

# Workshop

## Computational Materials Design Facility - CMDF

**Welcome to California,  
To Pasadena,  
To Caltech,  
To Beckman Institute  
To the Materials and Process Simulation Center**

**William A. Goddard III**

**Charles and Mary Ferkel Professor of  
Chemistry, Materials Science, and Applied Physics  
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319 or 316 Beckman Institute**

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email: [wag@wag.caltech.edu](mailto:wag@wag.caltech.edu)**



# Caltech History

**Throop University** founded in **1891** (at Green and Fair Oaks, near old town Pasadena, ~ 3 blocks from Courtyard Marriott).

vocational college, high school, grammar school

~**1905** **George Ellery Hale**, Astronomer came to Pasadena to build Mt. Wilson Observatory (because of clear air and lack of scattering due to city lights)

**1905-1907**: Hale hobnobbed with the rich people and leaders of industry that then all lived in Pasadena (long before Beverly Hills and Malibu). **Hale** Convinced them that California should have an MIT of the west (this is confidential, we do not like to let on that we were copying MIT)

In ~ **1907** changed name to **Throop Polytechnic Institute** (engineering college) and separated from the grammar and high school (now called **Polytechnic**, one of the best private schools in LA county)

In ~**1909** Throop moved to current site (previously a citrus grove)

~**1915** **Arthur Amos Noyes** came from MIT to start science (chemistry) at Caltech

~**1918** Noyes attracted **Robert A. Milliken** to Caltech

In ~ **1920** changed to **California Institute of Technology**

# Caltech Today

## Six Divisions:

- Chemistry and Chemical Engineering
- Biology
- Geosciences
- Physics, Math, and Astronomy
- Engineering and Applied Science
- Humanities and Social Science

~950 undergraduates

~1100 graduate students

~350 faculty



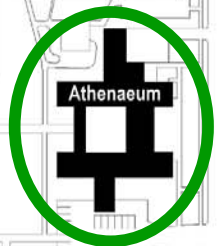
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Beckman Institute

