The Texas A&M University Computational Materials Science Summer School (CMS³): CyberTraining Program (NSF-OAC 1829799)

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Motivation

Grand Engineering Challenges

Economical solar energy | Energy from fusion | Carbon sequestration
Manage nitrogen cycle | Access to clean water | Improve urban infrastructure | Advance health informatics
Engineer better medicines | Prevent nuclear terror | Tools of scientific discovery

Require significant material advances

Materials Genome Initiative & ICME

- Shorten time-to-market for new materials
- Integrate computational tools and techniques
- How to solve key problems in a data/distractor-cluttered world

How to appropriately train research workforce?

Objectives

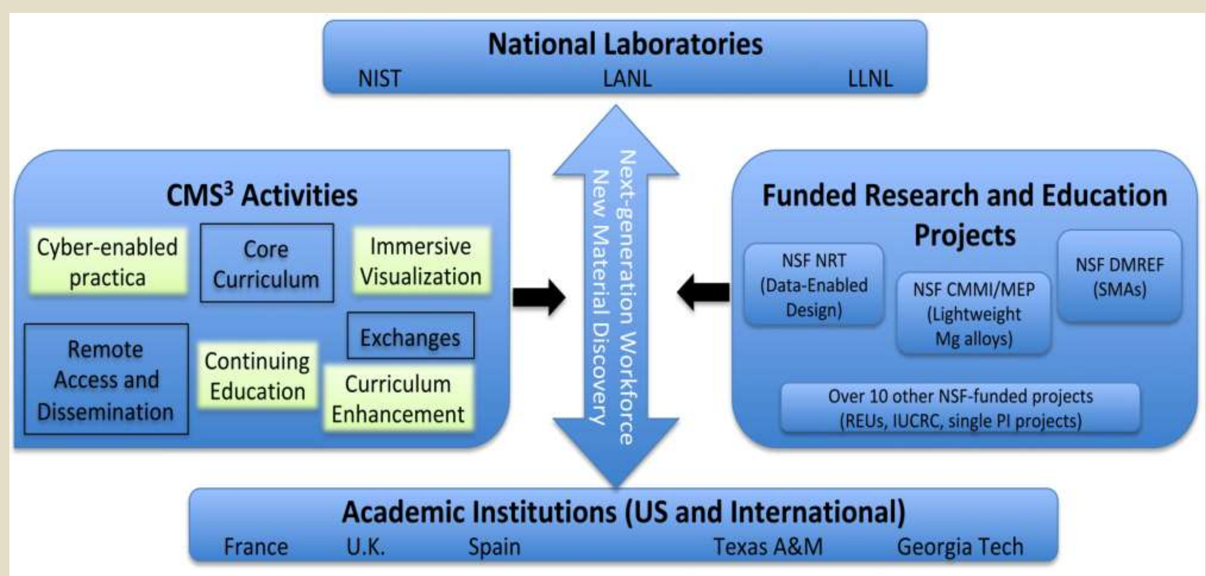
- Establish a **computational material science (CMS)** network among national laboratories and academic institution in developing next-generation workforce in materials research.
- Develop a **CMS curriculum**, that involves utilizing and supporting advanced **cyber-infrastructure (CI)** for effective scaleup of the practical component.
- Integrate the **theoretical foundations and practical training** into the graduate curriculum and continuing education at Texas A&M University
- Introduce **immerse visualization** through **virtual and augmented reality (AR/VR)** tools to help students with different backgrounds and learning styles interpret complex material data

