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
Director, Materials and Process Simulation Center, Beckman Institute
California Institute of Technology, Pasadena, California 91125
319 or 316 Beckman Institute
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email: 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
Note: make sure that you are parked legitimately.
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)
Mission: Develop Hierarchical Strategy for 1st Principles Design of Materials

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

1st Principles \(\rightarrow\) 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).

Accurate calculations for bulk phases and molecules (EOS, bond dissociation).

Chemical Reactions (P-450 oxidation).

Big breakthrough making FC simulations practical:

- reactive force fields based on QM
- Describes: chemistry, charge transfer, etc. For metals, oxides, organics.
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 (O₂), Polar Olefins

SEMICONDUCTORS: Dielectric Breakdown, Si/SiO₂/Si₃N₄ interfaces, B diffusion

CERAMICS: Ferroelectrics (BaTiO₃), 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: CH₄ 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: H₂ Storage, Polymer Electrolyte Membranes, Electrocatalysis

MultiParadigm Strategy enables application 1st 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: CH$_4$ to CH$_3$OH, Wax Inhibition/oil pipelines
- GM advanced propulsion: Fuel Cells (H$_2$ storage, membranes, cathode)
- Nissan Motor Co: Wear Inhibition in Automobile Engines (DLC)
- Intel Corp: Carbon Nanotube Interconnects
- Dow Corning: Mechanism synthesize Si(CH$_3$)$_2$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: CO + H$_2$ to CH$_3$OH over metal catalysts
- Owens-Corning: Fiberglas (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

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

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

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 difference 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
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.


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 $ZT = 5$.

• 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.

• Non-linear optical materials for applications with $\chi(2) \sim 10^{-3}$ esu or $\chi(3) \sim 10^{-17}$ (cm /volt)$^2$. 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.

• 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

<table>
<thead>
<tr>
<th>August 23 (Tuesday)</th>
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<tbody>
<tr>
<td><strong>DAY 1</strong></td>
<td>Beckman Institute (building #74) room 134 (Beckman Auditorium)</td>
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<tr>
<td><strong>Time</strong></td>
<td><strong>Speaker</strong></td>
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<tr>
<td>08:30-08:45</td>
<td>William A. Goddard</td>
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<tr>
<td>08:45-08:55</td>
<td>Emily B. Abbott</td>
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<tr>
<td>08:55-09:35* (40 mins)</td>
<td>Markus J. Buehler</td>
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<td>09:35-09:50</td>
<td>Richard P. Muller</td>
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**Session 1: Introduction**
Chair: Sergey Zybin

**Session 2: Computational aspects:** Data structures, performance and large-scale computing
Chair: Jonas Oxsgaard

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>09:50-10:05</td>
<td>Jef Dodson</td>
<td>Extended OpenBabel XOB: CMDF's central data structure</td>
</tr>
<tr>
<td>10:05-10:20</td>
<td>Lei Pan</td>
<td>Parallelization strategies in Python: Large-scale applications of CMDF</td>
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<tr>
<td>10:20-10:40 (20 mins)</td>
<td>Joey Czikmantory</td>
<td>The WIGLAF GUI Internet Hookup for CMDF</td>
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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

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Topic</th>
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<tbody>
<tr>
<td>11:00-11:30*</td>
<td>Adri C.T. van Duin</td>
<td>Reactive force fields: A new link from QM to MM</td>
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<tr>
<td>11:30-11:45</td>
<td>Si-ping Han</td>
<td>Incorporating ReaxFF into CMDF and applications</td>
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<tr>
<td>11:45-12:00</td>
<td>Daniel Yi</td>
<td>Time acceleration methods in CMDF: The temperature accelerated dynamics</td>
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<tr>
<td>12:00-12:15</td>
<td>Julius Su</td>
<td>eFF, a Force Field with Electrons</td>
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<tr>
<td>12:15-12:45* (30 mins)</td>
<td>Vaidehi Nagarajan</td>
<td>Application of CMDF in modeling of biological systems: Status and Outlook</td>
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<tr>
<td>12:45-01:00</td>
<td>Victor Kam</td>
<td>The CMDF SCREAM method: A new approach to place side chains</td>
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<tr>
<td>01:00-01:15</td>
<td>John A. Wendel</td>
<td>The DOCKING procedure in CMDF</td>
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<tr>
<th>Time</th>
<th>Session Activity</th>
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<tr>
<td>01:15-02:00</td>
<td>Lunch break (Bi courtyard; sandwich catering)</td>
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### Session 3: Scale coupling and applications: From QM to macroscale (part II)

**Chair:** Mario Blanco

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<tr>
<th>Time</th>
<th>Speaker</th>
<th>Topic</th>
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<tbody>
<tr>
<td>02:00-02:15</td>
<td>Li Tao</td>
<td>Coupling of DREIDING and ReaxFF and applications to biological systems</td>
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<tr>
<td>02:15-02:45*</td>
<td>Valeria Molinero</td>
<td>Mesoscale modeling of carbohydrates: Moving from atoms to beads</td>
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<td>02:45-03:00</td>
<td>Tod Pascal</td>
<td>Mesoscale DNA simulations</td>
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<tr>
<td>03:00-03:15</td>
<td>Barry Olafson</td>
<td>The Molscape GUI module for CMDF and bio-applications</td>
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<td>03:15-03:45*</td>
<td>Alberto Cuitino</td>
<td>Bridging to the continuum scale and ferroelectrical applications</td>
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<tr>
<td>03:45-04:15*</td>
<td>Santiago Solares</td>
<td>An application of multi-scale modeling: From quantum mechanics to classical mechanics</td>
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<tr>
<th>Time</th>
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<tr>
<td>04:15-04:30</td>
<td>Coffee and tea break (15 min.)</td>
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</table>
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 Oyaufuso  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 Bi2Te3, Sb2Te3

06:35-07:15  Valeria Molinero (Caltech), Paul von Allmen (JPL), and Ioana Cozmuta (NASA Ames), Markus J. Buehler (Caltech)
Panel discussion: **New trends and challenges in multi-scale modeling**

07:15-07:20  Markus J. Buehler  Closing remarks

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 vegitarian or Kosher
It is ~ 4 blocks from here (can walk)
### August 24 (Wednesday)

**DAY 2: Training sessions**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>09:00-09:15</td>
<td>Markus J Buehler</td>
<td>Opening remarks</td>
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<tr>
<td></td>
<td>Markus J Buehler,</td>
<td>Visual demonstrations of the CMDF framework</td>
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<tr>
<td></td>
<td>Jef Dodson,</td>
<td><em>How to interface your C, C++ and FORTRAN code with Python</em></td>
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<tr>
<td></td>
<td>Joey Czikkantory</td>
<td><em>How to integrate your code into CMDF: The three step procedure</em></td>
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<td><em>How to integrate your standalone executable code into CMDF</em></td>
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<td><em>Demonstration of the CMDF web interface WIGLAF: How to integrate your code into WIGLAF</em></td>
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<td><em>How to write CMDF Python scripts: Modeling cracking of silicon</em></td>
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<tr>
<td>Lunch</td>
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<td><em>Pizza served in 115 BI</em></td>
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<tr>
<td>12:30-04:00</td>
<td>Various</td>
<td>Training sessions in the BI sub-basement 056, 01</td>
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