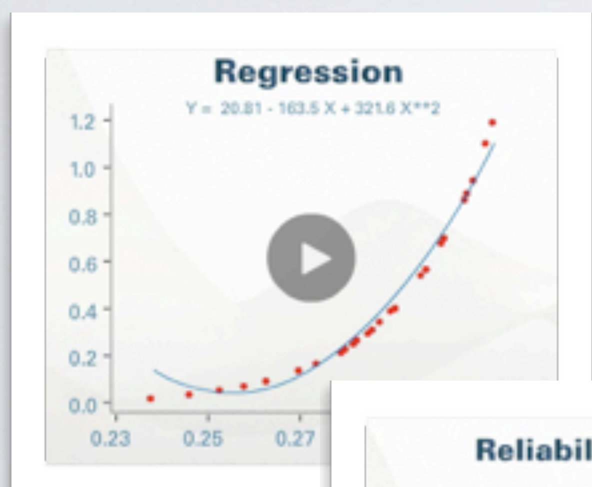


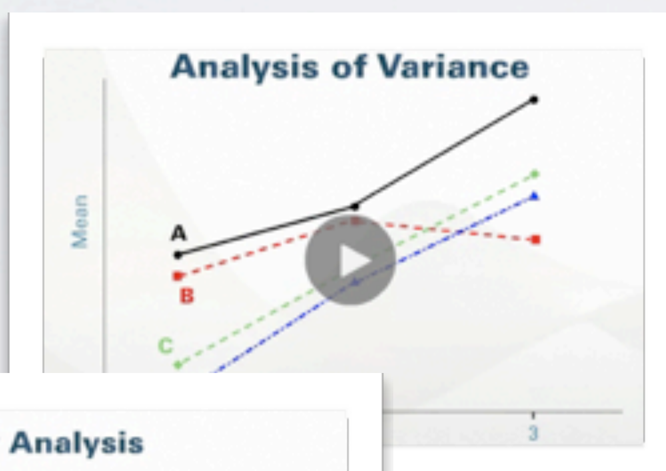
- Specialized Databases
  - Eco/Sustainability
  - Polymers
  - Medical Device Design
  - Aerospace/Defense
  - Nuclear

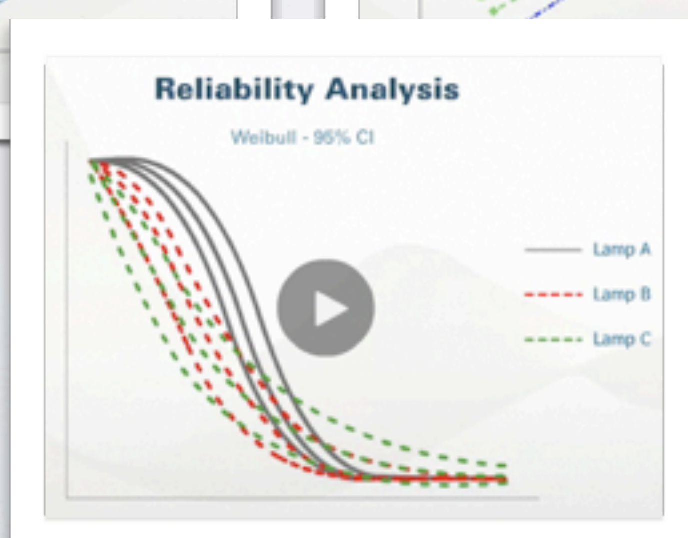


MATERIALS DESIGN STATISTICAL ANALYSIS

- Statistical Methods
  - Formal method of maximizing the information gained through experimentation
  - Avoids the tendency to use "trial-and-error" or "changing one variable at a time" approaches to experimental design
- Optimization







Minitab™

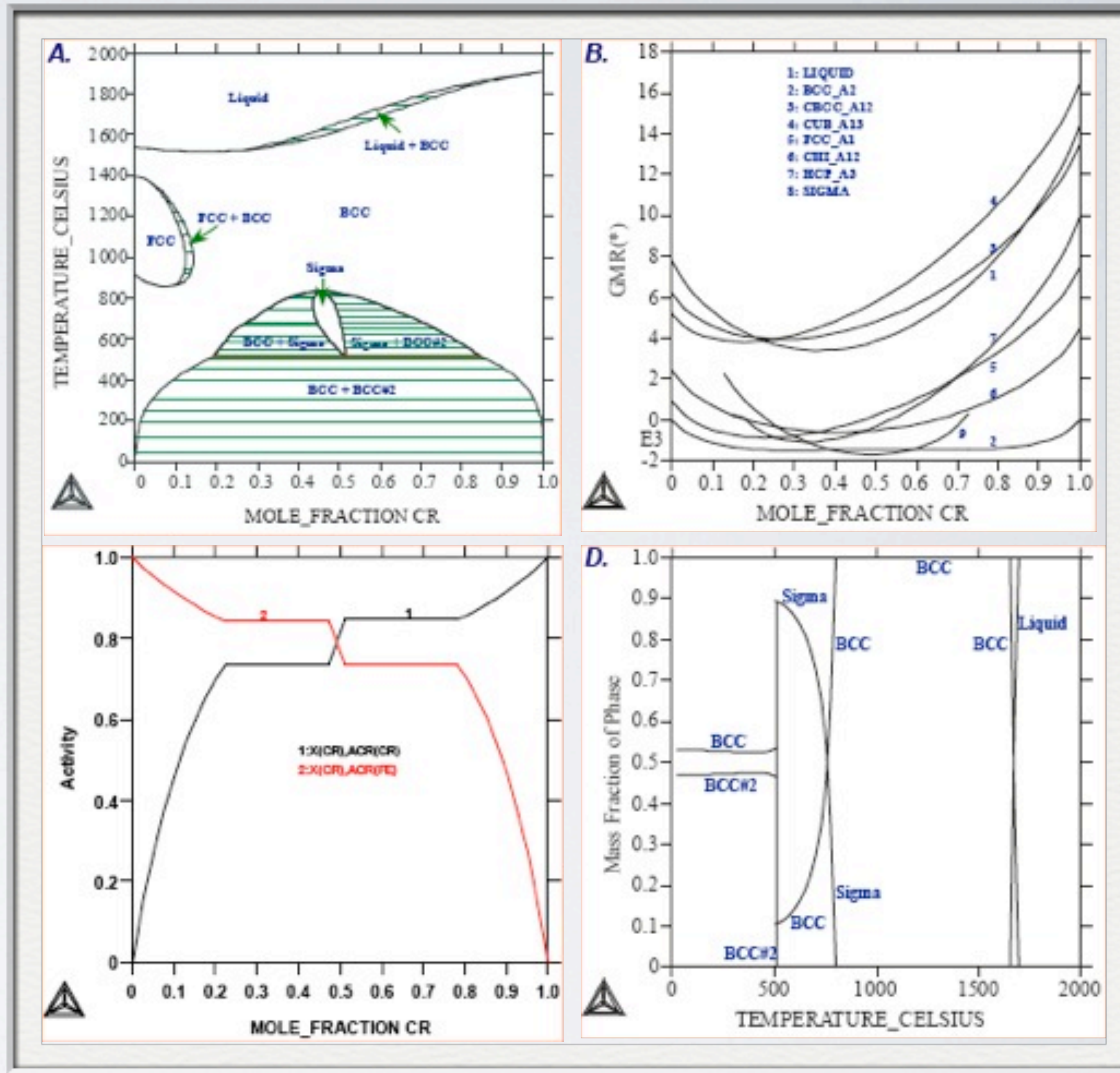
QUALITY. ANALYSIS. RESULTS.

