Advanced Scientific Computing Advisory Committee

Gaithersburg, MD

October 28, 2008

modeling & simulation

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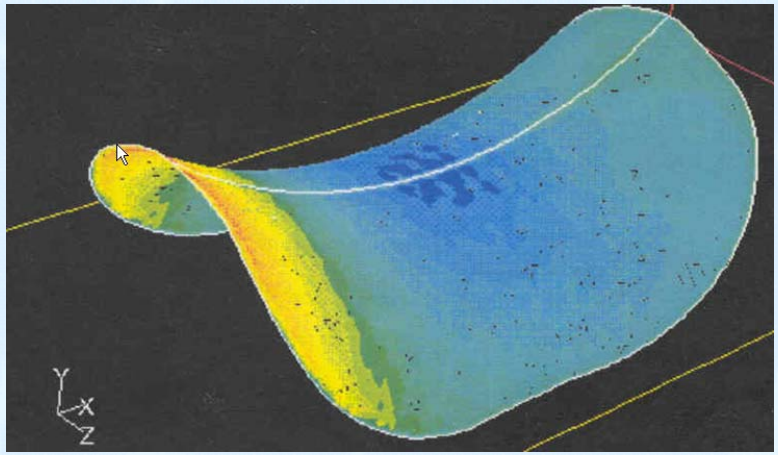
The Modeling & Simulation behind everyday Products



Tom Lange

Director, Procter & Gamble

Modeling & Simulation

Global Capability Organization R&D

modeling & simulation

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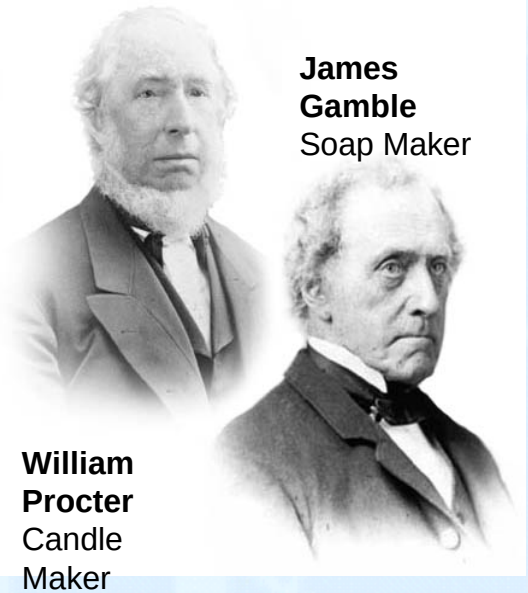
…Founded in 1837



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

‘Lighting’

…Started with *STAR* Candles

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...After a hundred years

C L E A N I N G

1937

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...By the time I was born

1957

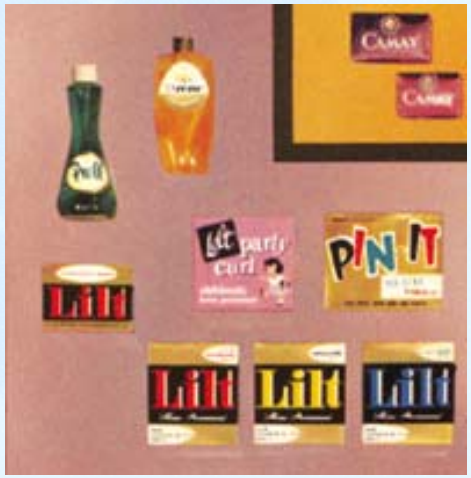
Clothes

CLEANing

Teeth & Hair

EATing

House



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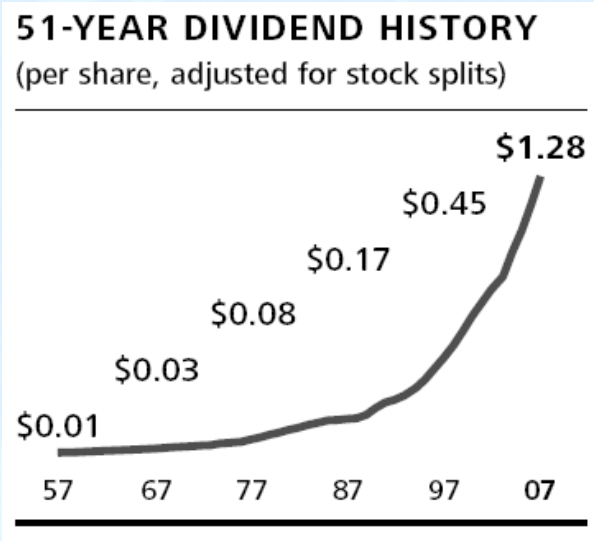
Investors Know Us By…

- **Sales:** $83.5 Billion FY June 30th, 2008
- **Net Earnings:** $12.1 Billion

P&G has paid dividends without interruption since 1890

51 consecutive years of increased dividend payment.



Worlds Largest Consumer Goods Company…Market Cap ~ $174 Billion
(COB Monday 10/27/2008)

Employ: 138,000 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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P&G Consumer Knowledge.... 300+ Worldwide Brands

Beauty

Health Care

Fabric Care & Home Care

Baby Care & Family Care

Snacks, & Pet Care

Blades & Razors Duracell & Braun

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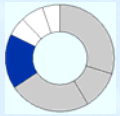
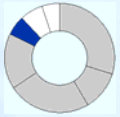
23 Billion $ Brands…

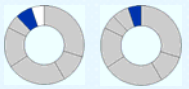

Beauty

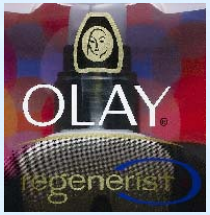

Health Care

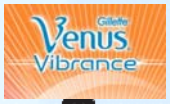

Fabric Care & Home Care

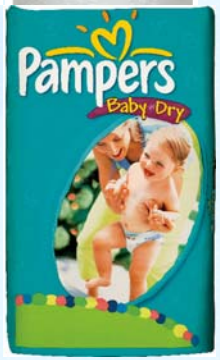

Baby Care & Family Care


Snacks, Coffee & Pet Care


Blades & Razors Duracell & Braun







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Why Brands?

