Modeling & Simulation

P&G Research and Development

Cleaning Up With HPC: Multiscale Simulations of Surface Active Molecules

Kelly L. Anderson

Senior Scientist, Corporate Modeling & Simulation

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Acknowledgments

- P&G
  - Bruce Murch
  - Tom Lange
- Michael Klein (Temple University)
  - Russell Devane
  - Xibing He
  - Axel Kohlmeyer

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Presentation Outline

- Introduction to:
  - P&G
  - M&S @ P&G
- Simulating Surfactants
  - Coarse Graining
  - Applications
- Conclusions
- Looking Forward

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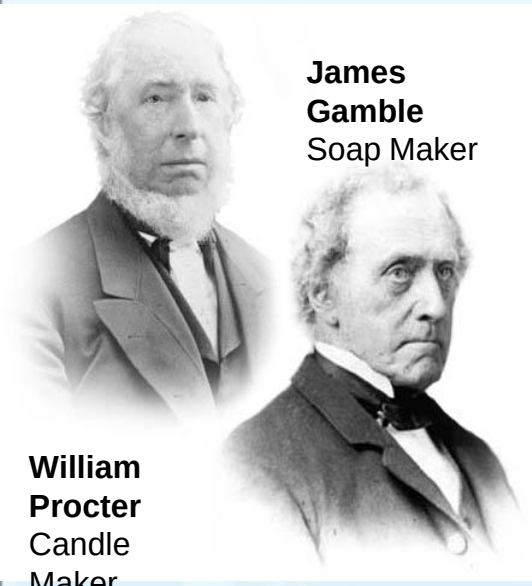
…Founded in 1837



James Gamble
Soap Maker

William Procter
Candle Maker

'Cleaning'

Introduced Ivory Soap In 1879

P&G is the 4th Oldest entity of the Fortune 50

…Started with *STAR* Candles

'Lighting'

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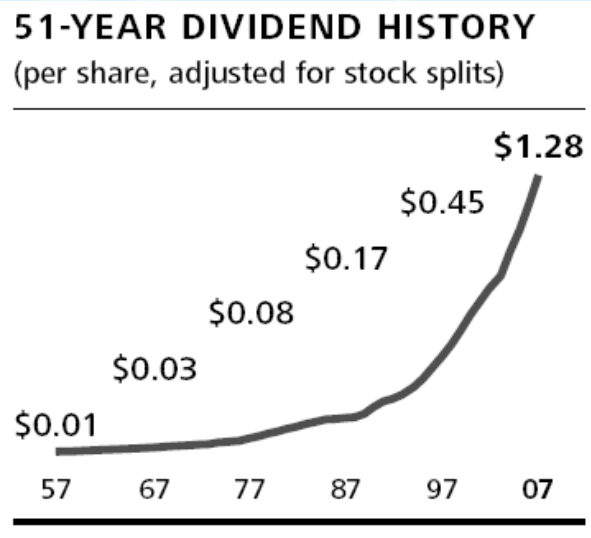
Investors Know Us By…

- **Sales:** $79.1 Billion FY June 30th, 2009
- **Net Income:** $13.4 Billion

P&G has paid dividends without interruption since 1890

56 consecutive years of increased dividend payment.

Worlds Largest Consumer Goods Company…Market Cap ~ $186 Billion
(COB Monday 4/26/2010)



Employ: 135,000 employees
Operate: in more the 80 Countries Worldwide
R&D Technical Centers: More than 28 R&D centers in 10 Countries on 4 Continents

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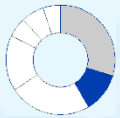
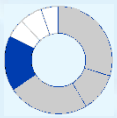
Consumers Know Laundry….

Beauty

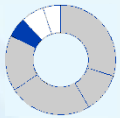


Health Care

Fabric Care & Home Care

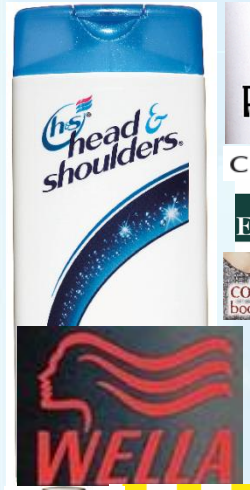


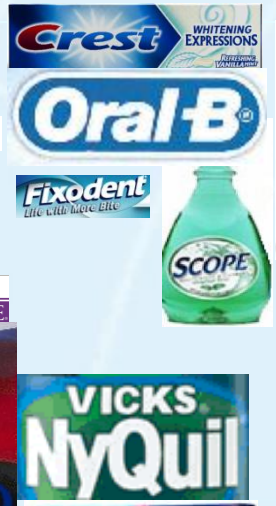
Baby Care & Family Care

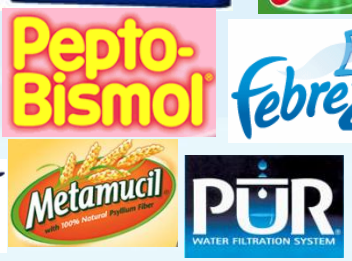


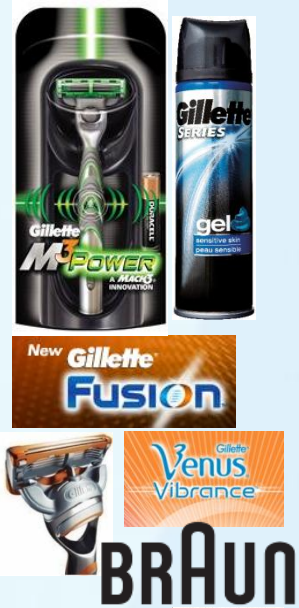
Snacks, & Pet Care

Blades & Razors Duracell & Braun









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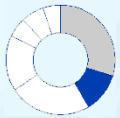
22 Billion $ Brands…

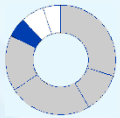
Beauty



Health Care

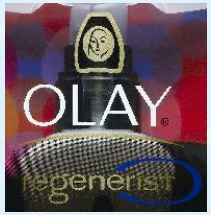
Fabric Care & Home Care

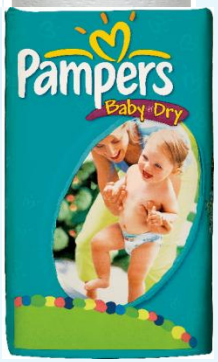
Baby Care & Family Care

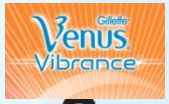


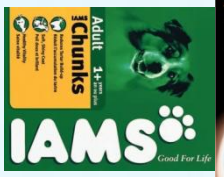
Snacks, Coffee & Pet Care

Blades & Razors
Duracell & Braun









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The Two Moments of Truth

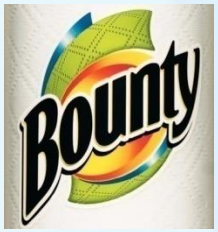
Second moment of Truth

- **Products must *perform* as expected (advertised) when used.**
- ***Performance* … leveraging <u>Fundamental Science & Engineering Contradictions</u>.**

Materials … strong but soft—even wet, stretch not break, breath but contain, break…not tear.

Liquids … mixtures can't separate, dispense easily… but stay where applied.

Packages … creative design is key, strong but light, never leak but open easily.



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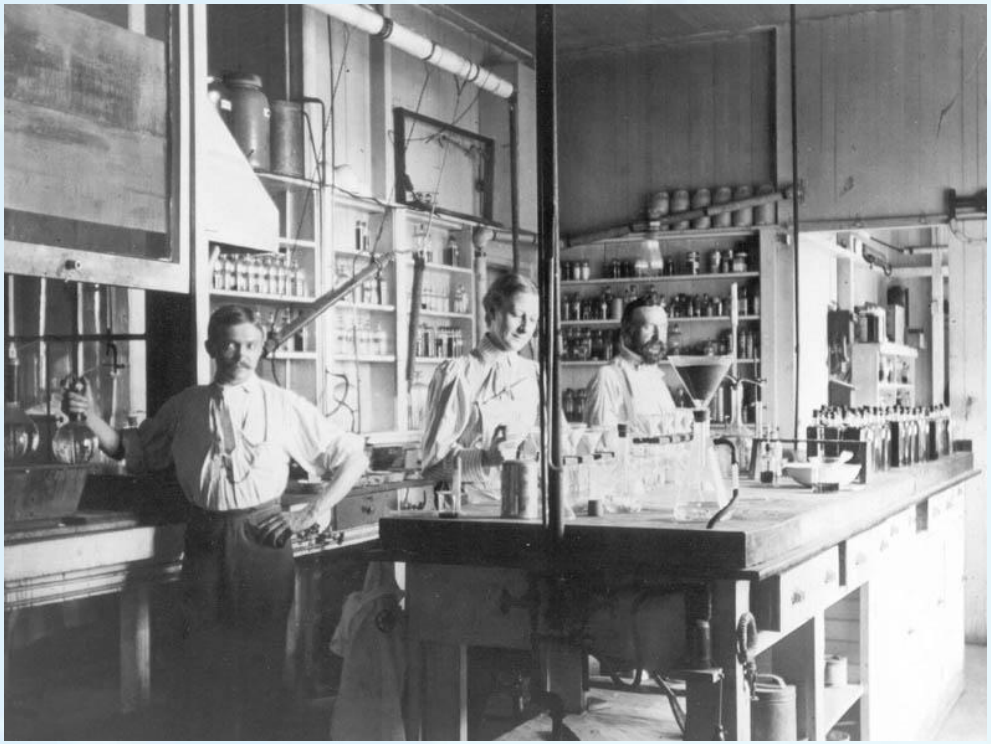
‘Innovation is our Lifeblood’