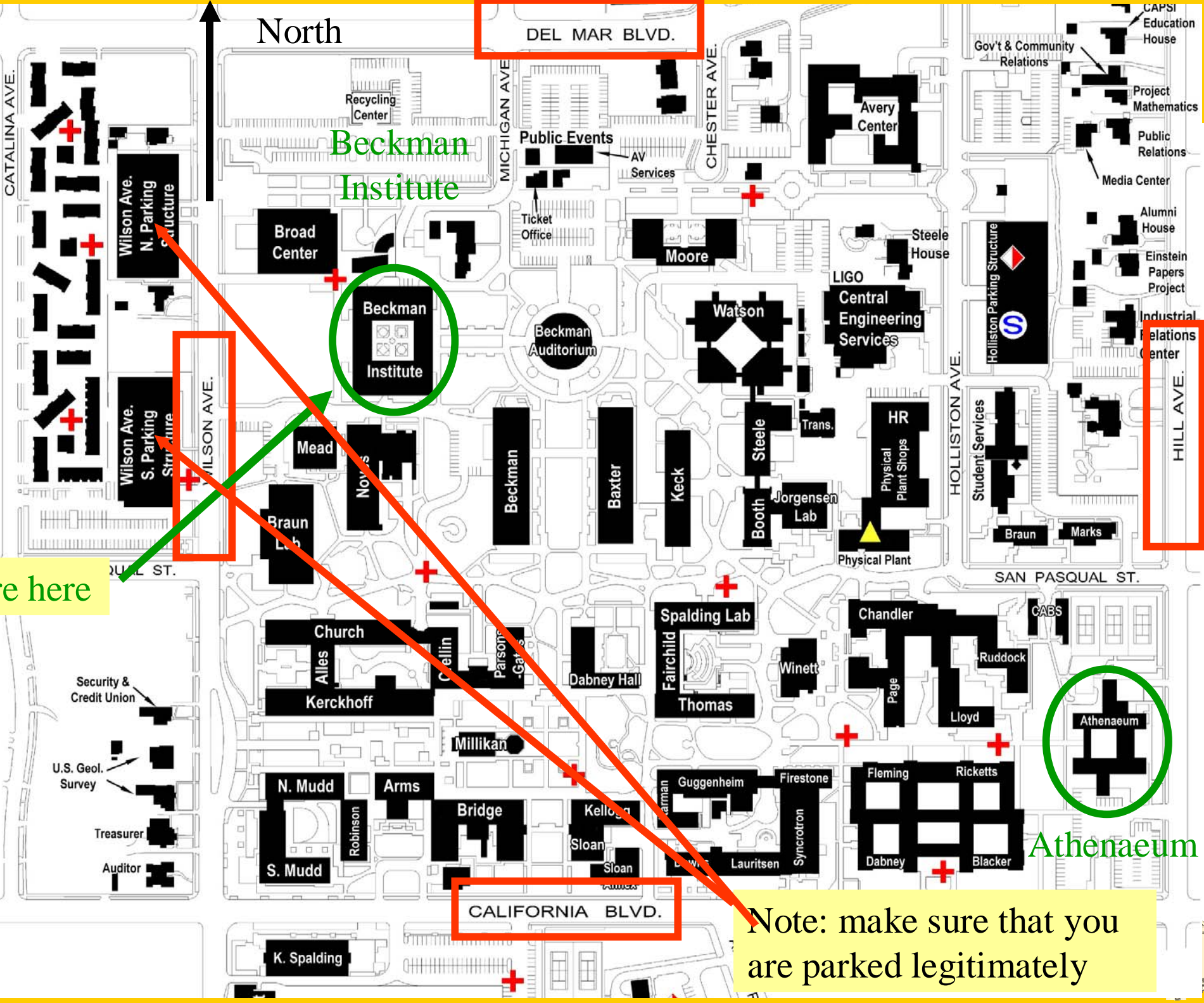


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# Beckman Institute

Gift by Arnold and Mabel Beckman (Arnold BS UIUC, ~1922, worked at Bell Labs ~ 1922-1924, PhD Caltech ~1928) Joined Caltech Faculty. Invented Electronic pH meter ~1932, Started Beckman Instruments ~1939.

Construction finished July, 1990

Resource Centers in Chemistry and Biology

- Imaging
- Lasers
- Materials
- Synthesis
- Etc.
- Materials and Process Simulation Center (MSC) Goddard Director  
no block funding, all from individual grants



# MSC is Unique: Critical Mass of Expertise in Most areas of Atomistic Theory and Applications to Materials, Chemistry, and Biology

Senior Staff:

William A. Goddard III, Director

Mario Blanco, Director Process Simulations and Oil Technology

Markus Buehler, Director Mesoscale and Materials Science Applications

Jonas Oxgaard, Director of Catalysis Technology

Adri Van Duin, Director Force Field and Materials Technology

Vaidehi, Director of Biotechnology and Pharma

Weiqiao Deng, Manager of nanoelectronics Technology

Darryl Willick, Manager of Computer Technology and Networks

Mamadou Diallo, Manager Molecular Environmental Technology

Boris Merinov, Manager of Fuel Cell Technology

Sergey Zybin, Manager of Energetic Materials technology

Total Staff: ~65 (~25 Graduate Students, 6 UG)

Trained in Chem., Phys., Mat. Sci., Appl. Phys., Biol., Envir. Engr., Chem. Eng., Comp. Sci., Elect. Engr.

