A Scientific and Engineering Computing Cluster Focusing on the Modeling and Simulation of Materials

UNT
UNIVERSITY OF NORTH TEXAS
Where is UNT?

- college town
- close to DFW metroplex
- 4th largest TX university: >35,000 students
UNT Chemistry

• Largest chem dept in region
• 23 full-time faculty
• ≈ 100 grad students and post-doctorals

Cundari Group participates in CASCaM, one of the largest and most diverse comp chem groups in the US!
New Chemistry Building

Completed in 2005!
Core Competencies
- Materials Modeling
- Interfacing with Experiment

CASCaM At A Glance
- 13 faculty
- cover all time and length scales
- ~50 researchers

Currently Funded Projects
- Catalysis
- Photonics
- Flexible electronics
- Combustion chemistry
- Material fatigue

Current Sponsors

[Images and logos of sponsors]
Targets hires to “fill” and “bridge” the gaps in current expertise domains.
Goals of the Modeling Cluster

1. **Extend** and consolidate current areas of strength
2. **Nurture** recent areas of modeling emphasis
3. **Diversify** UNT’s expertise in modeling
4. **Integrate** UNT’s modeling excellence with both on- and off-campus experimentalists

Make UNT a recognized leader in cross-disciplinary materials modeling research
Cross-Disciplinary Expertise

• Chemistry
  – Bagus
  – Borden
  – Cundari
  – Marshall
  – Wilson
  – Schwartz

• Engineering
  – Boetcher (M&EE)
  – Du (MS&E)
  – Feng (M&EE)
  – Needleman (MS&E)
  – Srivilliputhur (MS&E)

MS&E: Materials Science and Engineering
M&EE: Mechanical and Energy Engineering
Better catalysts are needed for more efficient destruction of NO\textsubscript{x} in automotive catalytic converters.

Model catalyst for destruction of the pollutant NO\textsubscript{x}.

Current Funding Sponsors

DR. THOMAS R. CUNDARI, Co-Director, CASCaM

Regents Professor of Chemistry
Editor, Reviews in Computational Chemistry
Editorial Board, Journal of Computational Information and Modeling

Catalysis, Energy Related Research, Project ISES, Biomodeling

Dr. Angela K. Wilson, Co-Director, CASCaM

Associate Professor of Chemistry
2003 NSF CAREER Award
2004 IJQC Young Investigator Award
2005 U.S. Chair for Chinese-American Frontiers of Science (National Academy of Sciences)

The Wilson group is a leader in the development of more accurate and efficient chemical modeling techniques.
Modeling is a window on species too unstable or processes too fast to be studied by experiment. Such insight leads to useful products.
Dr. Paul S. Bagus
Research Professor of Chemistry
Editorial Board, Journal of Electron Spectroscopy
Alexander von Humboldt Fellow

Nanomaterials

Using computer clusters to understand atomic metal clusters.

Current Funding Sponsors
Modeling fast chemical reactions is crucial in understanding combustion chemistry.


Chemistry in the atmosphere is difficult to study without scientific modeling.
Dr. Martin Schwartz
Regents Professor of Chemistry

Cetorelix: A cancer hormone antagonist

TPA dye developed by USAF scientists.

Developing novel electronics and medical materials.

Current Funding Sponsors
Research interests include natural convection, biomedical heat transfer and fluid flow, and energy-related fields. Dr. Boetcher has collaborations to study epileptic brain cooling and laser tissue welding with IMTEC, a 3M Company (a biomedical company) and the University of Oklahoma.

Model of brain cooling. Courtesy IMTEC.
Dr. Zhi-gang Feng
Assistant Professor of Materials Science and Engineering

Research interests: Modeling of turbulence and particulate flow, computational fluid dynamics.

Effect of buoyancy and viscosity on sedimentation of particles in a fluid
Dr. Jincheng Du

Assistant Professor of Materials Science and Engineering

Research interests: atomistic modeling of structure and dynamics of amorphous systems, *ab initio* calculations of materials surfaces, interfaces, and heterogeneous catalysts, electronic structure and phase transitions for ceramic oxides, classical and *ab initio* simulation of glass structure and properties.

Simulation of the displacement cascade in cristobalite during erbium implantation.

Model of dislocation in radiation damaged metal-oxide.

Current Funding Sponsors:
Dr. Srinivasan Srivilliputhur
Assistant Professor of Materials Science and Engineering
Editorial Board of Review, Metallurgical and Materials Transactions
NSF CAREER Awardee

Research interests: Large-scale computer simulations of material failure, deformation and failure of materials in the presence of complex chemical reactions, new energy research, corrosion.

Model of He “bubble” formation in single crystal bcc Fe

Current Funding Sponsors
Dr. Alan Needleman
Professor of Materials Science and Engineering
Member, National Academy of Engineering

Research interests: Computational modeling of deformation and fracture processes in materials over a range of size scales from the nano to the macro.

Effect of indentation on surface and bulk stress and dislocation

Current Funding Sponsors
Dr. Zhiqiang Wang
Assistant Professor of Material Science Engineering

Research interests: Mesoscale Modeling & Dislocation Dynamics

Mesoscale modeling of defects in fcc crystal
Dr. Yuri Rostovtsev
Assistant Professor of Physics

Research interests: Condensed Matter Theory, Quantum Optics
CASCaM = Collaborative

- Inside/outside UNT
- Other centers of excellence in modeling
- Theory + experiment
- With national lab and industrial partners
CENTC is first Phase II CBC; CASCaM is providing modeling expertise and training.