- Set up first product research lab in U.S. in 1890



- hold 30,000+ Patents, apply for ~ 3000 every year

- Invest over $2 Billion per year in R&D
  - 1995 Recipient of U.S. National Medal of Technology

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Explore Digitally, Confirm Physically

P&G Research and Development

..Molecules to Market

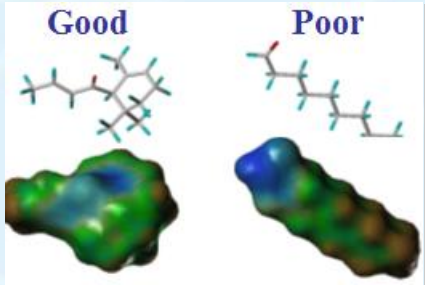
We build and test the ***FIRST*** prototypes…

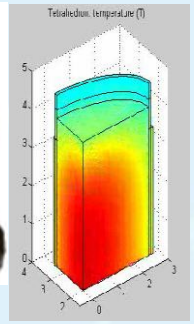
'VIRTUAL' ones that…

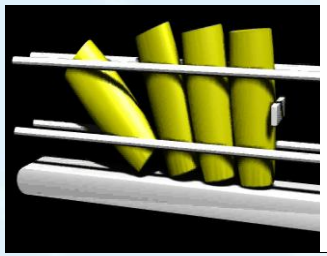
- **Fit**
- **Work**
- **Make Financial Sense**

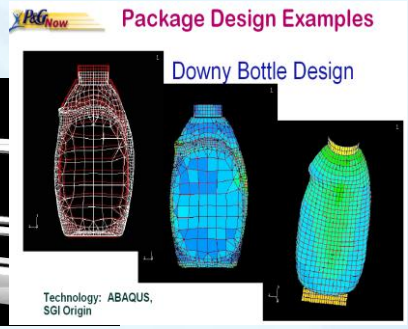
…***BEFORE*** they exist in the real world.

Product/Device/Package

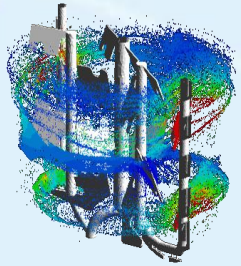


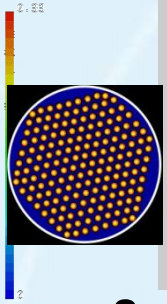


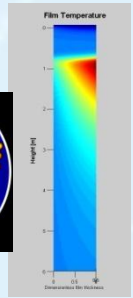


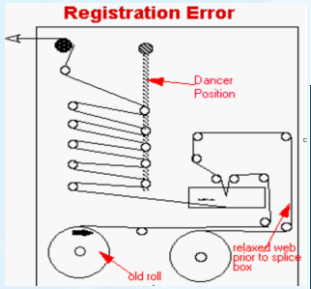


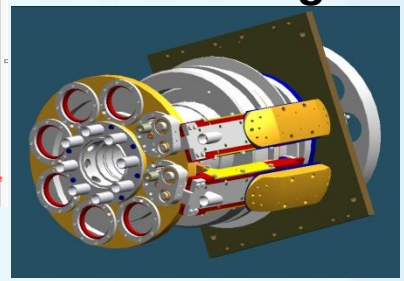
Mechanical & Converting



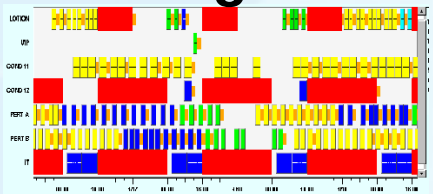




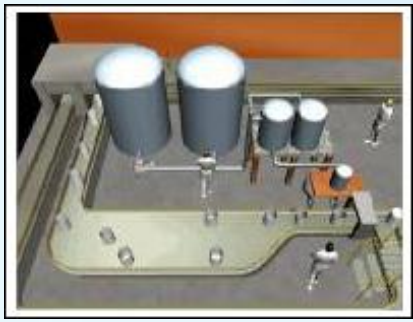




Process & Making



Supply Chain Throughput & Reliability



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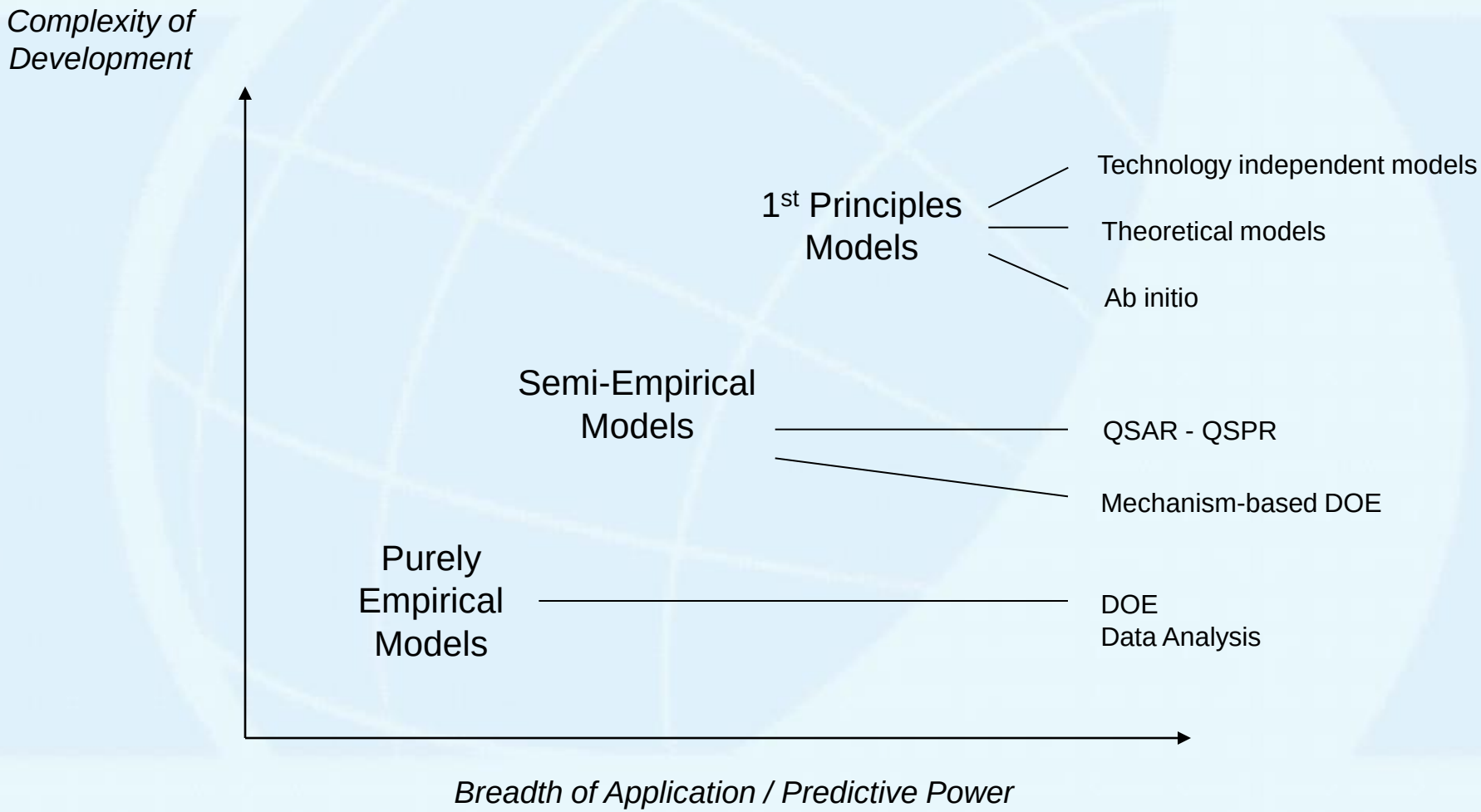
Types of Models