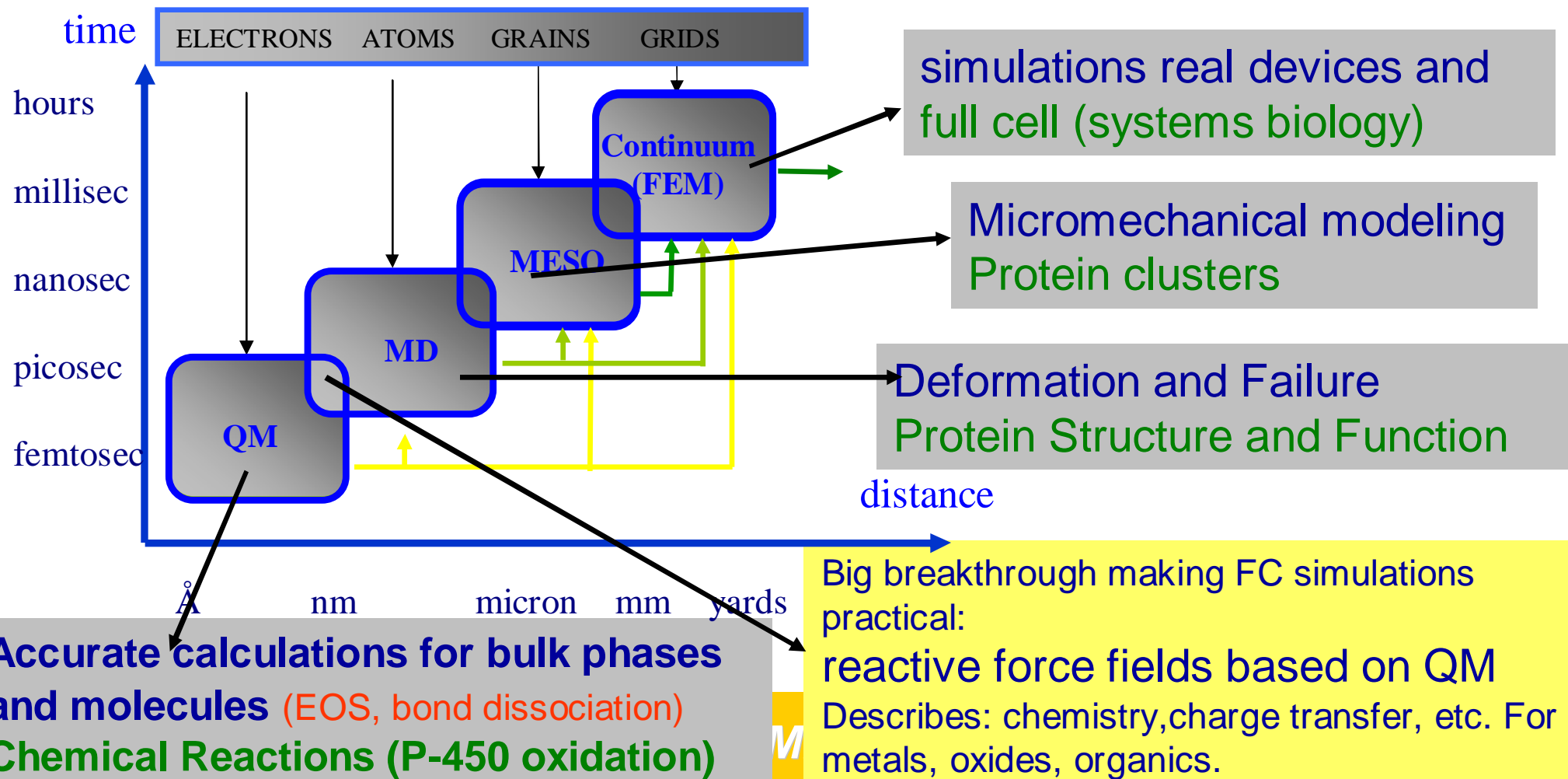
Critical Mass in QM, FF, MD, MesoDyn, Stat. Mech. Biochem., Catalysis, Ceramics, Polymers, Semicond., Metal Alloys, Nanotech. Environ. Tech.