Program Background and Overview

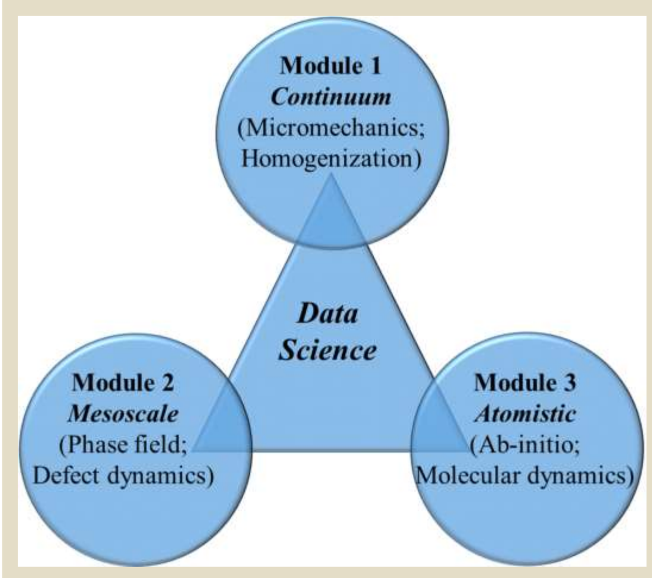
TAMU Computational Summer School Across the Scales

- Theory and practice of methods in computational materials science (and data-enabled techniques) across scales.
- **> 140 students** from the U.S., Europe, Middle East, Africa, Latin America participated to date
- **>35 instructors** from US and abroad

Scaled-up infrastructure and collaborative networks



Learning Outcomes



Multiplescale computational materials science.
Top-down approach:

- **Continuum level**: micromechanical homogenization.
- **Mesoscale**: phase filed modeling and discrete dislocation dynamics.
- **Atomic Scale**: first-principle quantum

The three modules structures, are enhanced with cross-cutting modules on **data enabled science**.

Enhancements in the program

1. Widening access to *practica*

Cyber-Enabled Practica:

Two type of student population: 1st On site limited to 20 students and 2nd 80 online students connected remotely by leveraging virtualization technology

Immerse Visualization

Utilizing emerging Virtual Reality (VR) technologies and applications to make education accessible to a wider variety of learning styles and to remote audiences.

2. Enhancing the curriculum of CMS³

Graduate curriculum Enhancement

- New Graduate course at Tamu focused on computational materials science.
- Incorporate pervasively elements of data science.

Profesional and continuing education

- TEES provides opportunities for professional and continuing education with a streamlined certification process.

Vertical Programs

Cyberinfrastructure

- The CMS³ cyberinfrastructure is structured around **four key concepts**:

1. Remote teaching:

- On-Site lectures will be streamlined live to remote students.
- Remote presentations and remote teaching applications through TAMU's videoconference network

2. Scaleup of Practica:

- High-Performnce Research Computing facility at TAMU will provide the needed computer resources for CMS attendees.
- Access via a web browser a full desktop hosted at Texas A&M University to perform exercises
- Remote attendances will be given local accounts and should not have to use VPN