MATERIALS DESIGN THERMODYNAMICS

- Predict Processing-Structure relationships
- Predict phase transformations
- Behavior of competing systems
- Microstructural modeling and optimization
- Combined with mechanistic models to predict properties

Thermo-Calc Software
www.thermocalc.com

CompuTherm LLC



ThermoCalc UsersGuide

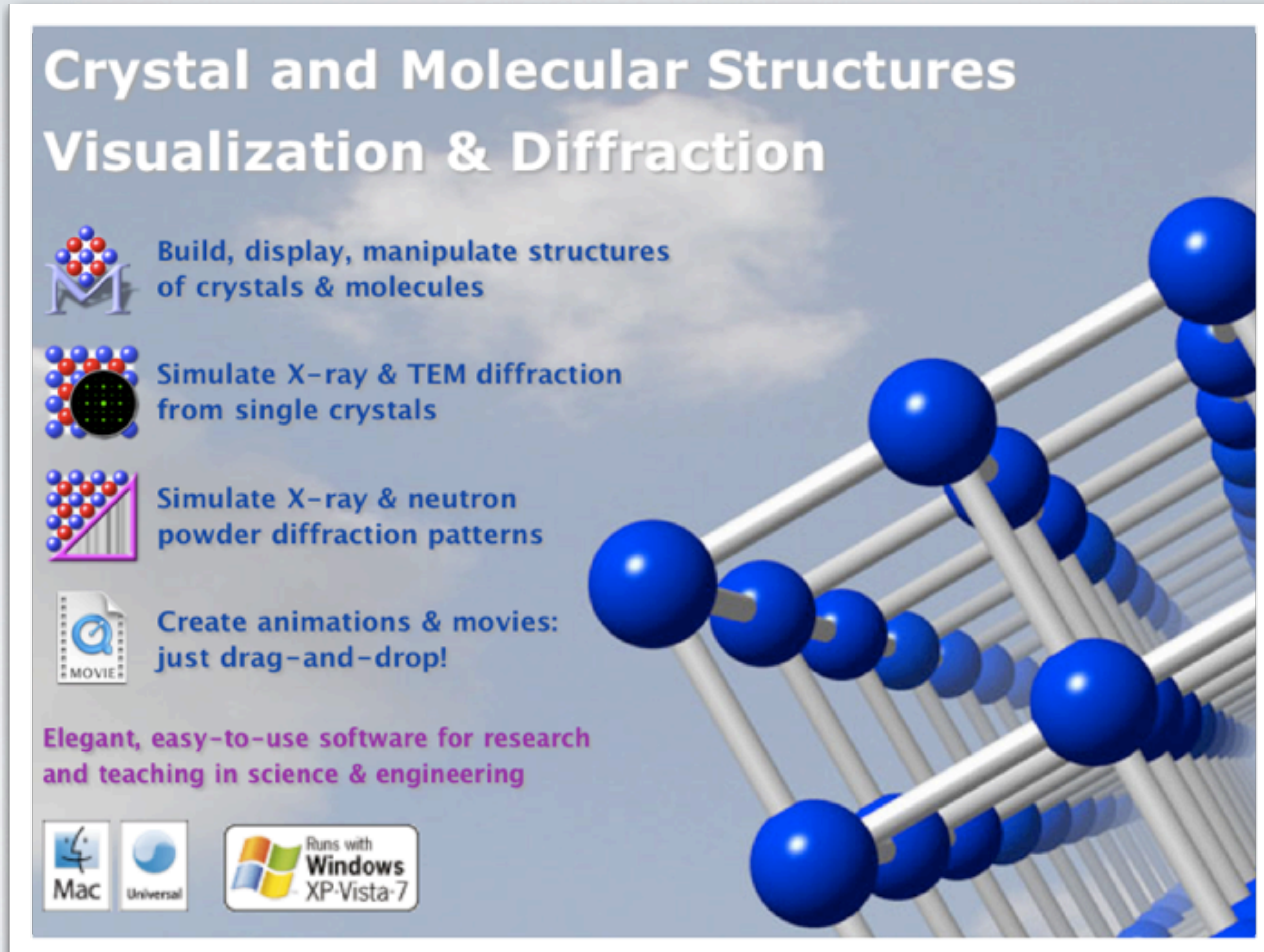
Materials Design resources

- Cambridge Engineering Selector by Granta
  - Annual license owned by department
- Minitab
  - Available in all on campus computer labs
  - Available for university computers for ~ $30/seat
- Thermocalc
  - Free databases are available, ie NIST Solder Database
  - License managed by departmental campus license server
  - Linux version used (Windows version available)
- PANDAT by Computherm
  - Advanced databases owned by the PI Manuel