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The Two Moments of Truth

OK…
Enough of the B School take on things…

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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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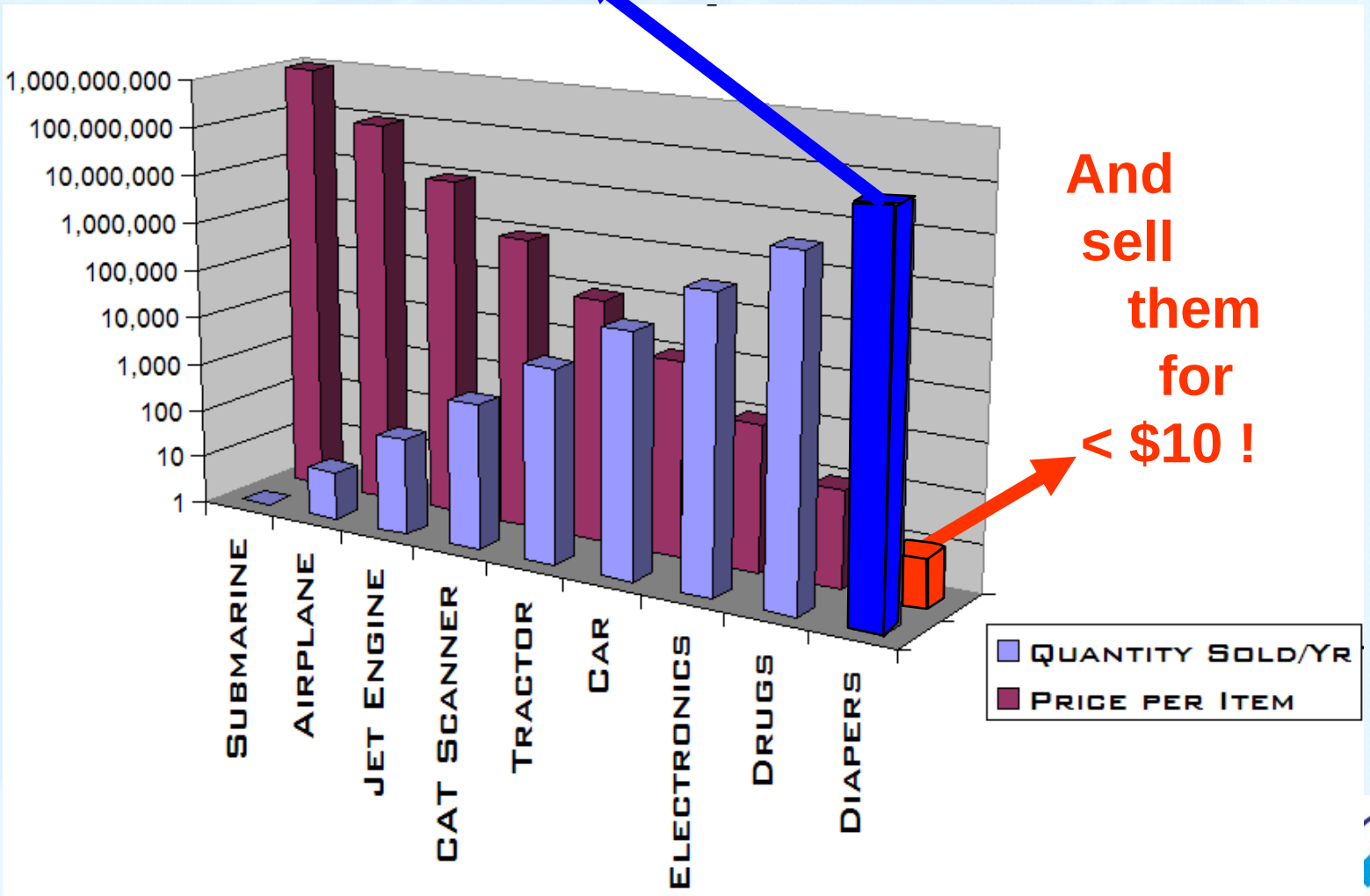
Scale: Sell a Billion $

We make **billions** of products a year…



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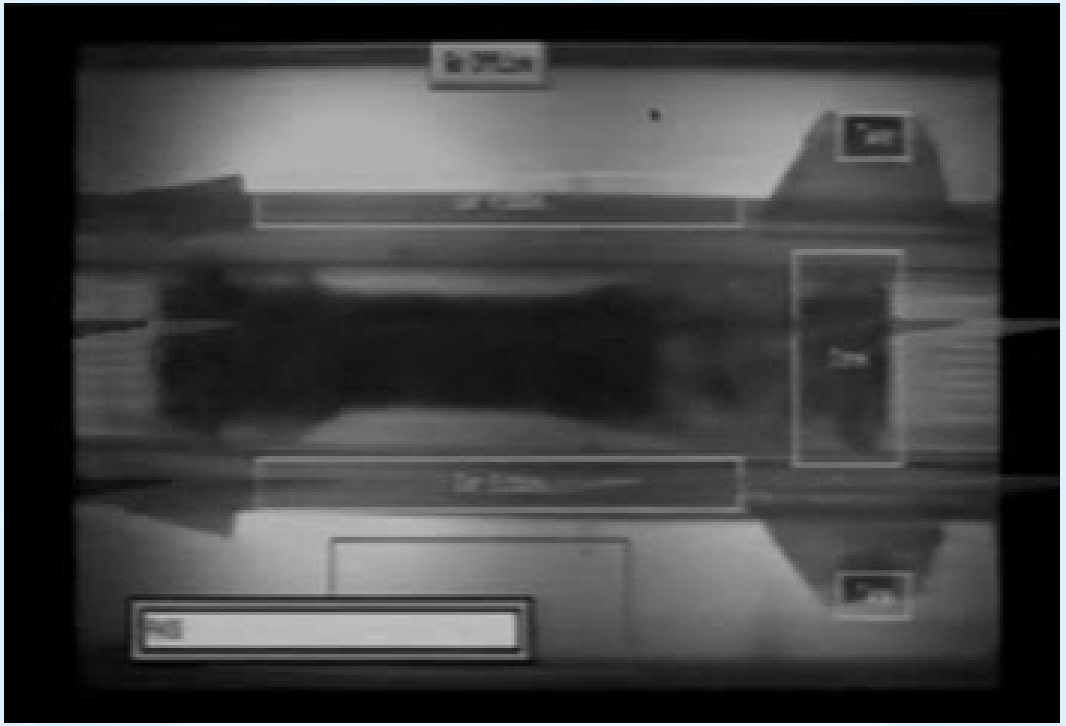
Make a Billion Diapers…

How long does it take to make a billion Pampers?