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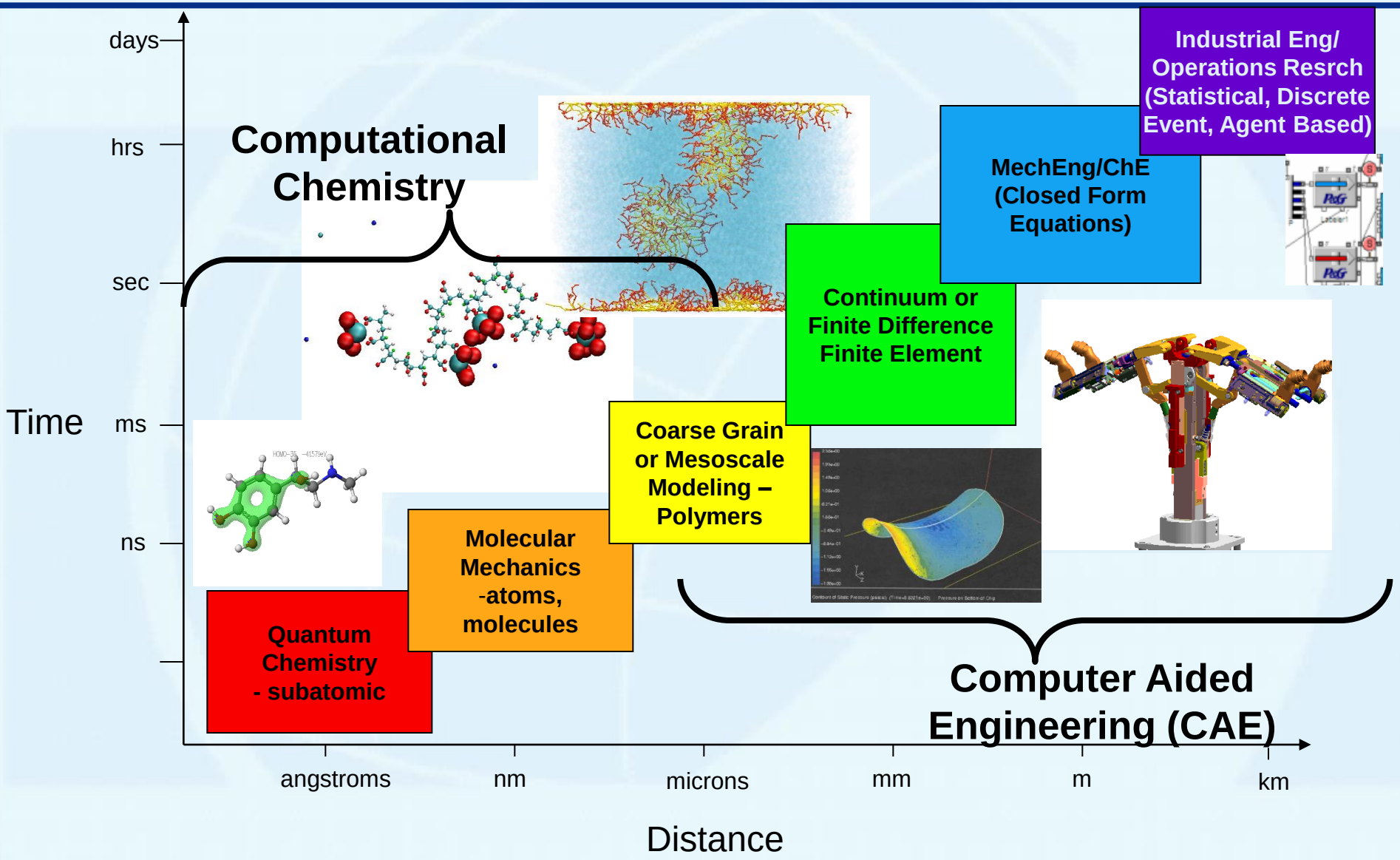
Scales of Modeling



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Motivation

Formulated liquids often contain:

- Solvent (water)
- Surfactants (generally mixtures)
- Polymer
- Other active ingredients (small molecules or inorganics)
- Perfumes or Pigments
- Organic solvents

Key Questions:

- How do we know if we are using the ‘right’ ingredients?
- How much of each ingredient should we use?
- How to predict ‘performace’
- How can we balance ‘performance’ with ‘cost’ during material selection and formula optimization stages?

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DoE INCITE Program (2007-2009)

Molecular simulations of surfactant assisted aqueous foam formation

Kelly L. Anderson
Sr. Scientist, Corporate
Modeling & Simulation

Argonne National Laboratory is managed by
The University of Chicago for the U.S. Department of Energy

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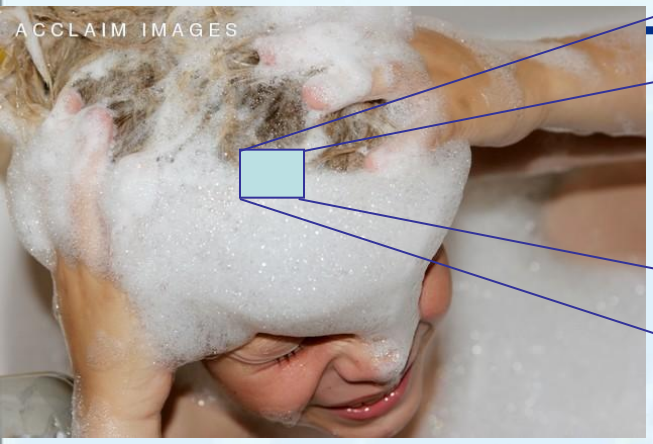
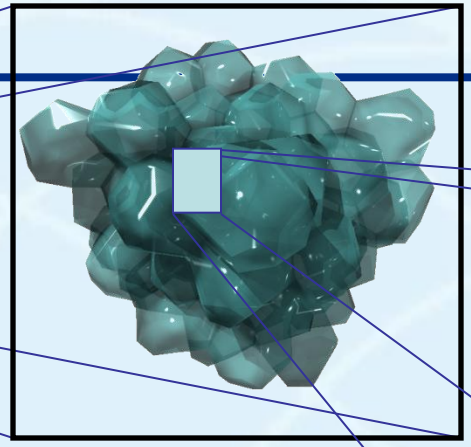
Multi-scale modeling of surfactant lather for shampoos

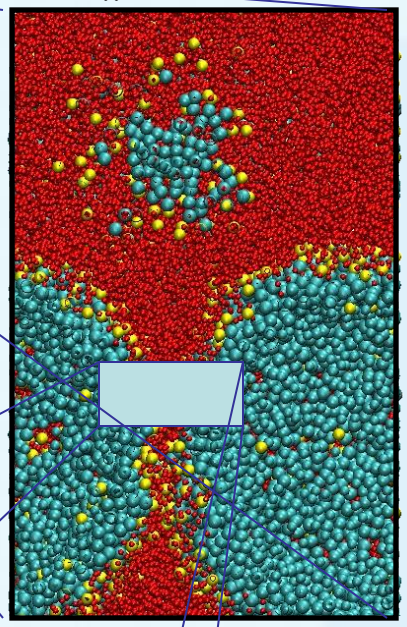


centimeters / seconds



millimeters / milliseconds

micrometers / microseconds

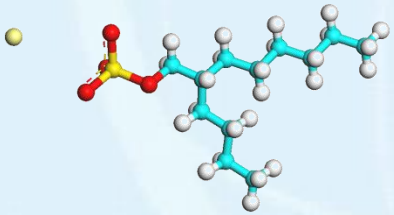


Color codes for Mesoscale / Atomistic simulations:

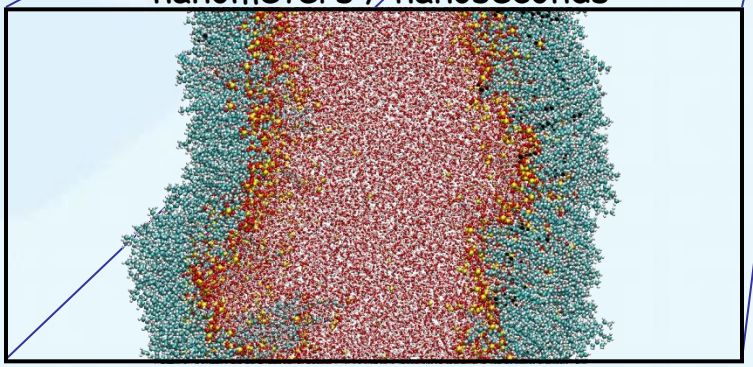
Aqua; Surfactant tail

Yellow; Surfactant head

Red; Water or Oxygen



nanometers / nanoseconds



New surfactants designed for consumer preference

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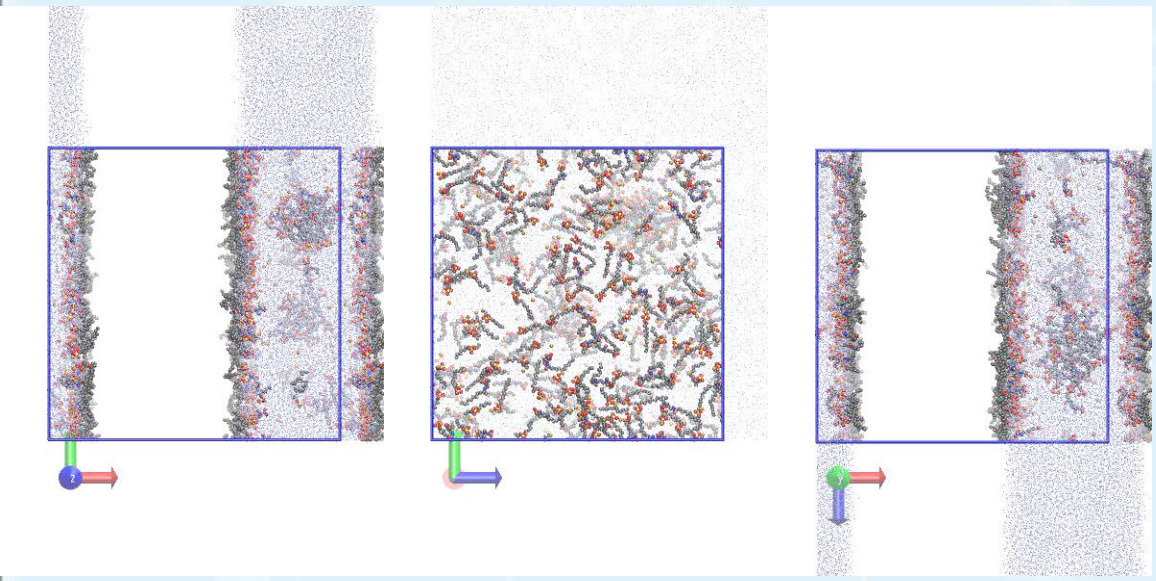
Why Coarse Grain

Simulating surfactant phenomena with all-atom detail requires way too much computer time!