  - Free DEMO version with built-in database for Al-Cu-Mg-Si
  - Uses same formalisms as Thermocalc, thus unencrypted databases are exchangeable

MATERIALS DESIGN ADDITIONAL RESOURCES

- Thermodynamic and Kinetic
  - FactSage by CRCT
    - Oriented toward physical chemistry, optimized for liquids/molten
  - DICTRA by Thermocalc
    - Simulates diffusion of multicomponent alloy systems
  - PrecipiCalc by QuesTek Innovations
    - Simulates 3D multi-particle precipitation kinetics
- Design Management
  - iSIGHT PRO by Engineous Software
    - Design integration and management software

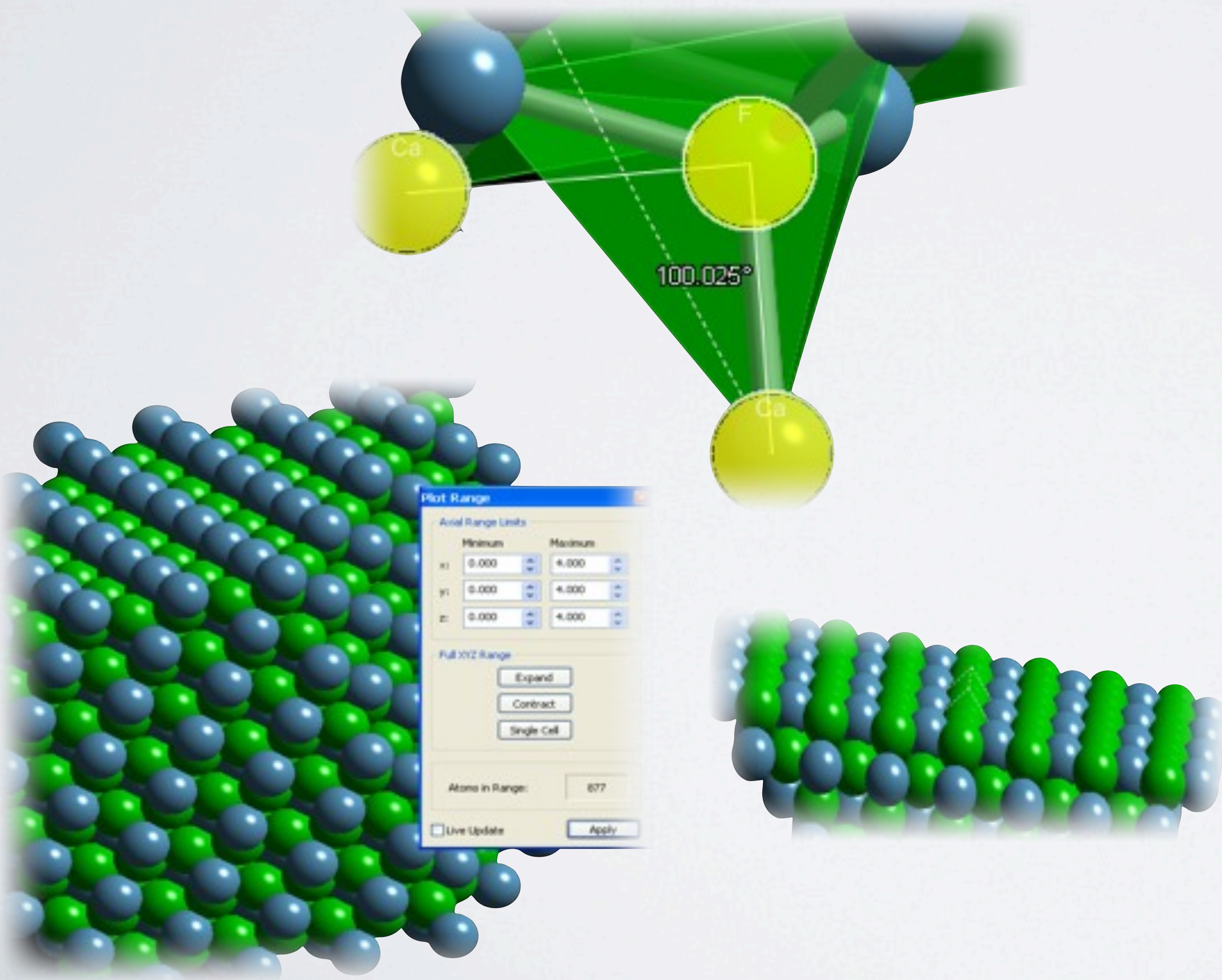
Applied Crystallography and Powder Diffraction



CrystalMaker® SOFTWARE

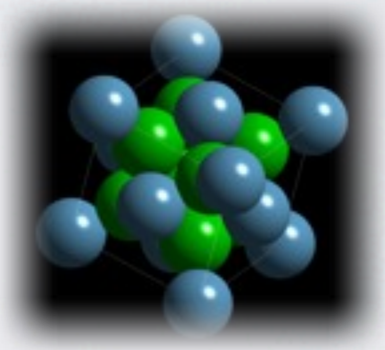
Applied Crystallography and Powder Diffraction

Visualize & Analyze: bond angles, density, slices, defect structures, etc.