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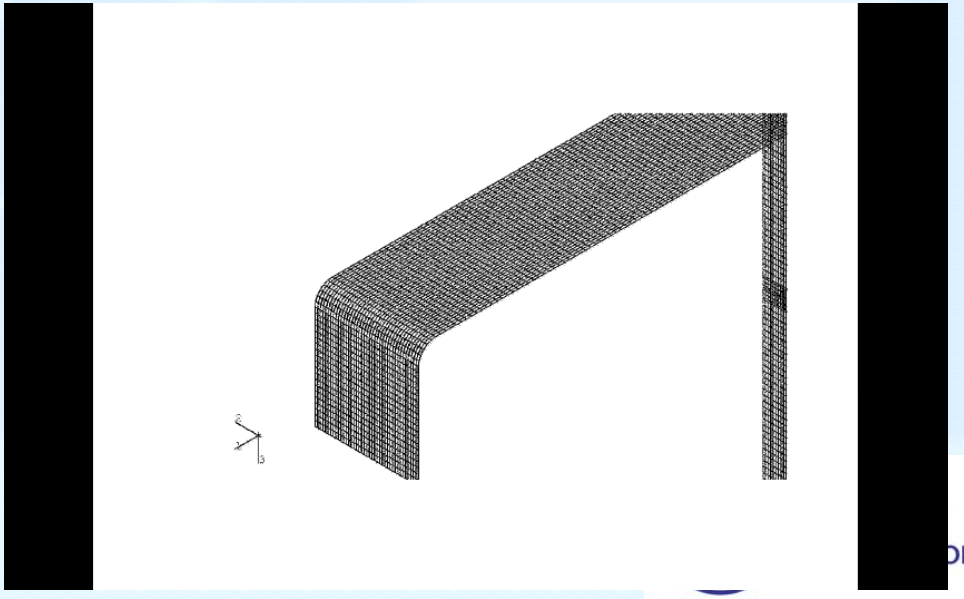
Splicing Webs…

What Happens…
When you miss!



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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 ish every year**

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

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Modeling & Simulation Has 'Transformed' Industries

1940's-1970's

Defense

1970's-1980's

Aviation

1980's-1990's

Automotive

1990's-2006+

Consumer Goods

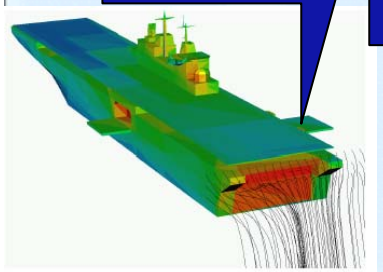
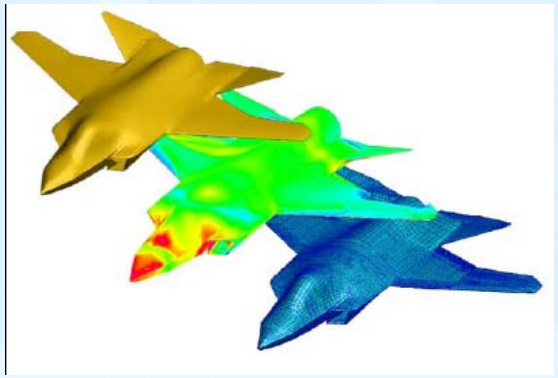
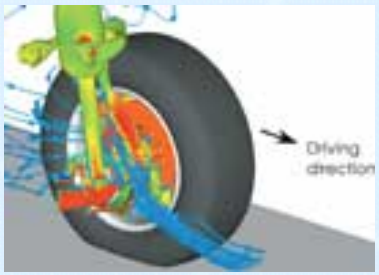
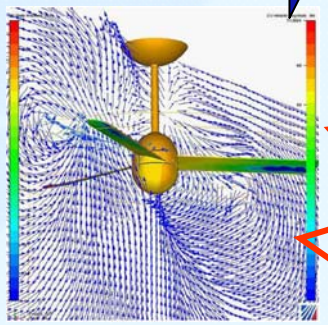


Figure 11: Simulation of full LHA and V/STOL aircraft with the FPV model.







Now CPG… FMCG

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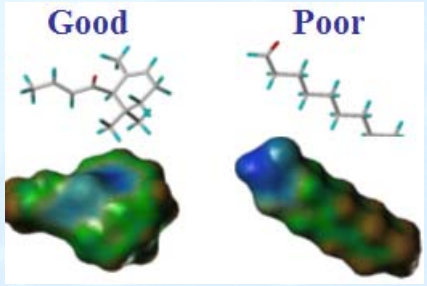
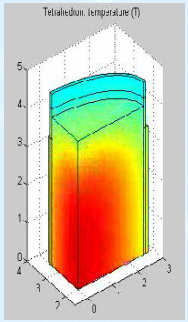
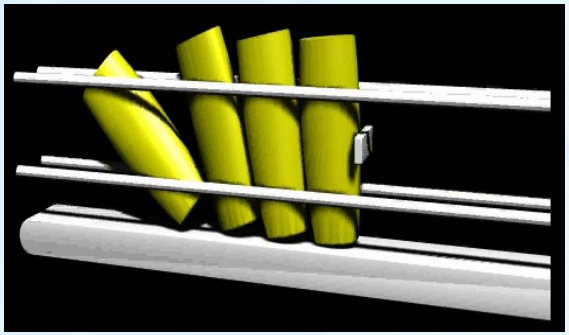
…Atoms to the Enterprise