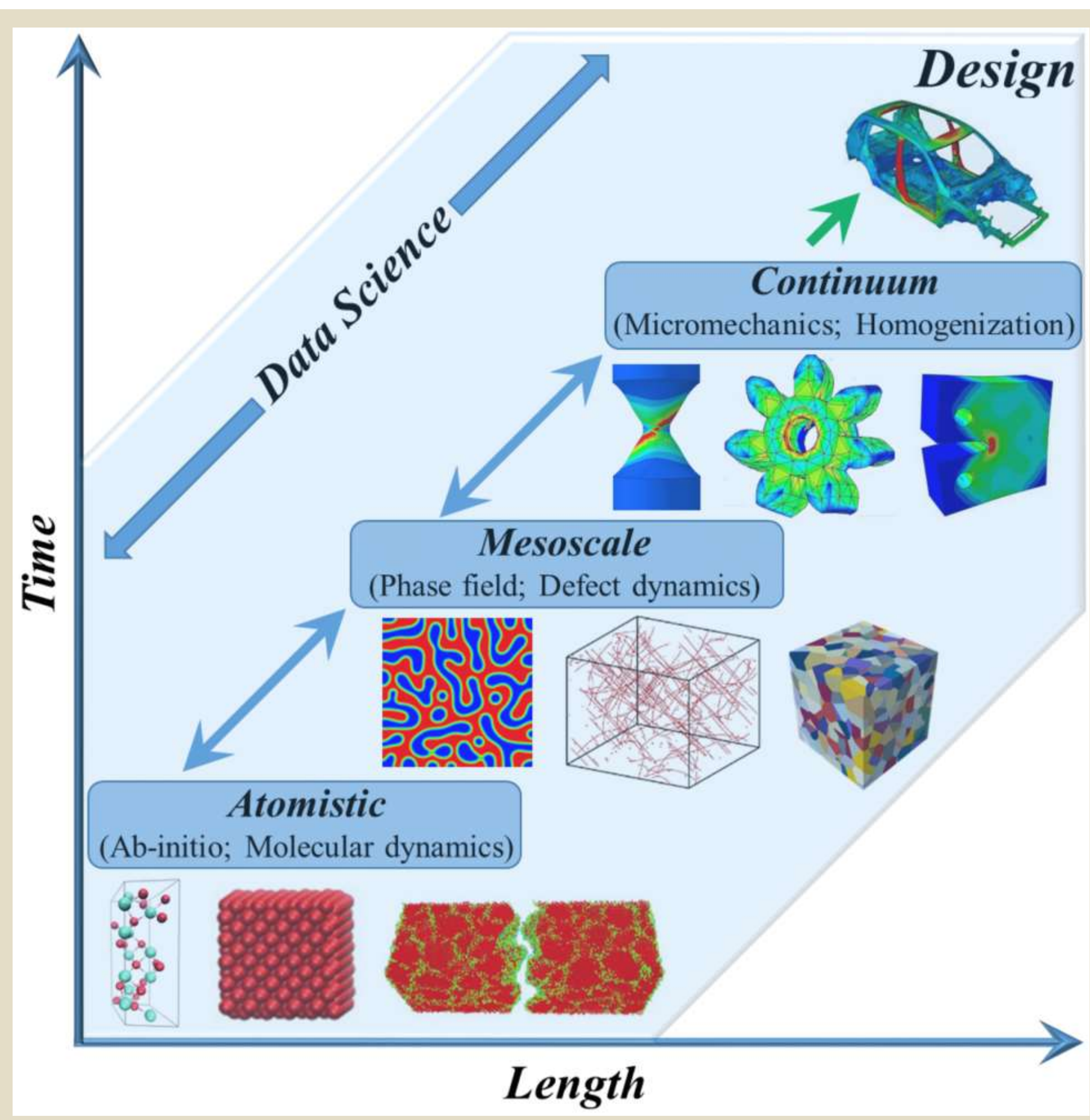
3. Immerse Visualization:

- VR technology that will be live streamed for students using their own smarphones and low-cost VR headsets.
- HTC Vive VR system for content creation and instructor delivery and Google Cardboard headsets for distributed student consumption.
- Instructors can utilize Vives to lead lessons regarding material science/mechanics concepts (e.g., material crystal structures, simulation results), while students use Google Cardboards to view interactive lessons in real time.

4. Broadening access to CMS³ Curricular Material:

- ICME specific infrastructure: (I) self-contained formulation of models, (ii) copies of codes under appropriate licenses, (iii) detailed description of how to use codes and (iV) addenda, e.g. any enhancement to the codes used. .
- CMS cyberinfraestructure will make experimental processing-structure-property-performance available

Synergistic Research themes



- CMS3 will leverage currently funded projects, including by NSF in three areas:
  (i) Lightweight materials
  (ii) Multifunctional materials
  (iii) Data-Enabled Science for materials
- The State of the art computational tools that form the backbone of CMS3 are very much those being employed by the CMS3 team members in their ongoing research efforts.

The forward-looking hands-on focused training in computational materials science across the Scales, along with the ongoing synergistic research efforts hold the promise to **enable new modes of discovery of new materials.**

CENTER FOR INTELLIGENT MULTIFUNCTIONAL MATERIALS & STRUCTURES
TEXAS A&M ENGINEERING EXPERIMENT STATION