Views using the "Model" menu

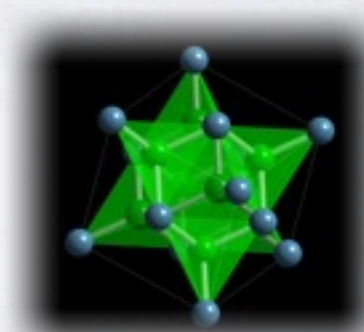
Space Filling



Ball and Stick

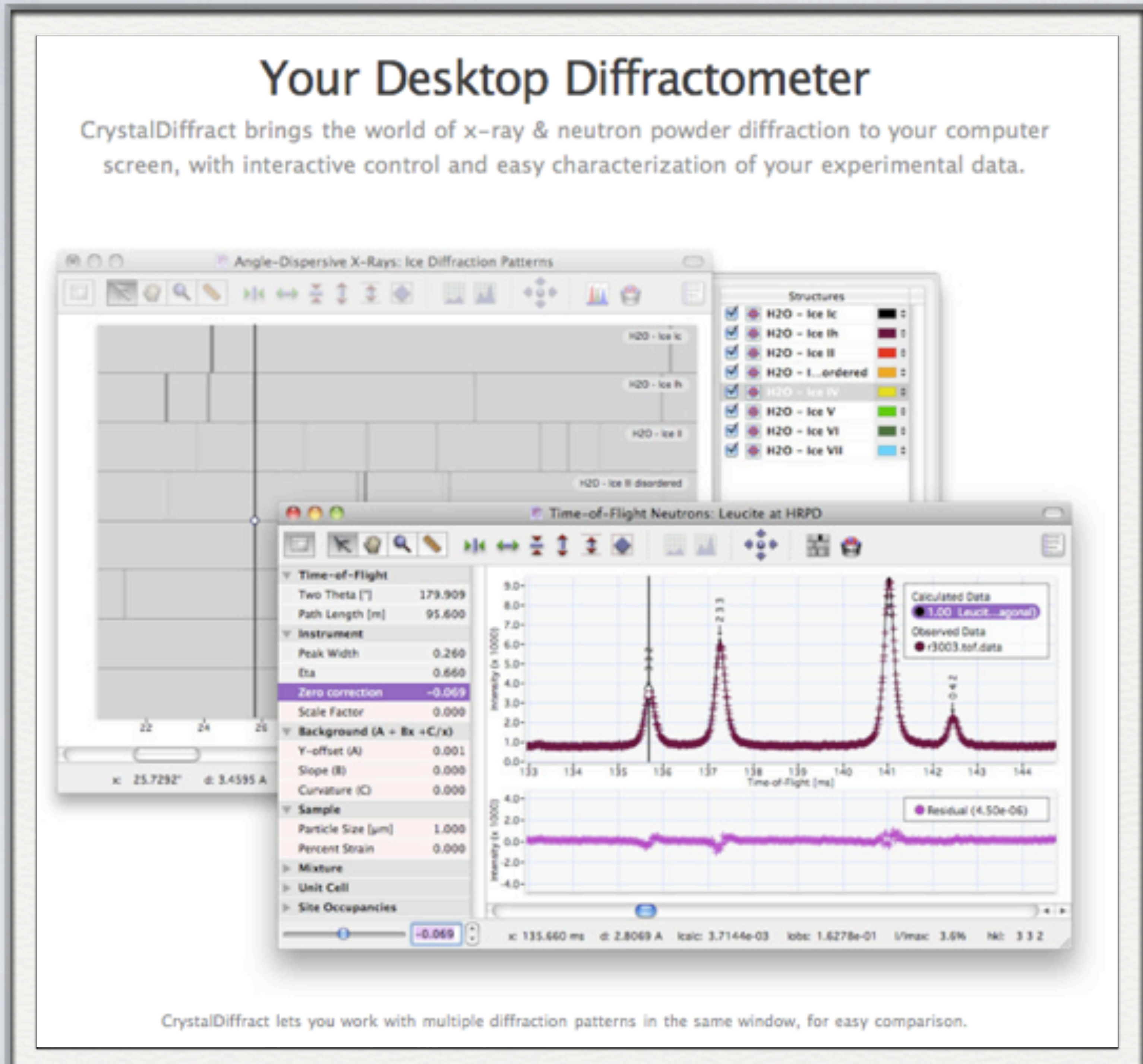
Stick

Polyhedral



CrystalMaker®
SOFTWARE

Applied Crystallography and Powder Diffraction



- Simulate x-ray or neutron powder diffraction patterns
- Analyze experimental data and check for impurity phases or other anomalies

Available to students through a departmental site license.