- This animation is of 8ns of 110k particles, 3 P&G surfactant molecules organizing in solution and at the air-water interface
- This simulation took a week on 1024 BG/L cores.
- We want to map out phase diagrams, dynamic IFT, ST, etc.
- 2 options: gross simpifications or coarse-grain

Procter & Gamble © 2010

Considerations for Blue Gene

- Particle based solver needs to be parallelized
- Domain decomposition w/ load balancing preferred
  - NAMD2
  - LAMMPS
  - Gromacs?
- Benchmarking showed both NAMD and LAMMPS run efficiently to 2k proc. (depending on system size, etc.)
- Pre-,Post- processing performed off-line on local Linux workstations.

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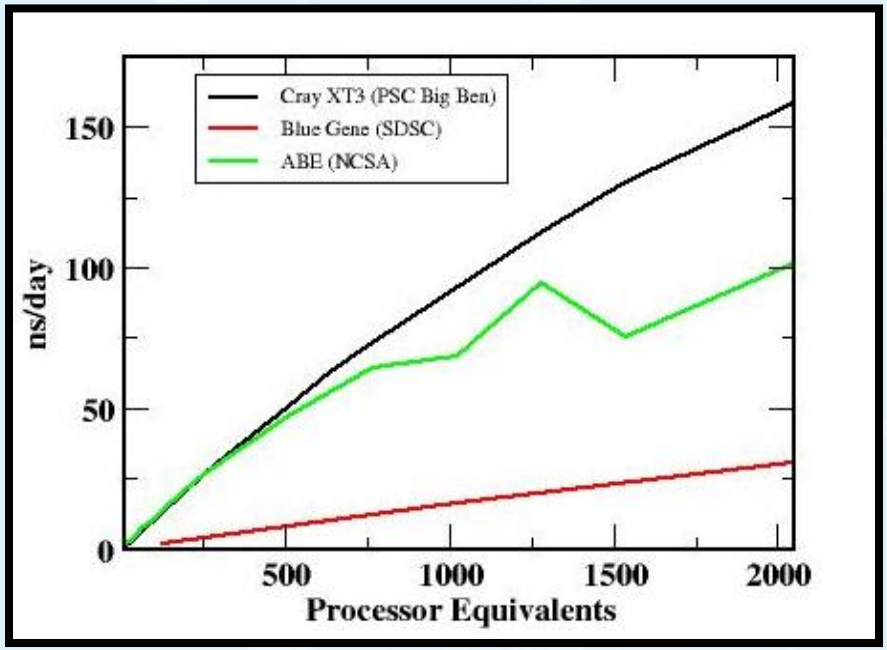
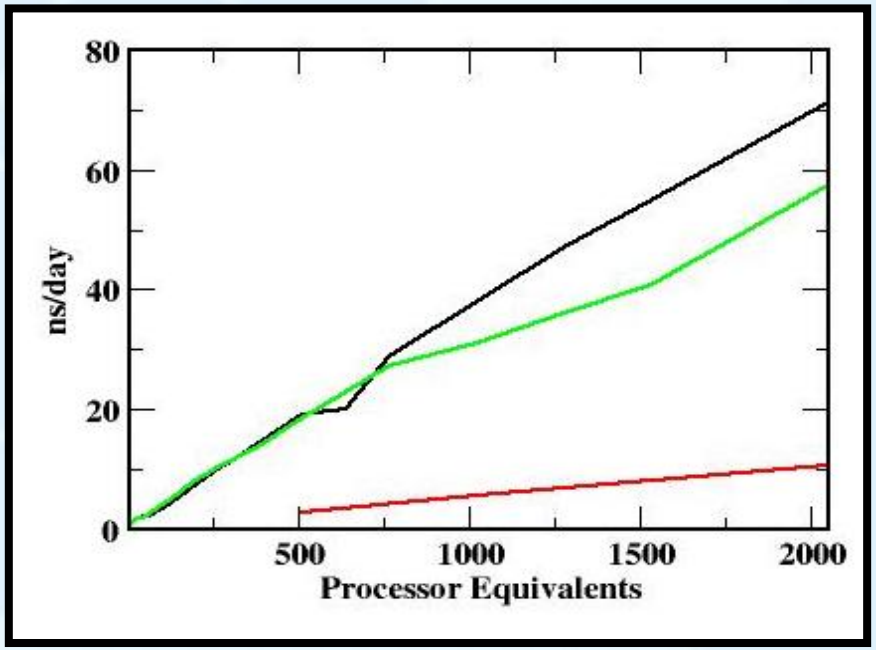
Computational Demand

Implementated In Lammps MD Code
(Sandia National Laboratory)

361260 CG PARTICLES



1003500 CG PARTICLES



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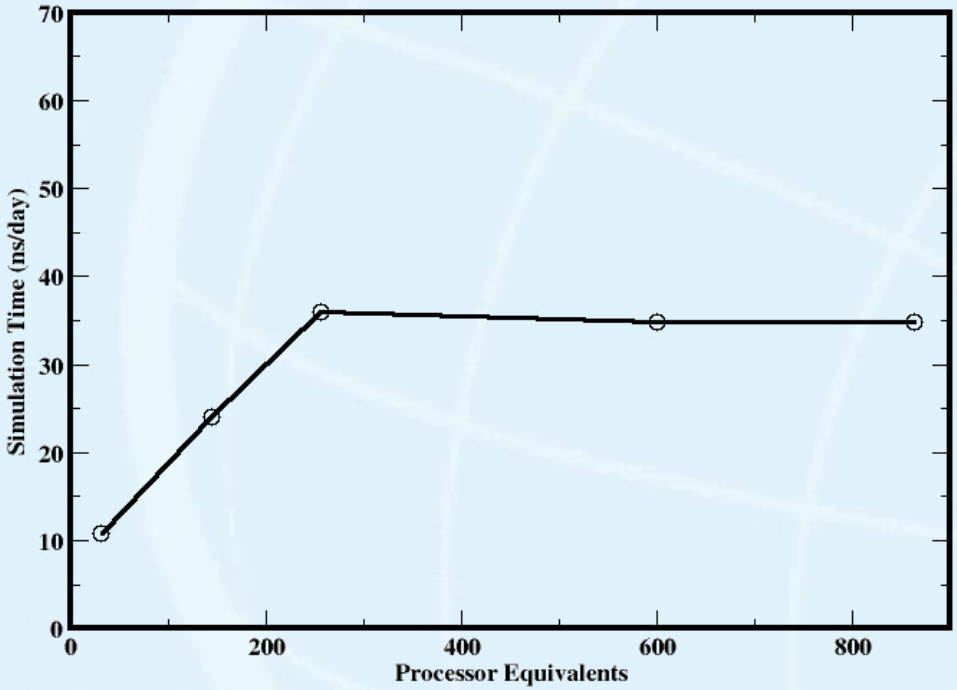
Courtesy: A. Kohlmeyer, R. Devane, Temple U.

Computational Demand

With Electrostatics: 300,000 CG bead lipid bilayer system
LAMMPS MD code (Sandia National Laboratory)



250 CPUs * 24 hours ≈ 5800 CPU hours/day
1 μs would consume ≈ 170,000 CPU hours
and take roughly 1 month

Keep in Mind!!