# Mission: Develop Hierarchical Strategy for 1st Principles Design of Materials

Need 1<sup>st</sup> Principles simulations of macroscale systems so can predict NEW materials never before synthesized and optimize them prior to experiment

1<sup>st</sup> Principles → connect Macro to QM. Strategy use an overlapping hierarchy of methods (paradigms) (fine scale to coarse)

Allows Design of new materials and drugs (predict hard to measure properties)



# Applications Using the Hierarchical Multiparadigm Strategy

- NANOSYSTEMS:** Nanoelectronics, Carbon Nanotubes for Interconnects and fuel cells
- BIOTECHNOLOGY:** Membrane Proteins (GPCR), non-natural Amino Acids, Pharma (VLS)
- CATALYSTS:** Methane Activation, Selective Oxidation, ElectroCat ( $O_2$ ), Polar Olefins
- SEMICONDUCTORS:** Dielectric Breakdown, Si/SiO<sub>2</sub>/Si<sub>3</sub>N<sub>4</sub> interfaces, B diffusion
- CERAMICS:** Ferroelectrics (BaTiO<sub>3</sub>), Zeolites, Fuel Cell electrodes
- POLYMERS:** Replace Nafion in PEM, Dendrimers, Nylon, PET deformations
- METAL ALLOYS:** Glass Formation, Plasticity (dislocations, crack propagation, spall)
- ENVIRONMENTAL:** Dendrimers for Selective Encapsulation, Humic acid
- INDUSTRIAL APPLICATIONS** (SonafiAventis, ChevronTexaco, Berlex Biopharma, Nissan, Intel)
- Polymers:** Gas Diffusion, Surface Tension Modification, Water solubility
  - Polymerization Catalysts for Polar Monomers**
  - Catalysts:** CH<sub>4</sub> activation, Alkylation phenols, zeolites (Acid sites/templates)
  - Semiconductors:** Dielectric Breakdown nanometer oxides, nitrides, B Diffusion in Si
  - Automobile Engines:** Wear Inhibitors (iron and aluminum based engines)
  - Oil Pipelines:** Inhibitors for Corrosion, Scale, Wax; Hydrates, Demulsifiers
  - Oil Fields:** Surfactants for low water/oil interface energy, Basin models
  - Electronics:** Carbon nanotube interconnects
  - Catalysts:** ammoxidation of propane
  - Fuel Cells:** H<sub>2</sub> Storage, Polymer Electrolyte Membranes, Electrocatalysis



MultiParadigm Strategy enables application 1<sup>st</sup> principles to complex systems



# Collaborations with Industry

## Stimulation to Solve Impossible Problems

- Aventis Pharma: Structures and Function of GPCRs
- Berlex Biopharma: Structures and Function of CCR1 and CCR5 (GPCRs)
- Chevron Corporation:  $\text{CH}_4$  to  $\text{CH}_3\text{OH}$ , Wax Inhibition/oil pipelines
- GM advanced propulsion: Fuel Cells ( $\text{H}_2$  storage, membranes, cathode)
- Nissan Motor Co: Wear Inhibition in Automobile Engines (DLC)
- Intel Corp: Carbon Nanotube Interconnects
- Dow Corning: Mechanism synthesize  $\text{Si}(\text{CH}_3)_2\text{Cl}_2$

### Previous

- Asahi Glass: Fluorinated Polymers and Ceramics
- Asahi Kasei: Ammoxidation Catalysis, polymer properties
- Avery-Dennison: Nanocomposites for computer screens Adhesives, Catalysis
- BP: Heterogeneous Catalysis (alkanes to chemicals, EO)
- Dow Chemical: Microstructure copolymers, Catalysis polymerize polar olefins
- Exxon Corporation: Catalysis (Reforming to obtain High cetane diesel fuel)
- General Motors - Wear inhibition in Aluminum engines
- Hughes Satellites/Raytheon: Carbon Based MEMS
- Hughes Research Labs: Hg Compounds for HgCdTe from MOMBE
- Kellogg: Carbohydrates/sugars (corn flakes) Structures, water content
- 3M: Surface Tension and structure of polymers
- Nippon Steel:  $\text{CO} + \text{H}_2$  to  $\text{CH}_3\text{OH}$  over metal catalysts
- Owens-Corning: Fiberglass (coupling of matrix to fiber)
- Saudi Aramco: Up-Stream additives (Demulsifiers, Asphaltenes)