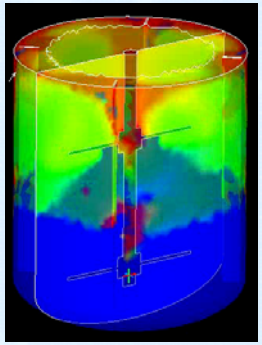
Product/ Device/ Package



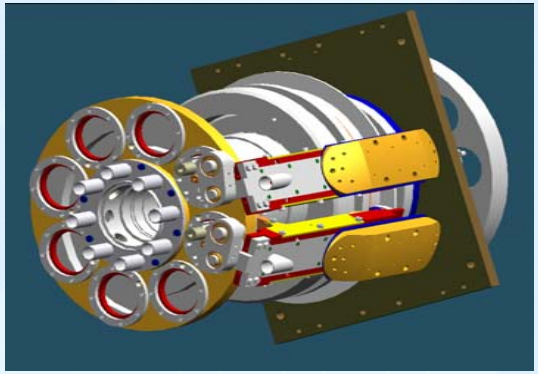




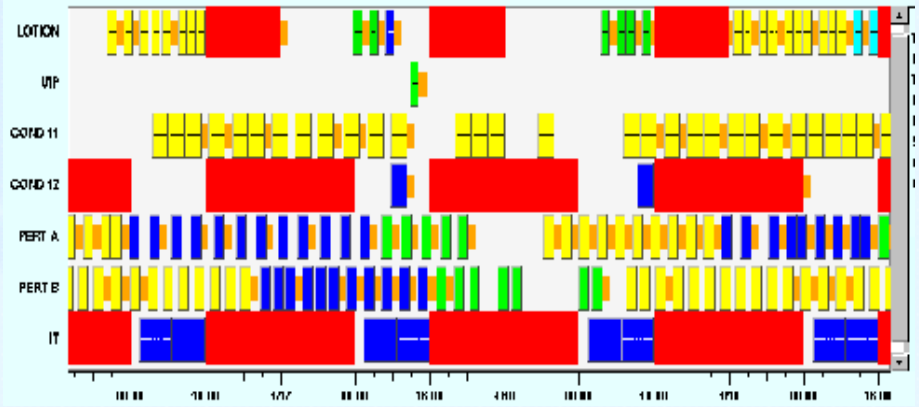
Process & Making

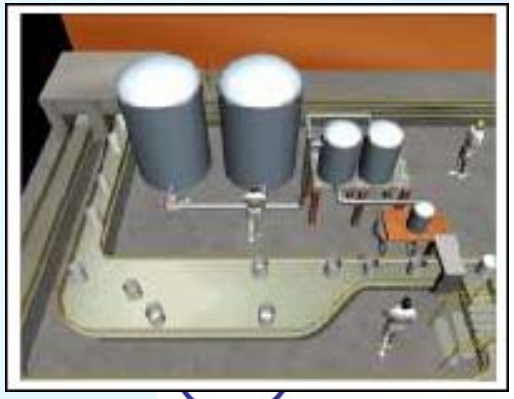


Mechanical & Converting



Supply Chain Through-put & Reliability





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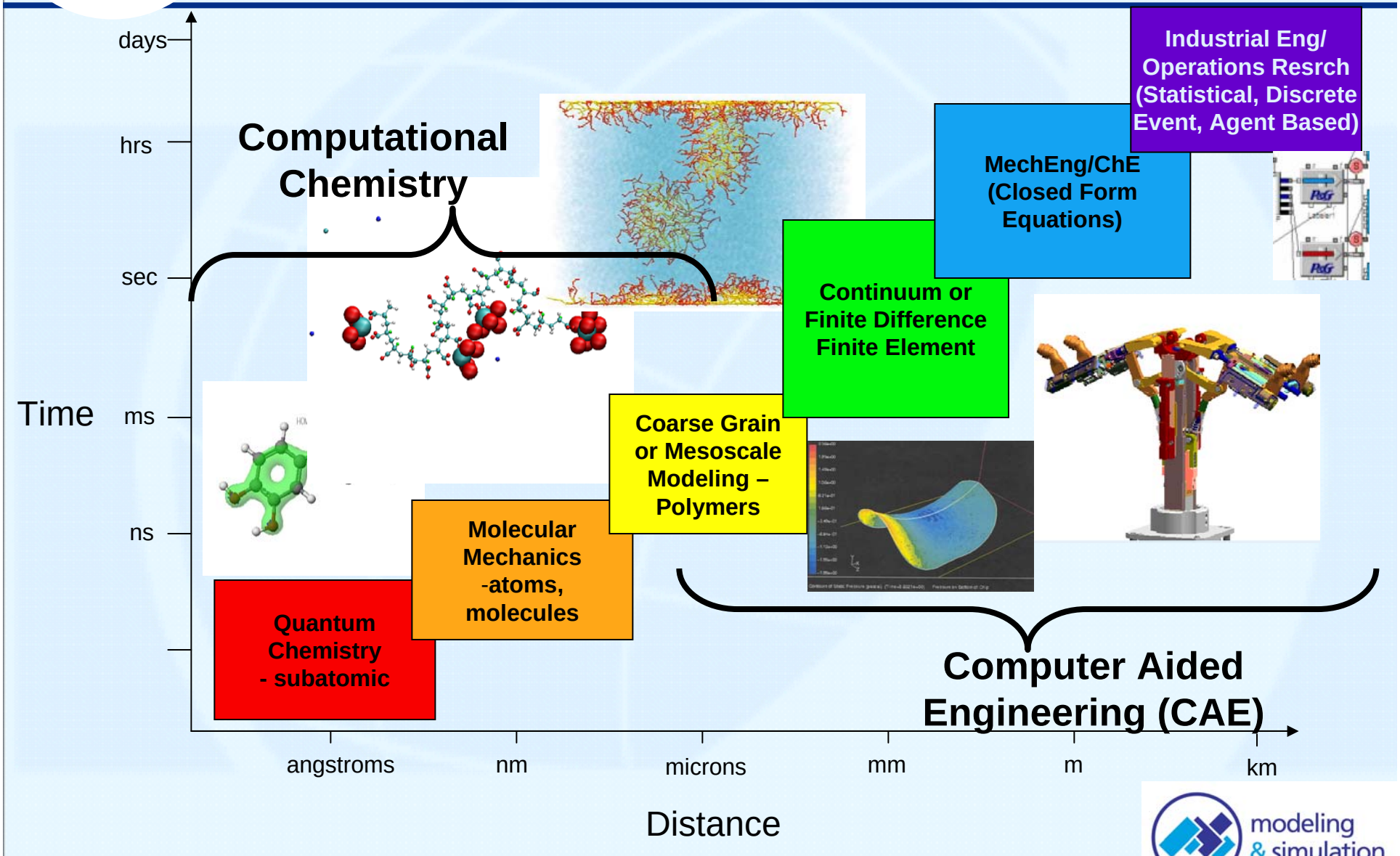
Scales of Modeling



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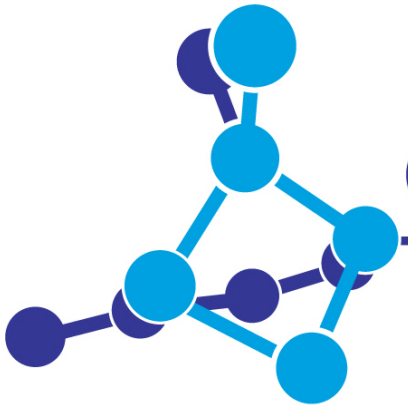
M&S 'Brands'



Computational Chemistry

CAE

computer aided engineering

modeling & simulation

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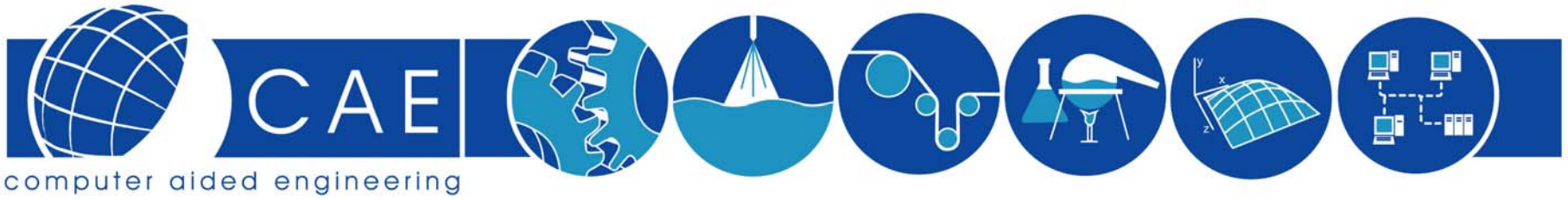
CAE Disciplines