Compared to AA-MD, this would be equivalent to roughly 3,000,000 atoms for 10 μs

Kraken (cray XT5) National Institute of Computational Science (NICS), UT/ORNL

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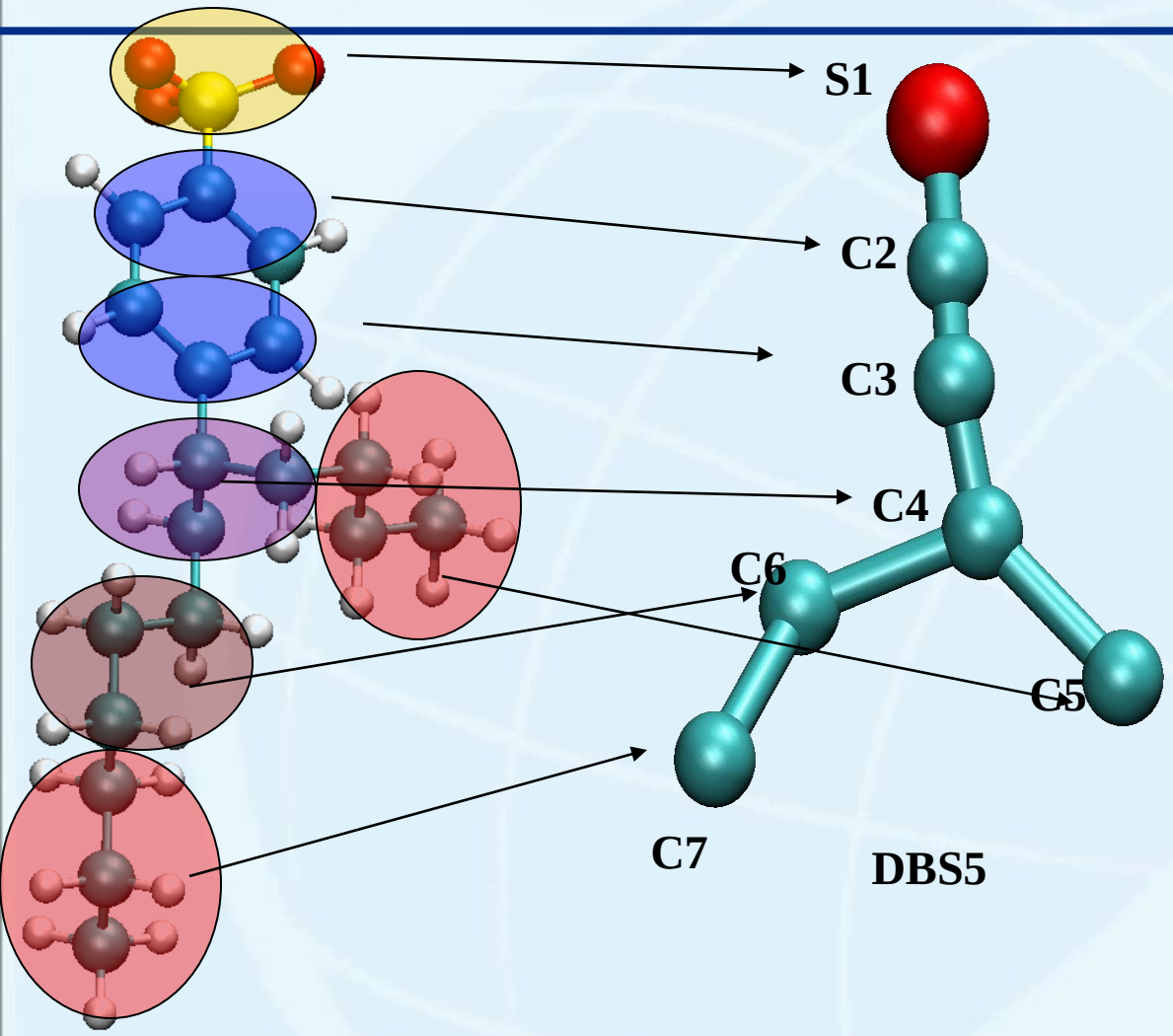
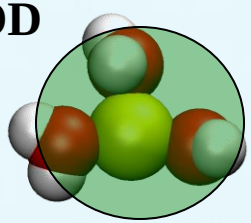
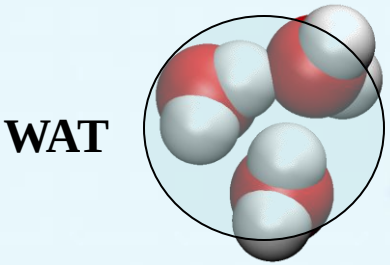
Courtesy: A. Kohlmeyer, R. Devane, Temple U.

Coarse-graining LAS







5-DodecylBenzeneSulfonate

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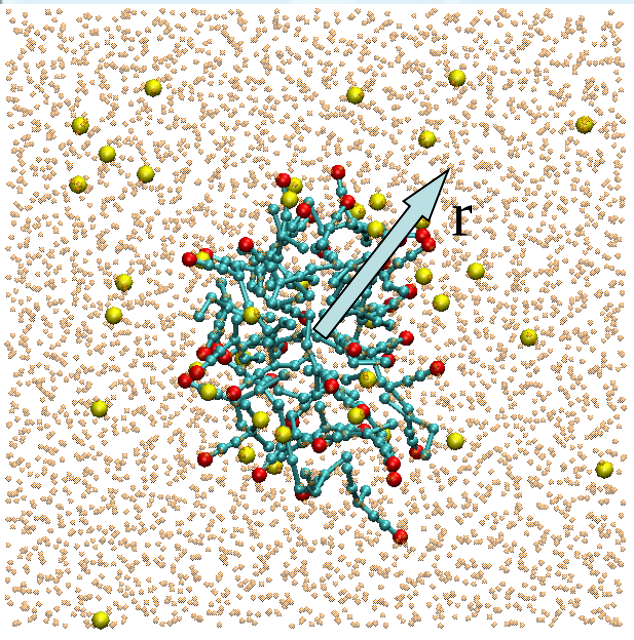
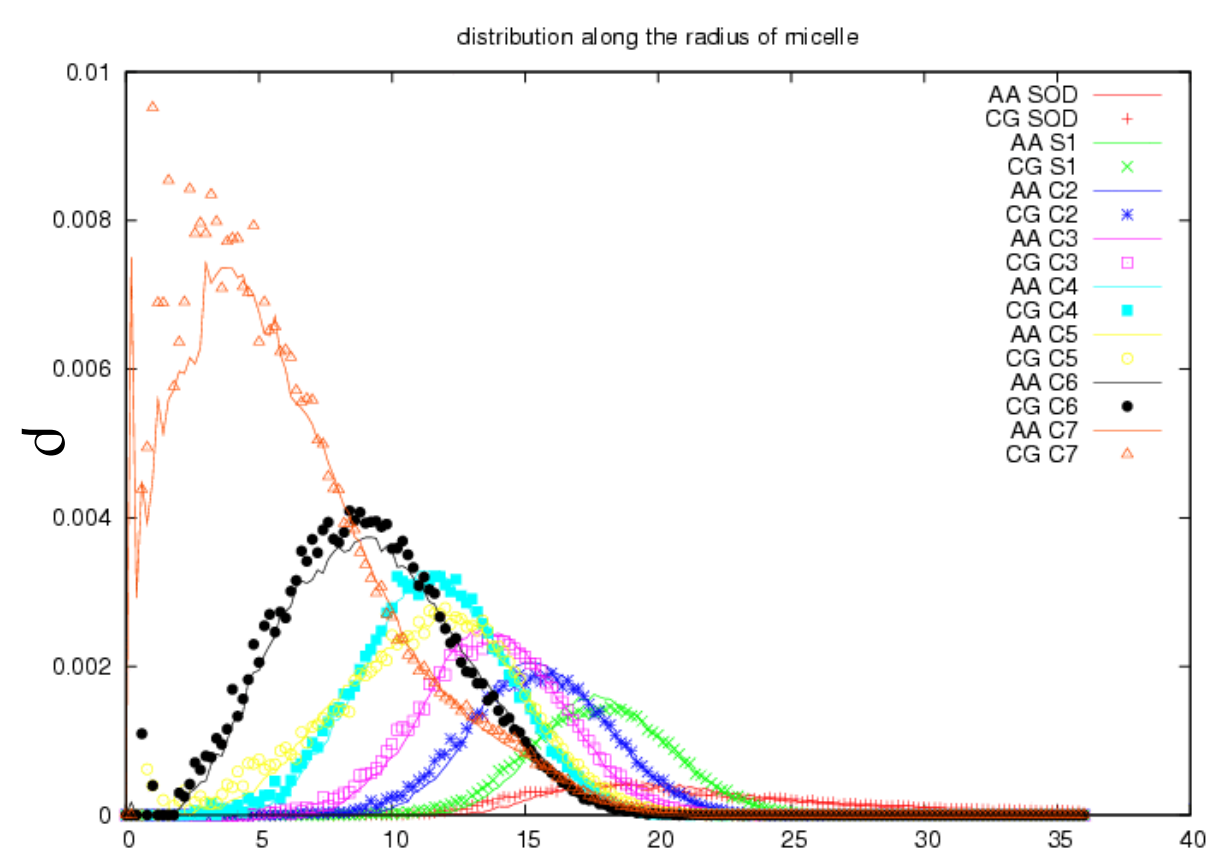
LAS parameter validation (micelles)

Run the same size of micelle system on All-atom (AA), Coarse Grain (CG) level and compare the structure





r (Å)