Each project (3 Years) supports full time postdoc and part of a senior scientist

Multiscale simulation essential for industrial applications

# Need Continued Improvement in Methods, Our Focus:

## 1: Quantum Mechanics

**Challenge: increased accuracy**

- New Functionals DFT (dispersion)
- Quantum Monte Carlo methods
- **Tunneling thru molecules (I/V)**

## 2: Force Fields

**chemical reactions**

- **ReaxFF- Describe Chemical Reaction processes**
- Describe Phase Transitions
- Mixed Metal, Ceramic, Polymer

## 4: Biological Predictions

1st principles structure GPCR  
proteins

1st principles Binding of Ligands

## 5: MesoScale Dynamics

**Coarse Grained FF**

Kinetic Monte Carlo

Hybrid MD and Meso Dynamics

Tribology

## 3: Molecular Dynamics

**Challenge: Extract properties essential to materials design**

- Non-Equilibrium Dynamics
  - Viscosity, rheology
  - Thermal Conductivity
- Solvation Forces (continuum Solv)
  - surface tension, contact angles
- Hybrid QM/MD
- Plasticity
  - Formation Twins, Dislocations
  - Crack Initiation
- Interfacial Energies
- Reaction Kinetics
- **Free energies of complex systems**

## 6: Integration:

Seamless across the hierarchies of simulations, Python-based scripts

# Point of the Workshop

**Applications require new theory, new methods, new software**

**Excellent training for graduate students: develop new theory and methods, write software, apply it to important application, get good job as professor or on staff of government lab or industrial lab.**

**Problem: now have 40 years of software development at Caltech and elsewhere. How can the old software be optimized and maintained. How can one use it for developing new paradigms for new problems**

**How can a new student enhance and improve the software when it is badly documented , complex, difficult to decipher all the interdependencies, and usually developed by someone no longer at Caltech and now longer available.**

**How can the old software be used in conjunction with developing new software**

# CMDF: Overview and Philosophy

The CMDF project aims toward developing a multiparadigm simulation environment allowing seamless coupling of simulation codes and methods based on completely different paradigms (QM, FF, finite elements)

Newly developed methods can be applied to predict material properties from first principles to be fed into more macroscopic simulations