CrystalMaker SOFTWARE

Non-MSE Curricula

L E V E R A G I N G

- Computational Chemistry
  - Department of Chemistry
- Statistical Mechanics Methods for MD Simulations
  - Chemical Engineering
- Fundamentals of DFT
  - Department of Physics
- Continuum Mechanics
  - Department of Mechanical and Aerospace Engineering
- Design of Experiments
  - Department of Mechanical and Aerospace Engineering
  - Department of Industrial Engineering
- Optimization
  - Department of Mechanical and Aerospace Engineering

GRADUATE COURSES COMMONALITY

- Each student carries out some calculations for the course and then works on material of his/her own choosing
- Oral presentations of results to the class
- Final reports
- Approach allows students to be exposed the strengths and weaknesses of each method as applied to a wide range of materials without requiring too many computationally expensive calculations per student

MAXIMIZING GRADUATE EDUCATION

O P P O R T U N I T I E S

- Integrate Research and Education
  - Graduate students given opportunity to use the tools in their research
  - Advanced tools for advanced students
- Leverage outside resources by cross-listing courses outside of the department

Education at The Undergraduate Level

Elevating Undergraduate Education
Status, Challenges, Barriers, and Opportunities

Undergraduate Students

Uniformity of Backgrounds

- Institutional
  - Primarily from State of Florida high schools
- Educational
  - State of Florida accreditation standards
- Experience
  - Limited programming experience
  - No computational MSE experience
- Typical MSE Undergraduate Characteristics
  - Yearly class size: 30-50 students
  - All College of Engineering Students required to have laptops
  - “Digital Natives” - millennial learners

Goal: Increase technical depth of undergraduate students

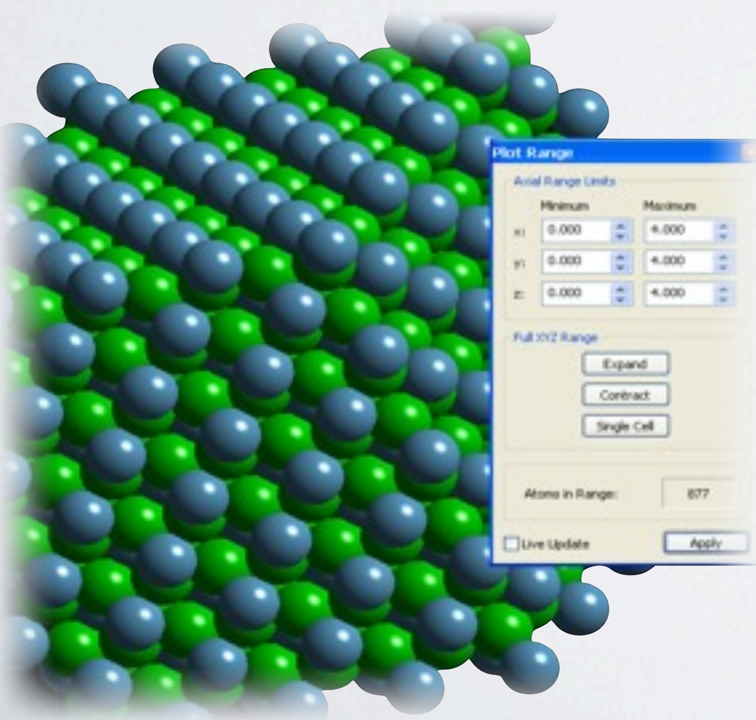
Undergraduate Courses

Integration of Computational Methods

Physical Ceramics/ Intro to Inorganic Materials

- Junior level course
- Uses structure processing and properties of inorganic materials, including metals, alloys, and ceramics.

CrystalMaker® SOFTWARE



Materials Selection and Failure Analysis

- Senior level capstone design course
- Philosophy and practice of engineering selection of materials. Case studies in product liability and failure analysis.