40 DBS5
40 SOD
4595 WAT

Distribution of particles (groups) along the radius of micelle

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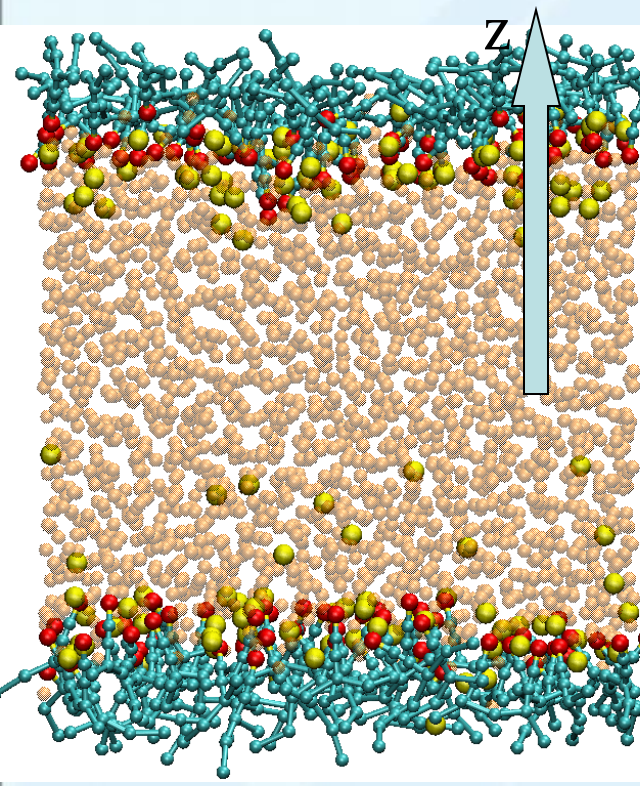
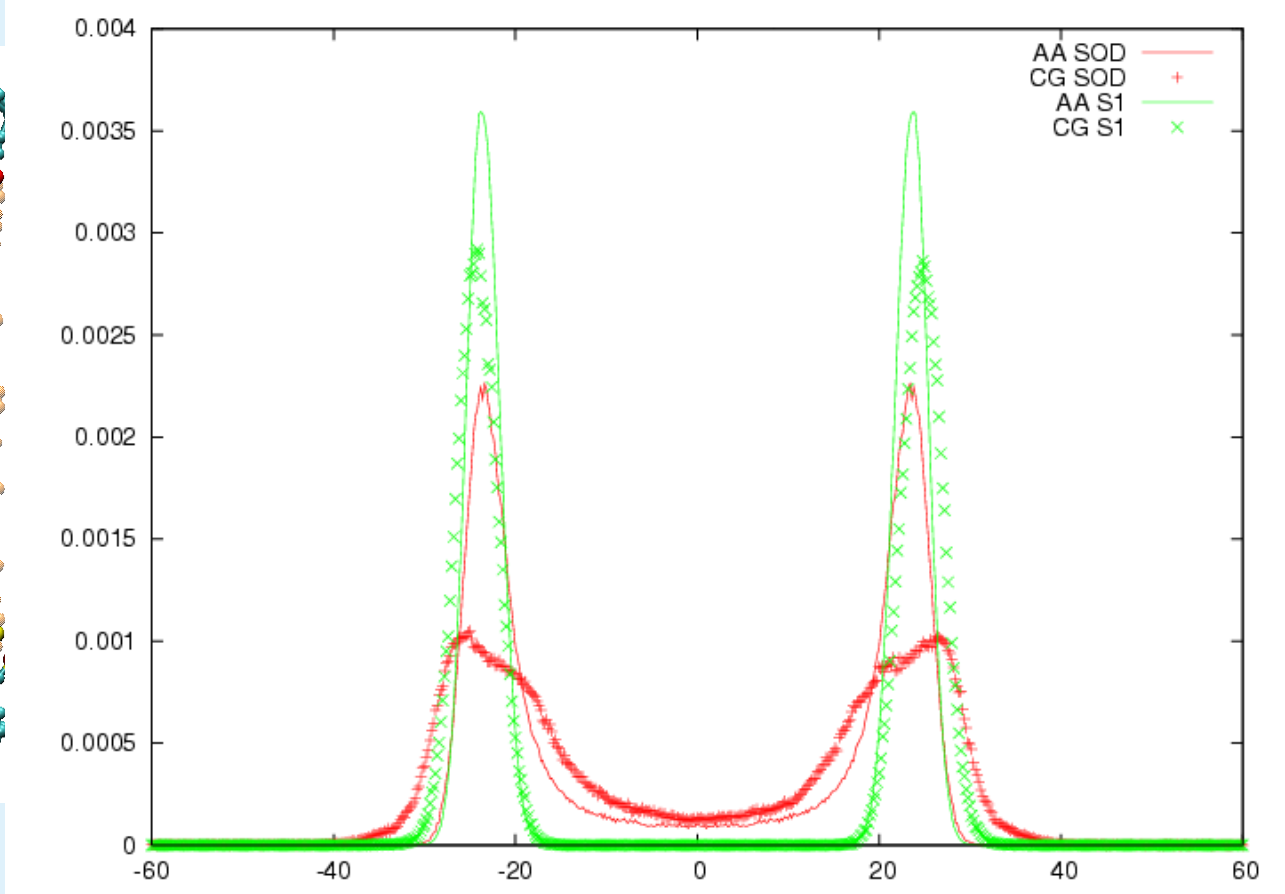
LAS validation (film)

Surface tension: γ_exp = 34.5 dyne/cm,γ_cal = 36.0 dyne/cm





128 DBS5
128 SOD
2135 WAT

Distribution of head group and counter ions across film (not as good)

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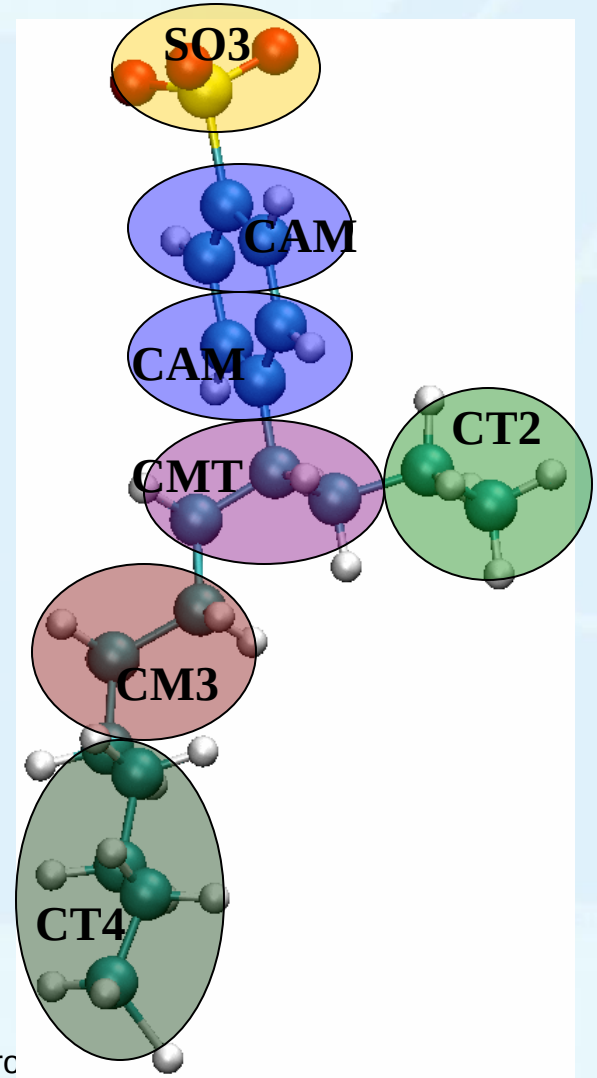
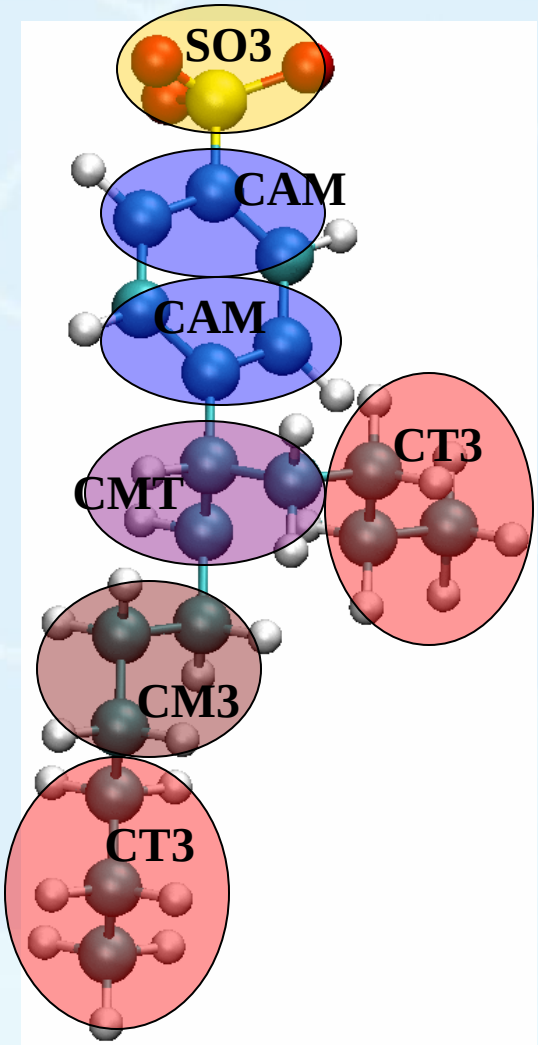
Coarse-grained beads for LAS