Application: *de novo* design of materials with optimized

Mechanical properties

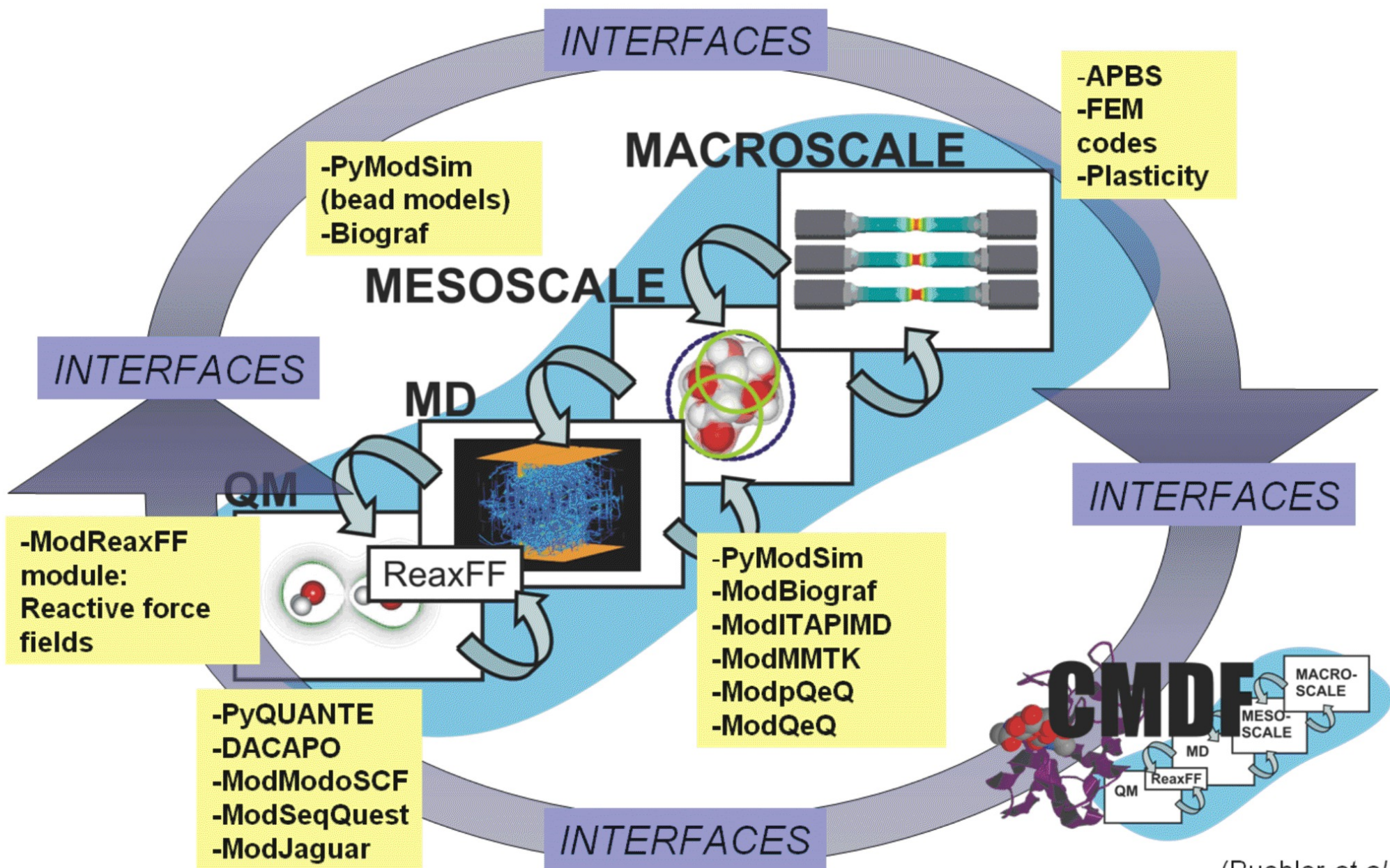
(specifically, coupling of chemistry with the mechanics of cracking)

Thermo-electrical properties

Nonlinear optical properties

Ferroelectric properties and others

# The computational Materials Design Facility



(Buehler et al.)

# Philosophy on Maintaining and Optimizing Software

Development of new theory, methods, software at universities is quite appropriate: provides excellent training for graduate students

But documenting, cleaning up the code, moving to new hardware is not proper training of graduate students.

Original solution: spin off a company to do the software optimization and documentation, get paid by customers

MD: Accelrys (started in Pasadena as Biodesign in 1984, changed to Molecular Simulations Inc (MSI) in 1987, acquired (Polygen ~1990, Biosym 1995) merged with Pharnacoopia ~1998, renamed Accelrys ~2002

QM: Schrödinger (started in Pasadena 1990), now in Portland and NYC

Biofunctionomics: Eidogen-Sertanty (started in Pasadena 2000 as Bionomix), now in San Diego

# How has industrial spin-offs worked?

Not great.

Documentation and validation generally much better.

But the source is generally not available to other developers and hence the software stagnates.

Rather than developing new methods and software, most companies spend most of their resources selling the old products, trying to convince companies that the software is useful and worth the price.

Most new methods and software still come from universities but often is not well integrated.

# Philosophy for CMDF and other software developments at Caltech

Distribute the software free to collaborators at universities and Government labs, using Gnu or similar type licenses

Work together with other developers allowing them access to source and to add new features modules etc.