Undergraduate Courses

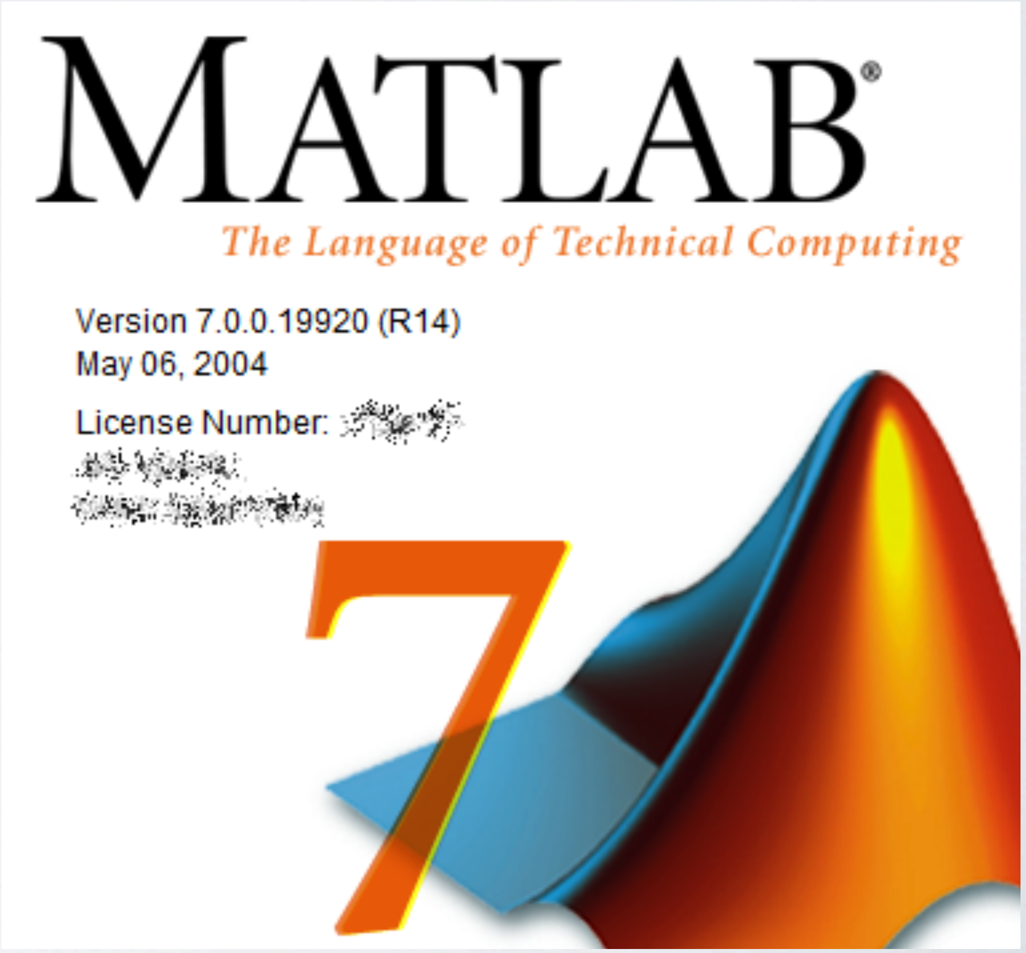
INTEGRATION OF COMPUTATIONAL METHODS

Error Analysis and Optimization

- Junior level course
- Statistical approach for materials research, basic and relevant statistical concepts, error analyses, factorial matrices, reducing the variance, nested designs, sampling plans, mixture designs, optimization technology, response surface method and Taguchi

Transport Phenomenon in Materials Processing

- Senior level course
- Science and application of momentum, heat and mass transport in materials and materials processing



Undergraduate Courses

W O R K   I N   P R O G R E S S

- Analysis of Computational Requirement
- Concurrent Modeling and Experimentation
- Energy Minimization in Thermodynamics

Undergraduate Courses

COMPUTATIONAL REQUIREMENT

- Assessment
  - Students taking a variety of programming languages
  - Majority of student taking Visual Basic
- Action
  - Trade programming language for a numerical methods course
  - Promote the use of MatLab
- Motivation
  - Common platform creates continuity in curriculum

Undergraduate Courses

EXPERIMENTATION & COMPUTATION

- Assessment
  - Limited computational tools used across curriculum
  - No computational tools used in laboratory classes
    - Materials Laboratory (1 year course), Processing course (1 semester), Characterization course (1 semester)
- Action
  - Add computational thermodynamics
    - ex. calorimetry, analysis of microstructure, phase transformations
  - Add design of experiments (statistical analysis)
    - ex. final project optimize a performance index in a composite
  - Students should use computational tools to predict behavior and then validate with experiment
- Motivation
  - Link the relationship between experimental and computational data

Undergraduate Courses

ENERGY MINIMIZATION

- Assessment
  - No computational tools used in thermodynamics & kinetics course
- Action
  - Add computational thermodynamics (if cost allow)
    - Computational thermodynamics used in graduate curricula, thus infrastructure is in place
  - Add a numerical project (M. Asta)
    - ex. final project optimize a performance index in a composite
- Motivation
  - Gain a deeper understanding of energy minimization through numerical analysis
  - Understand the limitation and power of computational thermodynamics

Challenges and Barriers

U N I V E R S A L (UNDERGRAD AND GRAD)

- No unified agreement in community - ABET?, Textbooks?
- Recognized that it is important to integrate into undergraduate curriculum but where and how to do it?
    - Elective versus Core or both?
- Computational tools expected by employers are disconnected from what is offered in academia
- Location of educational resources is ambiguous

Challenges and Barriers

U N I V E R S A L (UNDERGRAD AND GRAD)

- No unifi ... oks?
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- Comput ... onnected from wh
- Location

Table I. Tools Cited by Employers, Categorized and Ranked by the (Normalized) Frequency of Cites, along with Corresponding Results from the Computational Faculty Survey

Category	Example	Employer	Faculty*
Mechanics (mostly FEA)	DEFORM, ABAQUS	80%	14%
Thermodynamics (CALPHAD)	ThermoCalc, Pandat	53%	7%
Density Functional Theory	VASP, ABNIT	47%	21%
Programming Language/Integration	Matlab, Fortran, iSight	40%	43%
Casting	ProCAST, MAGMAsoft	40%	—
Molecular Dynamics/ Monte Carlo	LAMMPS	27%	14%
Fluid Flow/ Heat Transfer	COMSOL, Fluent	20%	7%
Diffusion/ Microstructural Evolution	DICTRA, PrecipiCalc, JMatPro	20%	—
Statistics	Informatics	13%	7%
Materials Modeling Suite	Materials Studio	13%	—
General Visualization	Mathematica, Tecplot	7%	29%
General Data Processing	Spreadsheet	7%	21%
Special Purpose	K-Flow, WARP 3D	7%	—
Materials Selection	CES Materials Selector	—	36%
Crystallography	CaRIne	—	7%

*Some of the responses did not provide specific software/categories, and therefore we expect some degree of undercounting in this data.