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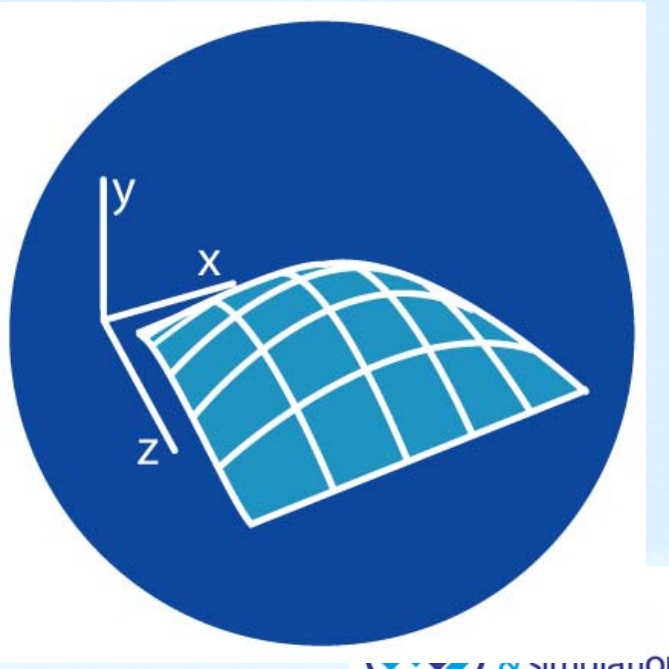
Empirical & Optimization

- Supply Chain Analysis
- Planning & Scheduling Analysis
- Plant Throughput Analysis
- Reliability Engineering
- Consumer Response modeli
- DOE
- Optimization



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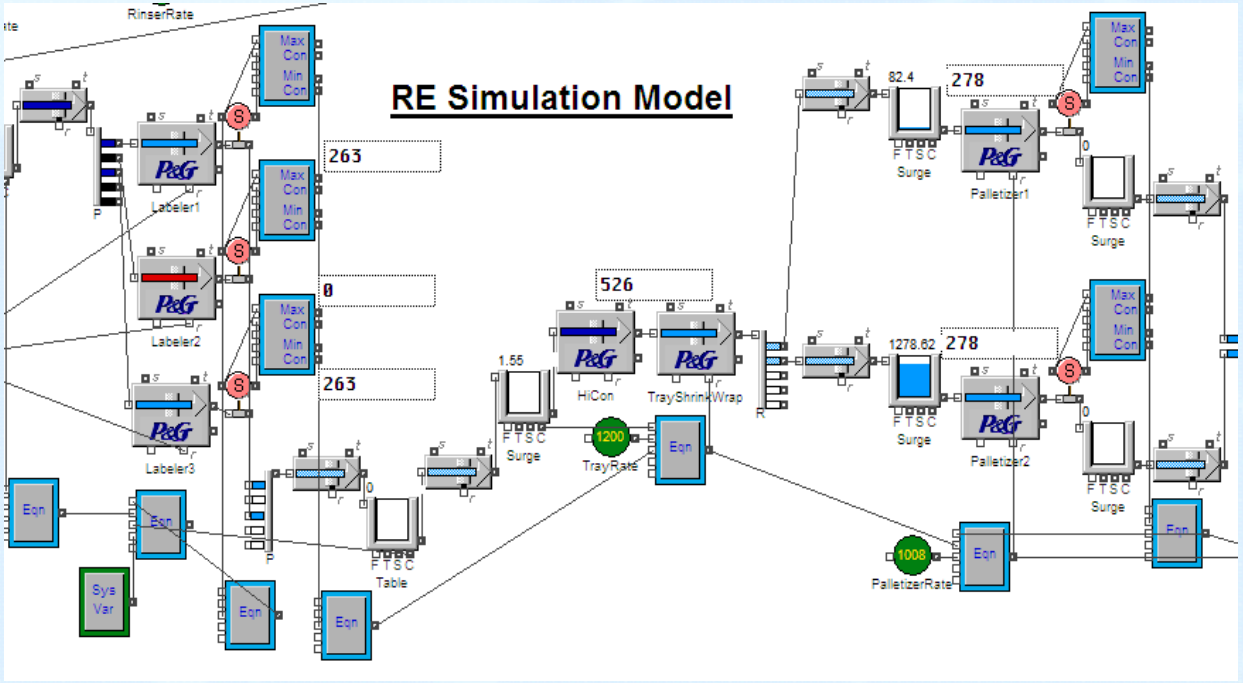
Process Reliability



2003

Council for Chemical Research (CCR)

2003 Research Collaboration Award

***Collaboration began in 1994

2002

T&B Award

Winner of Several Joint Awards with Los Alamos National Laboratories

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Solid Mechanics:

- **Rigid Body Kinematics**
- **Finite Element Analysis (FEA):**
  - Implicit
  - Explicit
  - Linear
  - Non-linear
  - Massive Contact
  - Complex non-metal Material Models: High Strain Rates 1/500 Seconds, Elastic-plastic, Hysterisis: Visco-Elastic, Visco-Plastic