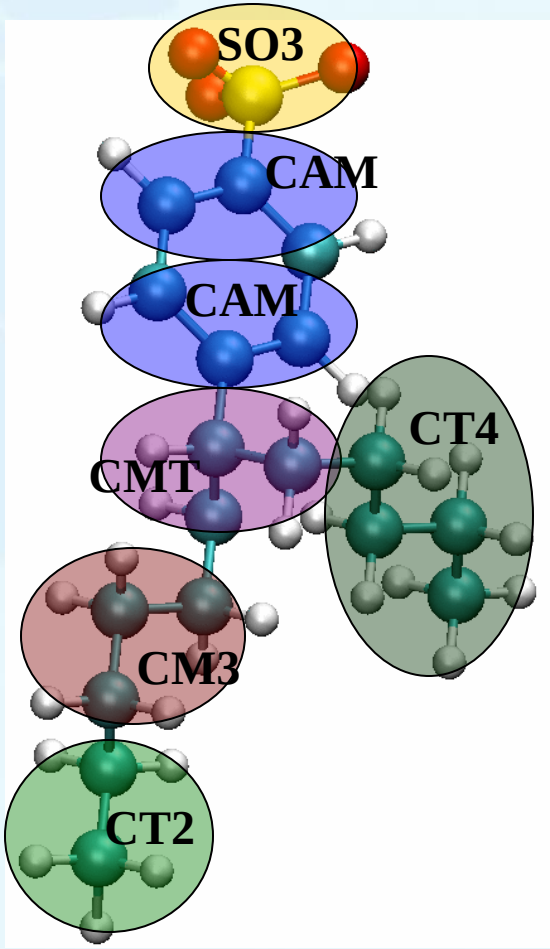
4-DodecylBenzeneSulfonate



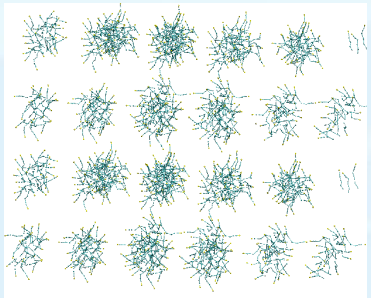
5-DodecylBenzeneSulfonate



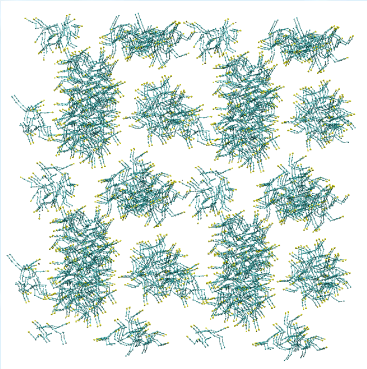
6-DodecylBenzeneSulfonate



Virtual Phase Diagrams



10 wt%



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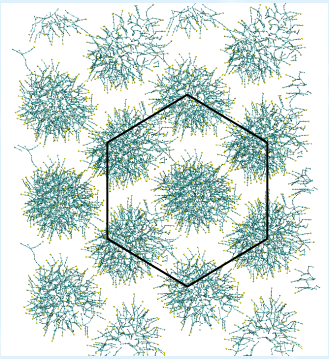
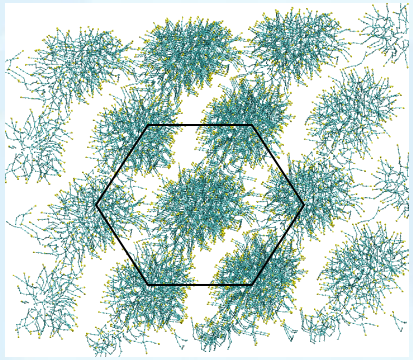


30 wt%



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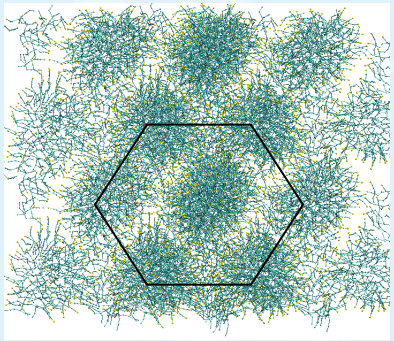
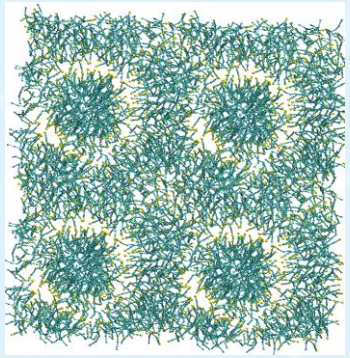
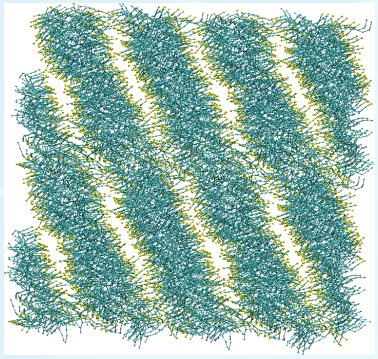


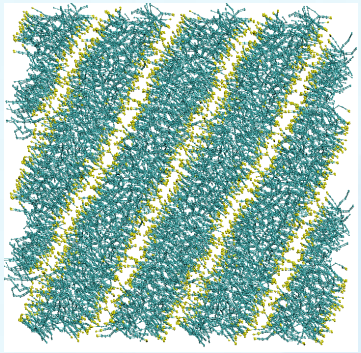
50 wt%



60 wt%



70 wt%



80 wt%

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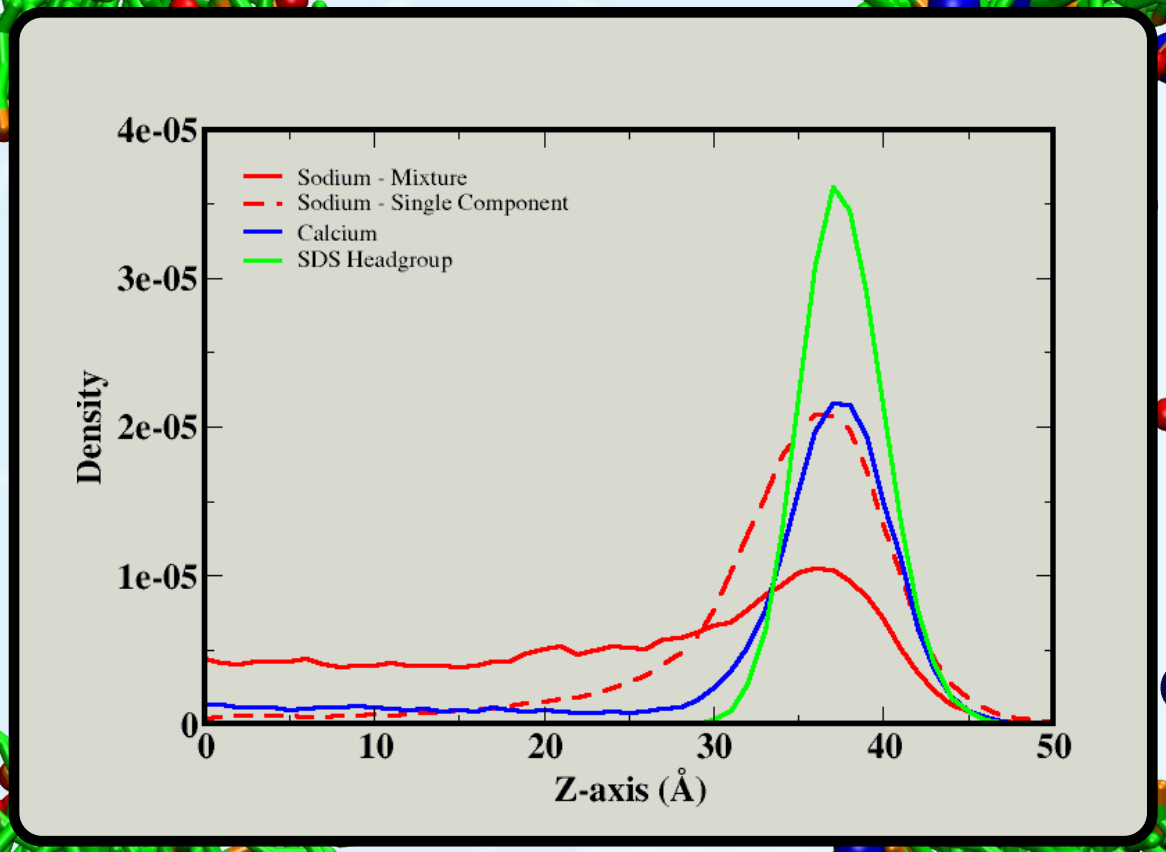
Modeling & Simulation