Work together with other applications scientists to improve methods and software where needed

Encourage developers and applications people to interact with Caltech and other centers to recognize new opportunities required for new applications.

# Problem: How to pay for developments

Funding for CMDF: special DARPA grant (Steve Wax and Carey Schwartz) to start project

Predicting Real Optimized Materials (PROM) project: DARPA (Steve Wax and Carey Schwartz)

DOE-ASCI:

Also: ONR (Goldwasser) and ARO (Mann)

If you like what we have done, please let them know:

DARPA: "Wax, Steve" <swax@darpa.mil

DARPA: "Schwartz, Carey" <cschwartz@darpa.mil

ASCI: Robert Voigt <rvoigt@compsci.wm.edu

ASCI: "Mailhiot, Christian " <mailhiot1@llnl.gov

ASCI: "Meiron, Dan " <dim@its.caltech.edu

ONR: "Goldwasser, Judah" <goldwaj@onr.navy.mil

ARO: "Mann, David" <David.Mann1@us.army.mil

# Applications Goals for DARPA PROM

- **Thermoelectric materials** for power applications with thermal and electrical conductivity, thermoelectric power, and Seebeck coefficient leading to a **figure of merit of  $ZT = 5$** .

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- **Thin film ferroelectrics** for applications ranging from tunable microwave devices to IR detectors to achieve a **tunability/loss tangent ratio of 100 at 100 GHz**. Here the composition and nanostructure would be modified to maximize tunability (ability to change the dielectric constant with an electric field) while minimizing the dielectric loss tangent.

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- **Non-linear optical materials for applications with  $\chi(2) \sim 10^{-3}$  esu or  $\chi(3) \sim 10^{-17}$  (cm /voltage)<sup>2</sup>** We believe that achieving such performance will require self-assembled arrays of quantum dots such as InAs/GaAs and hence we will consider the NLO properties of such configurations.

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- **High Energy Density Materials** to predict the chemistry, combustion and energy release of real propellant and explosives with **high specific impulse (ISP>300 s) and low sensitivity**.

# Problem: How to pay for developments

The DARPA, ASCI, ONR, ARO funding all for short term projects.

There is a problem with continued funding of new developments, integration, documentation, etc

We expect that university collaborators will often do joint proposals with us to develop new funding

We expect that government labs will also find ways to provide funding for new developments and new applications.

Probably ~\$500K/year is needed to have robust support, this would be \$100K/year for 5 laboratories. This would pay for people at Caltech and elsewhere involved in maintenance and development

# Plan for today

## 1st Workshop on Multi-Paradigm Multi-Scale Modeling in the Computational Materials Design Facility (CMDF)

Talks marked by asterisk \*: 30 min talks given by senior people

### August 23 (Tuesday)

**DAY 1** Beckman Institute (building #74) room 134 (Beckman Auditorium)

Time	Speaker	Title
<b>Session 1: Introduction</b>		
Chair: Sergey Zybin		
08:30-08:45	William A. Goddard	Overview over Caltech's MSC's activities
08:45-08:55	Emily B. Abbott	Opening Remarks by the Associate Director of Corporate Relations (Caltech)
08:55-09:35* (40 mins)	Markus J. Buehler	Introduction and Overview: Multi-scale multi-paradigm modeling in CMDF
09:35-09:50	Richard P. Muller	Python in scientific computing: Historical perspective

### **Session 2: Computational aspects: Data structures, performance and large-scale computing**

Chair: Jonas Oxgaard

09:50-10:05	Jef Dodson	Extended OpenBabel XOB: CMDF's central data structure
10:05-10:20	Lei Pan	Parallelization strategies in Python: Large-scale applications of CMDF
10:20-10:40 (20 mins)	Joey Czikmantory	The WIGLAF GUI Internet Hookup for CMDF