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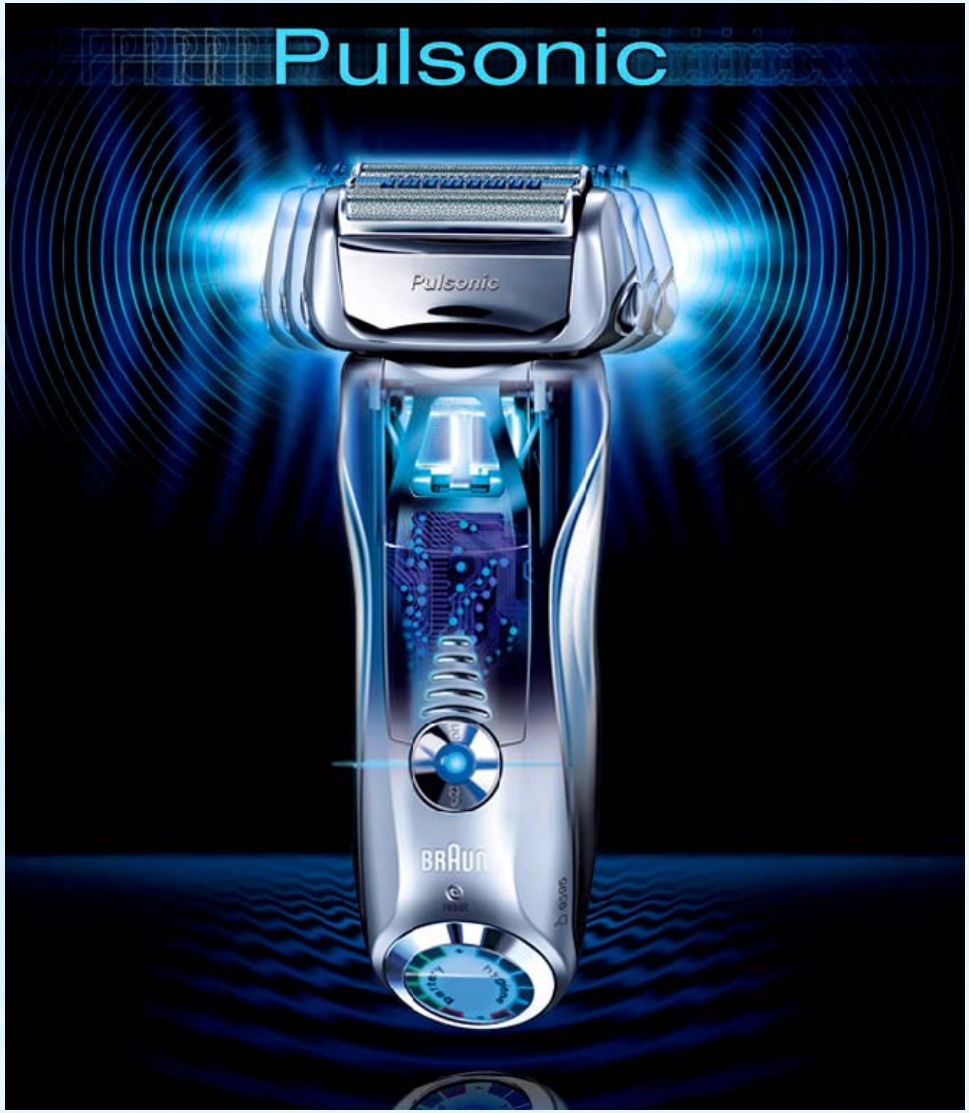
The new premium shaver …



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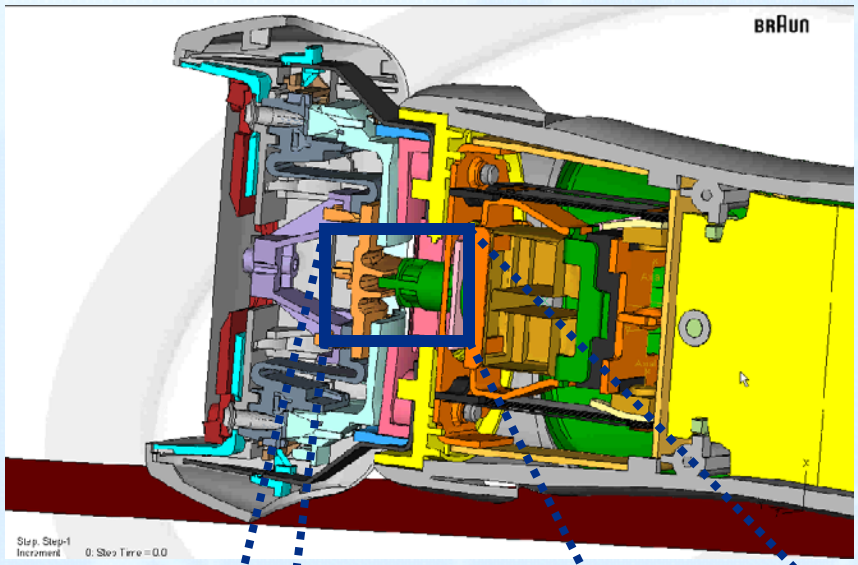
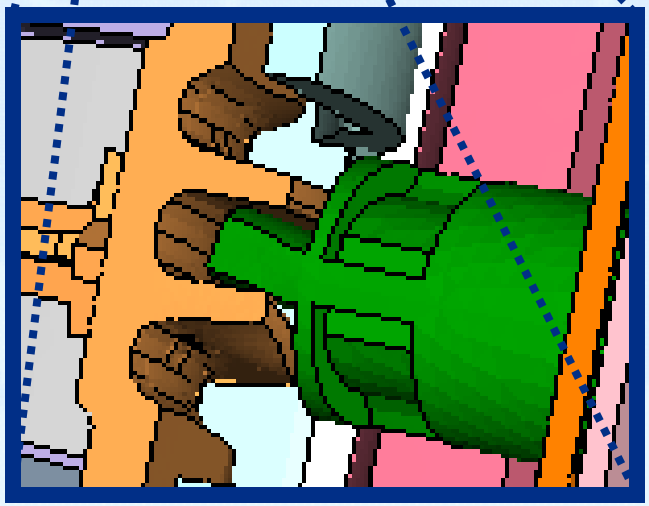
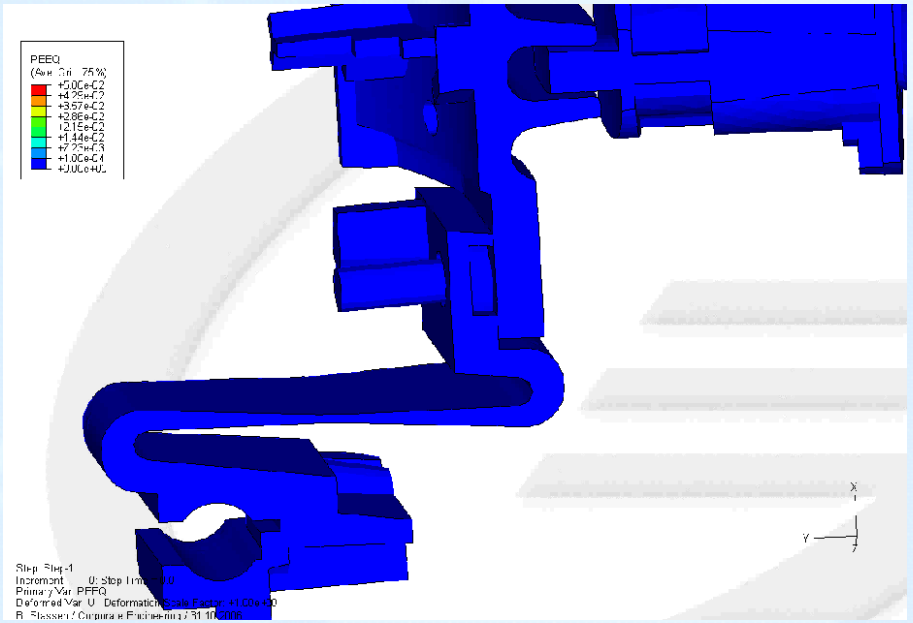
Braun Drop







Lots of Small Parts...
…Everyone must work!