P&G Research and Development

Monovalent/Divalent Ions



SODIUM

SODIUM/CALCIUM

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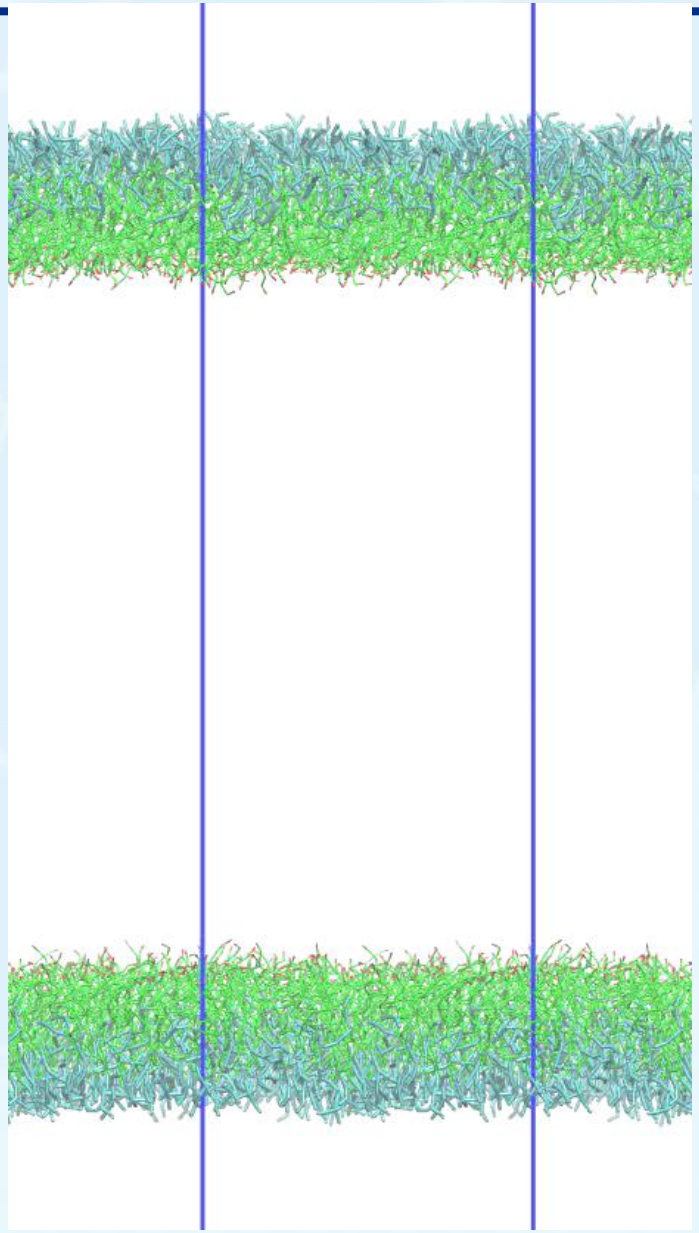
Budding



- Air
- Surfactant
- Water
- Surfactant
- Air

Film compression leads to budding of micelles

Complements of Wataru Shinoda (Temple / AIST)

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WRAP-UP

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Modeling *(in my ideal world)*

- Technology development with computational chemistry:
  - Screening of reactions for new materials (*ab initio, qm/mm*)
  - New materials 'performance' prediction (*ab initio, qm/mm, molecular dynamics, monte carlo, mesoscale methods, virtual DOE*)
- Virtual Formulation:
  - 'Performance' optimization against many criteria (*molecular simulations, mesoscale methods, virtual DOE*)
  - Interactions with other ingredients, target substrate (*molecular, mesoscale*)
- First principles Computer Aided Engineering (CAE):
  - Processing – parameters derived from mesoscale simulations
  - Packaging – material properties from molecular simulations

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Modeling *(in the real world)*

Current business relevance

- CAE
  - Processing (*empirical parameters*)
  - Packaging (*empirical parameters*)
- Formulation
  - 'Performance' against many criteria (*empirical parameters, proprietary methods*)
  - Interactions with other ingredients, target substrate (*difficult analytical measures*)
- Technology development
  - Screening of reactions for new materials (*some simulation, but mostly intuition*)
  - New materials 'performance' prediction (*qspr, hts*)

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The Undone (where we need help)

- Forcefields
  - Organic – Inorganic
  - Amphoteric materials
  - Implicit solvents
  - Formalized comprehensive coarse-graining methodologies
- Molecular simulation features
  - Scalable long range electrostatics
  - Run-time analysis, call-backs to visualization / other software
- Easier access to HPC environments
  - Client-server simulation software from outside your firewall?
  - Cloud computing that our lawyers will let us use?

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INCITE Conclusions

- Although much can be done today with empirical methods, we are just starting to show successes with first principles based modeling of suds.

- Have demonstrated that Intrepid / Jaguar systems can work for a variety of well-parallelized MD simulation codes.

- We have developed coarse-grained models of our key surfactants and polymers, and are using them in "production mode" in complex formulations.

- Continued fundamental research is key to enabling future virtualization of materials design for soft-condensed matter applications in formulated products.

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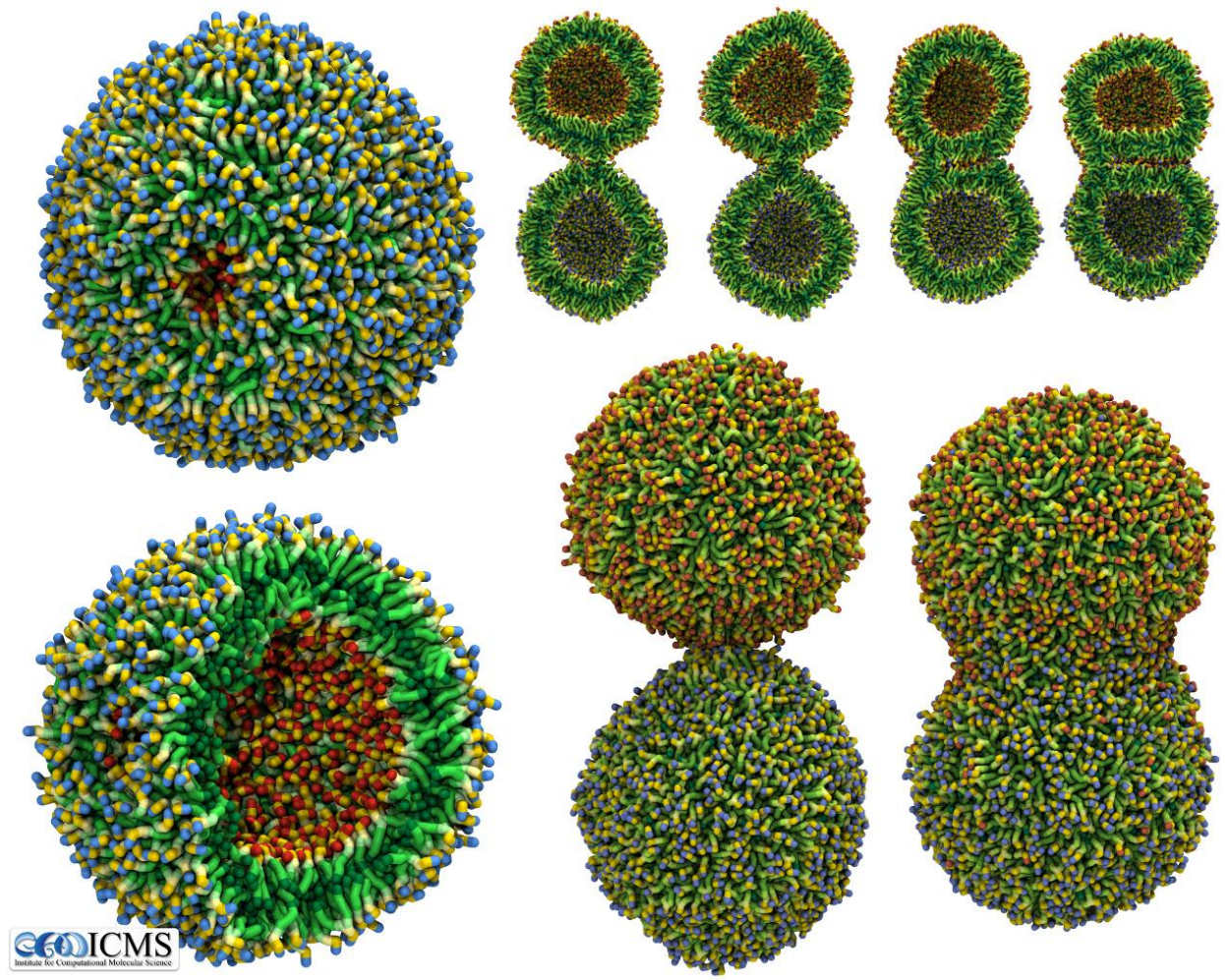
Looking forward

DOE INCITE proposal for CY2011:

Coarse Grained Molecular Dynamics Studies of Vesicle Formation and Fusion

- Protein mediated fusion
- Polyelectrolyte interactions
- Small molecule impacts
- Mechanistic study of product (in)stability



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Science Impact of Access to Leadership Computing

Advancing Industrial R&D by:

- Enabling new discoveries (virtually)
- Running current simulations faster than possible on in-house systems
- Validating the ‘physics’ of current in-house production simulations with larger volume / longer running simulations
- Providing common platform for collaborations with DOE staff and Academic partners
- Justification for more in-house computing

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Competitive Impact of Access to Leadership Computing

- Accelerates product innovation / development for shorter time to market
- Allows us to respond to a competitive threat
- Enables us to meet customer (internal or external) expectations
- Lowers innovation costs

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Questions?

Comments?

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