The $15 million grant to the Center for Enabling New Technologies through Catalysis will continue to foster research to find easier and better ways of manipulating strong chemical bonds found in most materials.
Lockheed Nanotechnology Group

- Multi-institutional NSF-CCI proposal submitted
- NSF-IMI: CHiPS(NCSU)+CASCaM(UNT)
Center for Catalytic Hydrocarbon Functionalization

- Goal: Viable catalyst to convert methane (natural gas) into methanol (liquid)

1 of 40 EFRCs

Comp Teams
- Goddard (CalTech)
- CASaM (UNT)

UNT Team
- Cundari
- Du
- Srivilliputhur
Project ISES

Modeling aerospace materials from continuum to atomic, closely interfaced with leading-edge characterization via UNT’s CART
Multi-scale Modeling of CO$_2$ Storage

Modeling from a high-level ab initio simulation of a single CO$_2$/H$_2$O pair to CFD modeling of CO$_2$ in aqueous brines
CO$_2$-formatics

- Coupling bioinformatics tools & traditional comp chem methods to CO$_2$/protein binding
- Can we develop novel, bioinspired strategies for CO$_2$ sequestration?

Joint DOE-BER Grant to Wilson & Cundari
Designer Electronics

- “Flexible” electronics for next-generation apps
- Joint NSF-DMR grant to design (Cundari, Du), synthesize (Omary) & construct (Gnade, UTD) flexible electronics
CASCaM = Diversity of Experience

Ian Haken
• CASCaM Research Student
• Intel Finalist
• Developed improved schemes for molecular “fingerprinting”

Paul Bagus
CASCaM Research Professor
• Pioneer
• Developed first practical computational chemistry program

CASCaM = Today’s Pioneers + Tomorrow’s Scientific Leaders
CASCaM Across the Globe

CASCaM = A Global Resource for Modeling Excellence
CASCaM Expertise

**Diversity of Chemistry**
- Inorganic/Organometallics
- Organics
- Materials Chemistry
- Biological Chemistry
- Physical Chemistry

**Diversity of Methodology**
- Molecular mechanics
- Semiempirical quantum mechanics
- Ab initio & density functional theory
- Bioinformatics
- Artificial intelligence
- Molecular dynamics

Diversity Of Experience = Greater Employment Potential!
Both on- and off-campus, CASCaM focuses on the integration of cutting-edge theory and simulation, integrated with experiment and characterization to provide comprehensive solutions to technical problems.
Hiring Plan

Five – seven (5-7) faculty hires over next 3 years

– Junior and senior faculty hires

– Focus areas of application
  a) Aerospace materials
  b) Biomaterials
  c) Catalysis

– Goals for hiring
  • Fill in “gaps” in modeling expertise: time/length scales & methodologies
  • Diversify expertise base: applications, development, theory, coding
  • Complement on-campus experimental strengths
Targeted Hire Areas

Modeling of materials interfaces/surfaces
  • 1 senior hire

Multi-scale/multi-physics materials modeling
  • 1 senior hire

Mesoscale/microstructure evolution
  • 1 junior hire

Continuum scale lifetime prediction
  • 1 junior hire, 1 senior hire

Informatics
  • 1 senior hire

Computational Chemistry
  • 1 senior hire (2008)

Additional Staff
  • 1 ➔ Visualization, programming, code development, etc.
  • 1 ➔ administrative assistant ➔ PR, recruiting, outreach, dissemination, etc.
• Over 3,000 sq ft. of server rooms **within the chemistry building**

• Over 2,000 cores (5 Teraflops) housed in the chemistry building **devoted to computational chemistry research**

• Ph.D.-staff member to manage computational chemistry facilities and provide training

• Computational Chemistry Instructional Facility (CCIL)

• UNT’s Center for Advanced Scientific Computing and Modeling (CASCaM) is expanding and will invest in ~5,000 cores in 2009-2010 → ca. $1.5M.

• Computational chemistry faculty also heavily use other facilities – UNT’s Research Faculty clusters, National TeraGrid facilities, and DOE (“Grand Challenge”) facilities.
Timeline*

Year 0
Start renovation
1\textsuperscript{st} installment of new UNT research computing facility
Computational chemistry senior hire

Year 1
Continue renovation
2\textsuperscript{nd} installment - computing facility
Junior hire – Mesoscale modeling
Senior hire – Multiscale modeling

Year 2
Complete renovation
Junior hire – Continuum modeling
Senior hire - Informatics
3\textsuperscript{rd} installment – computing facility

Year 3
Senior hire – Surfaces/Interfaces modeling

• Timeline is tentative and for illustrative purposes; flexibility in hiring will be key;
• Year 0 = 2008 – 2009
Summary

✓ Hires will build upon existing expertise @ UNT
  ▪ Expertise across many applications areas
  ▪ Expertise across many time/length scales
  ▪ 5 - 7 faculty hires, next 2 – 3 years

✓ Core faculty are highly collaborative
  ▪ Modeling and expt
  ▪ Modeling and modeling

✓ Upgrades to infrastructure & equipment

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