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Behind Every Great Package…

…Is more than meets the eye!

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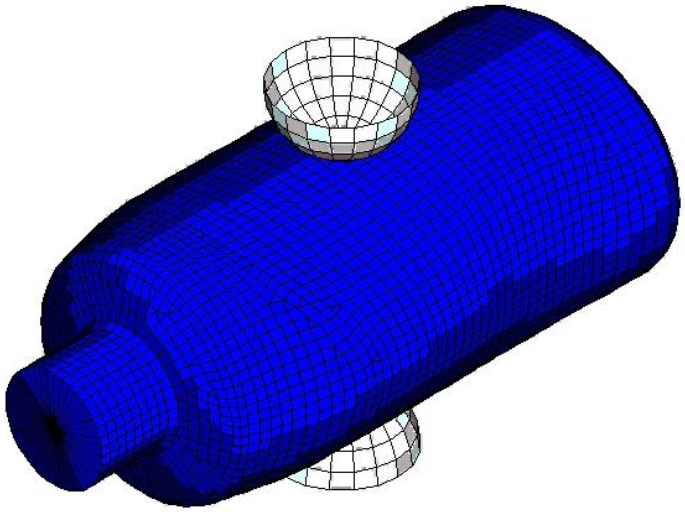
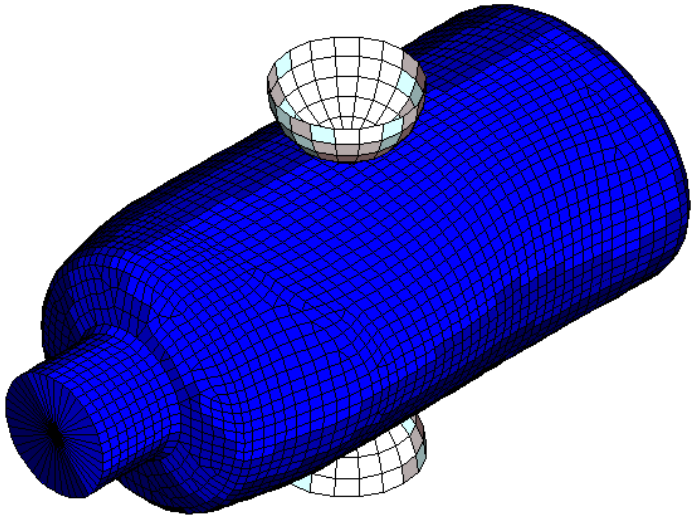
Hair Colorant Bottle: checking squeeze performance.