10.40-11.00 *Coffee and tea break (20 min)*

# More....

## Session 3: Scale coupling and applications: **From QM to macroscale (part I)**

Chair: Mario Blanco

11:00-11:30*	Adri C.T. van Duin	Reactive force fields: A new link from QM to MM
11:30-11:45	Si-ping Han	Incorporating ReaxFF into CMDf and applications
11:45-12:00	Daniel Yi	Time acceleration methods in CMDf: The temperature accelerated dynamics method (TAD)
12:00-12:15	Julius Su	eFF, a Force Field with Electrons
12:15-12:45* (30 mins)	Vaidehi Nagarajan	Application of CMDf in modeling of biological systems: Status and Outlook
12:45-01:00	Victor Kam	The CMDf SCREAM method: A new approach to place side chains
01:00-01:15	John A. Wendel	The DOCKING procedure in CMDf

01:15-02:00 *Lunch break (BI courtyard; sandwich catering)*

## Session 3: Scale coupling and applications: **From QM to macroscale (part II)**

Chair: Mario Blanco

02:00-02:15	Li Tao	Coupling of DREIDING and ReaxFF and applications to biological systems
02:15-02:45*	Valeria Molinero	Mesoscale modeling of carbohydrates : Moving from atoms to beads
02:45-03:00	Tod Pascal	Mesoscale DNA simulations
03:00-03:15	Barry Olafson	The MolScape GUI module for CMDf and bio-applications
03:15-03:45*	Alberto Cuitino	Bridging to the continuum scale and ferroelectrical applications
03:45-04:15*	Santiago Solares	An application of multi-scale modeling: From quantum mechanics to classical mechanics

04:15-04:30 *Coffee and tea break (15 min.)*

# And More.....

04:15-04:30 *Coffee and tea break (15 min.)*

## **Session 4: Novel computational approaches and prediction of properties of complex materials**

Chair: Weiqiao Deng

04:30-05:00*	Paul von Allmen	EZTB in CMDF and Sensitivity Analysis
05:00-05:15	Fabiano Oyafuso	Calculations of Thermal Conductivity
05:15-05:35 (20 mins)	Hatem Helal	The Jaguar module in CMDF and application to modeling LE4
05:35-05:50	Frank Ducheneux	Implicit solvation methods for discrete systems
05:50-06:05	Qingsong Zhang	The pQEq force fields
06:05-06:20	Chris George	I-V calculations in CMDF
06:20-06:35	Seungwon Lee	Thermoelectrical properties of Bi <sub>2</sub> Te <sub>3</sub> , Sb <sub>2</sub> Te <sub>3</sub>
06:35-07:15	Valeria Molinero (Caltech), Paul von Allmen (JPL), and Ioana Cozmuta (NASA Ames) Markus J. Buehler (Caltech)	<i>Panel discussion: New trends and challenges in multi-scale modeling</i>
07:15-07:20	Markus J. Buehler	<i>Closing remarks</i>

Starting 7:30 *Dinner (Burger Contintental; 535 S. Lake Ave, Pasadena, 91101, CA; Phone (626) 792-6634)*

Note: BC is NOT a burger place (but you can get them).

It is middle eastern (Lebanon) food

Please sign up if you are attending (it is covered in the registration fee)

Let us know if you need vegetarian or Kosher

It is ~ 4 blocks from here (can walk)



# Tomorrow, not so formal, hands-on

August 24 (Wednesday)

## DAY 2: Training sessions

Beckman Institute (building #74 room 115 BI)

Time	Speaker	Title
09:00-09:15	Markus J Buehler	Opening remarks
09:15-11:15	Markus J Buehler, Jef Dodson, Joey Czikmantory	Visual demonstrations of the CMDF framework <i>How to interface your C, C++ and FORTRAN code with Python</i> <i>How to integrate your code into CMDF: The three step procedure</i> <i>How to integrate your standalone executable code into CMDF</i> <i>Demonstration of the CMDF web interface WIGLAF: How to integrate your code into WIGLAF</i> <i>How to write CMDF Python scripts: Modeling cracking of silicon</i>
Lunch	Pizza served in 115 BI	
12.30-04:00	Various	Training sessions in the BI sub-basement

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