*Thornton, K et. al 2009

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Challenges and Barriers

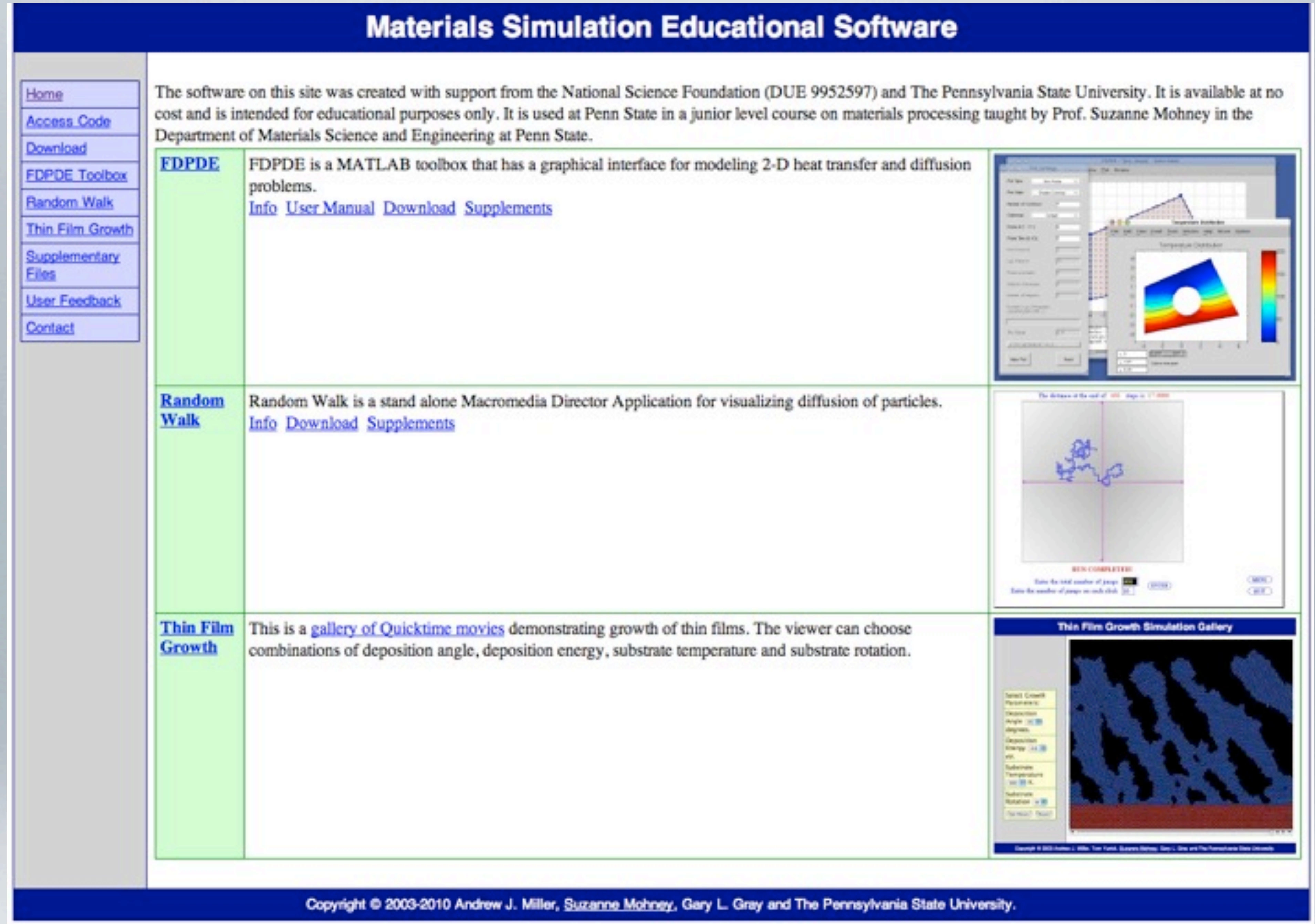
U N I V E R S A L (UNDERGRAD AND GRAD)

- Infrastructure: Space, location, environment
- Technology Support: IT
- Licensing: Single seat, departmental, perpetual
- Platforms: PC, UNIX, Mac
- Energy Barrier for Faculty
- Cost: Economies of scale, cost-benefit analysis

User-Friendly

&

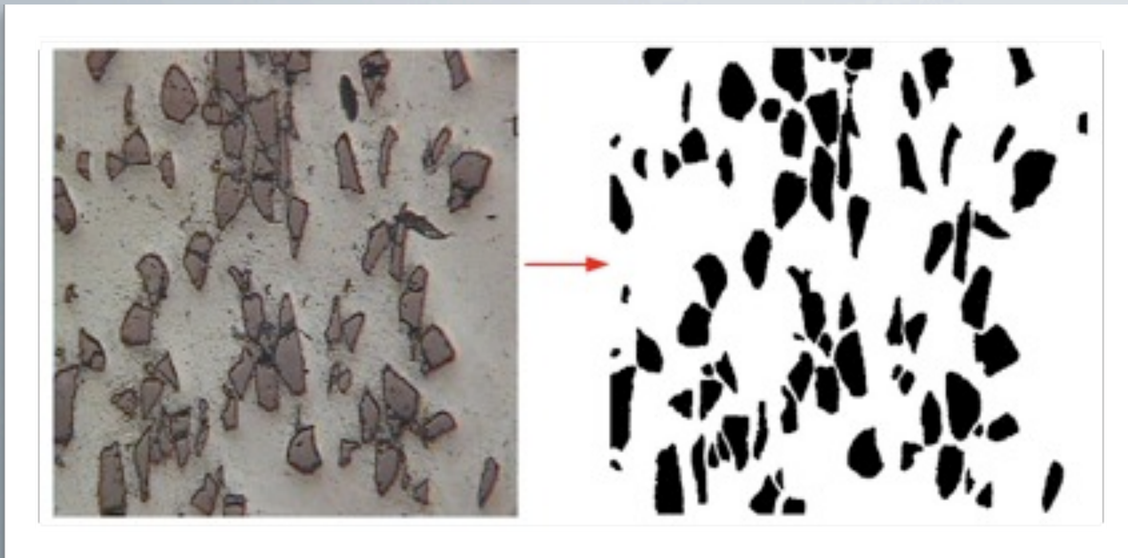
Open-Source

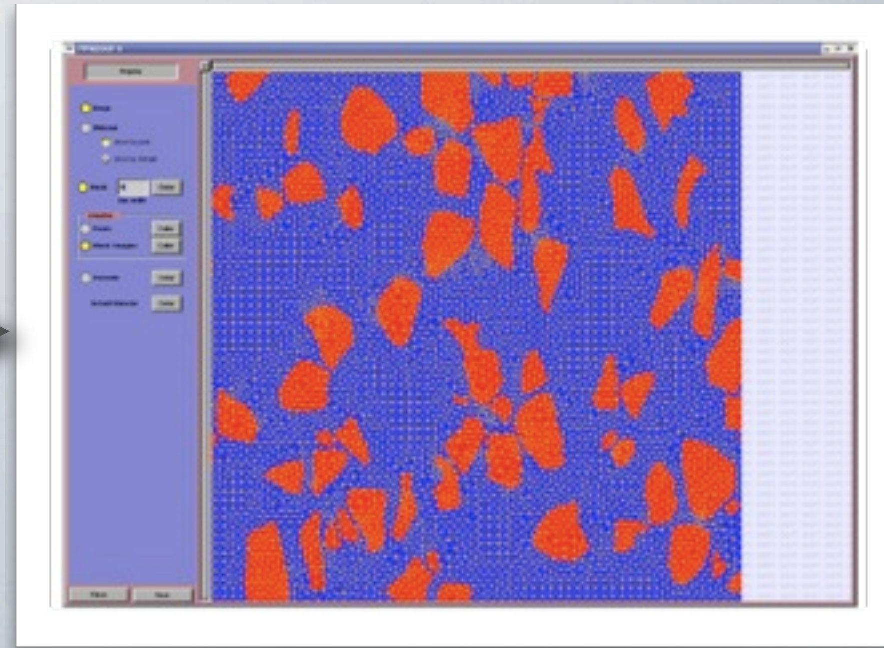


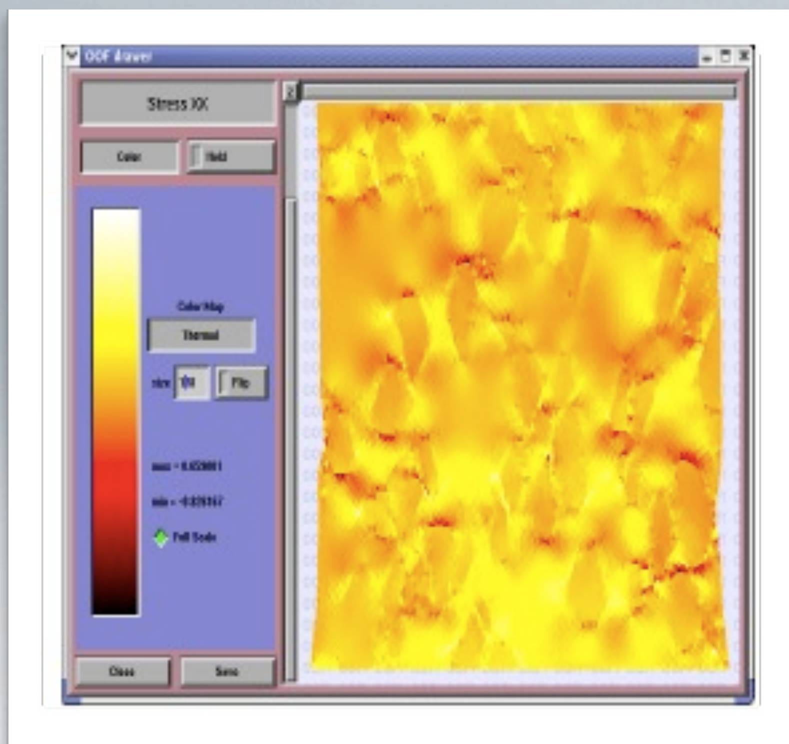
2D-Heat Transfer and Diffusion

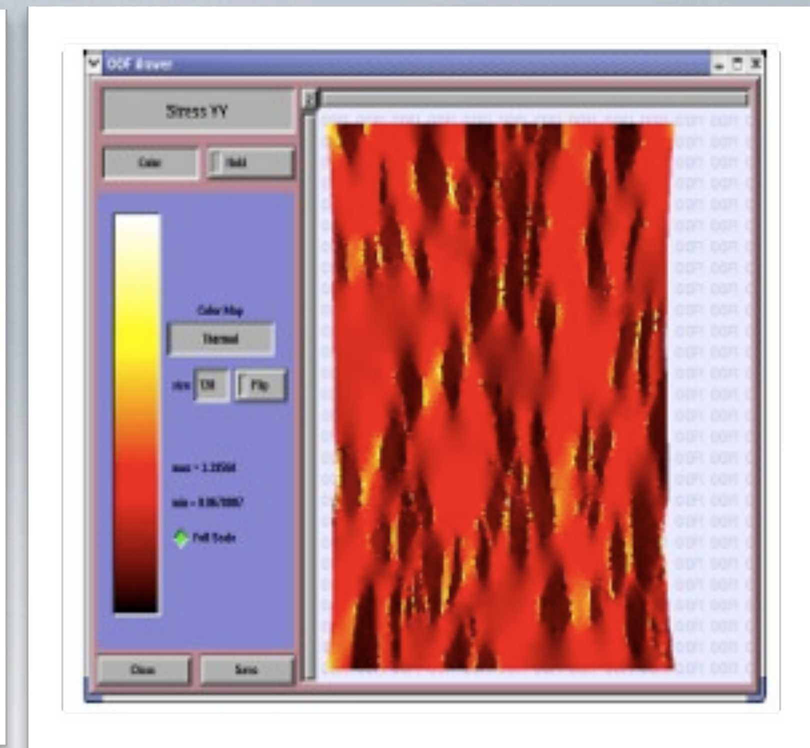
P E N N S T A T E

http://www.esm.psu.edu/matls-sim/main.php









OOF: Finite Element Modeling For Materials Science N I S T

http://www.nist.gov/msel/ctcms/oof/index.cfm

Suggestions for Immediate Action

TOP 5 ACTION ITEMS

1. Seek a Unified Platform
2. Leverage non-MSE courses
3. Use research-grade software in graduate courses
4. Use basic or open-source programs to teach fundamentals
5. Integrate computational tools as early in the curriculum as possible

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