Material A: insufficient spring-back

Material B: sufficient spring-back

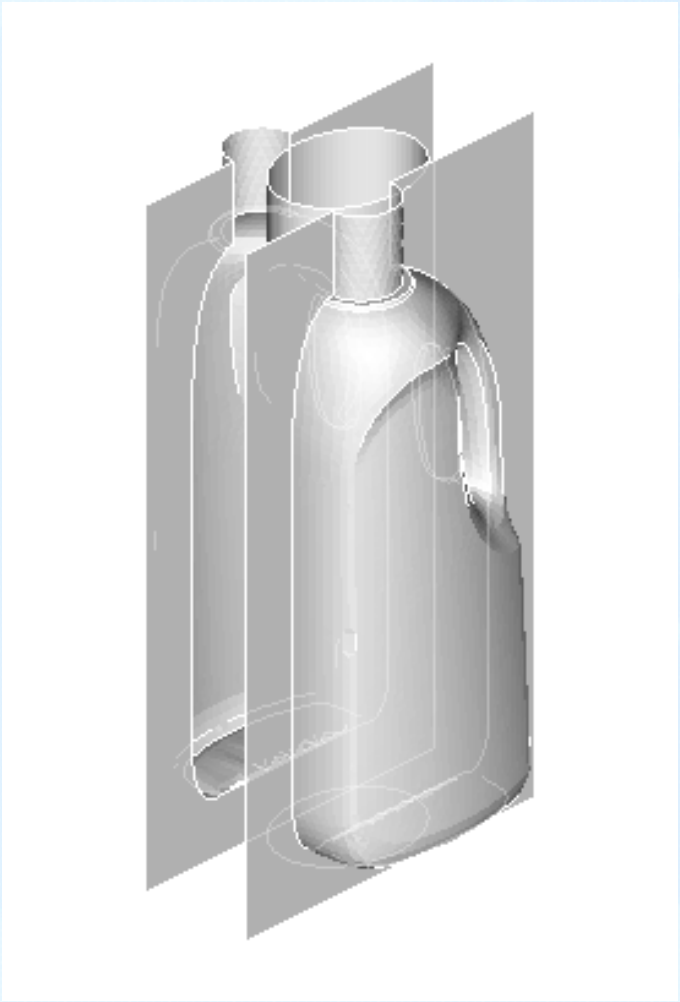


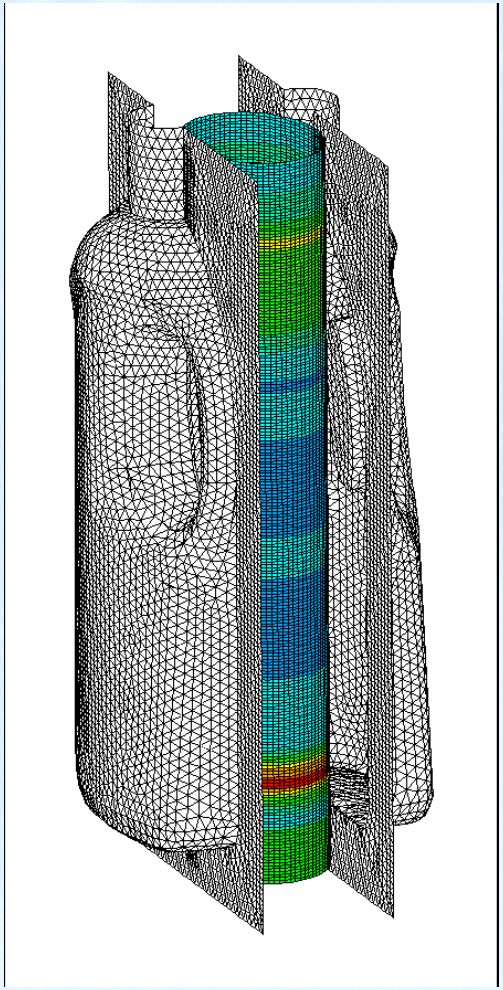


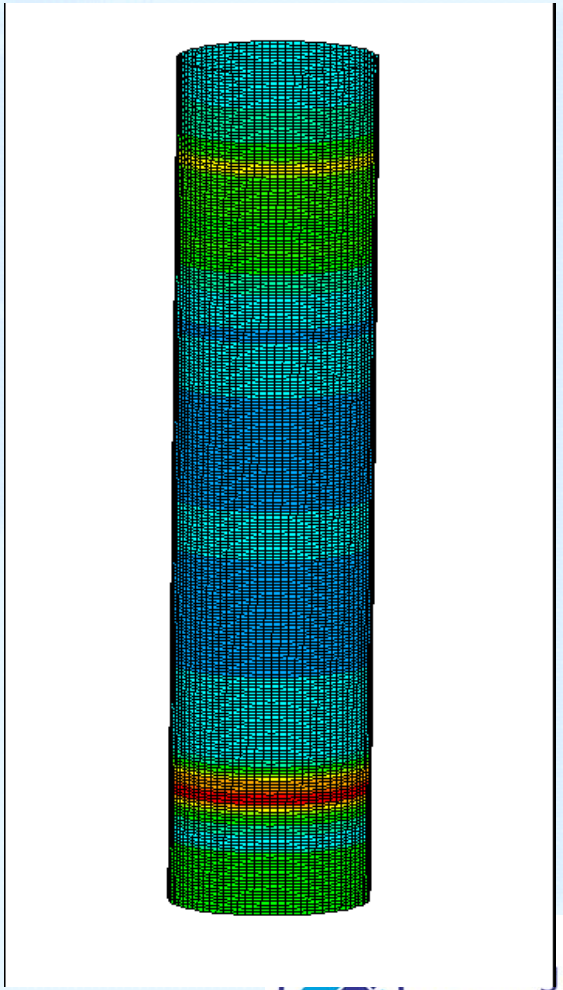
Stress

Bottle Optimal Weight System.

Optimizing the bottle weight : profiling the parison .

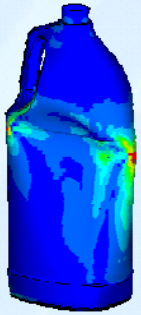




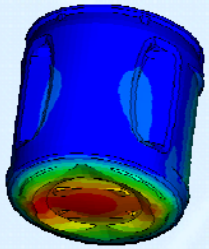


Load Cases

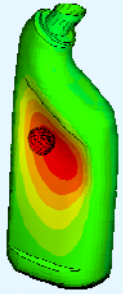
Top Load Empty

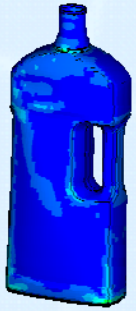


Pressure

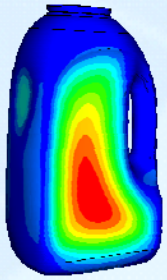


Squeeze

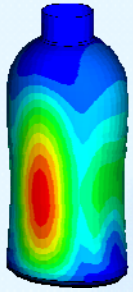




Top Load Filled



Vacuum



Hydrostatic

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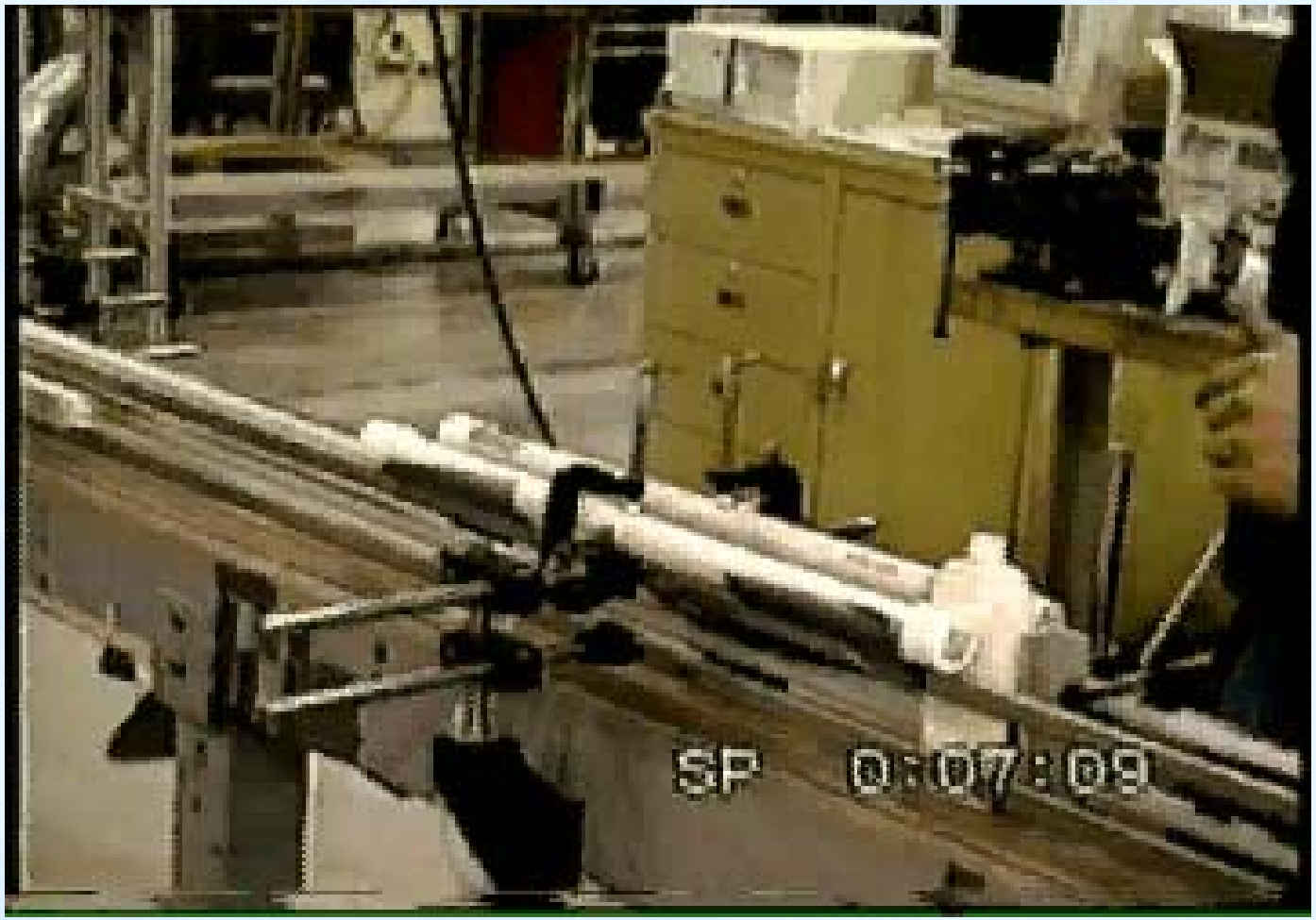
Can We Pack it?



Bottle Race Track
'Circa 2000'

modeling & simulation

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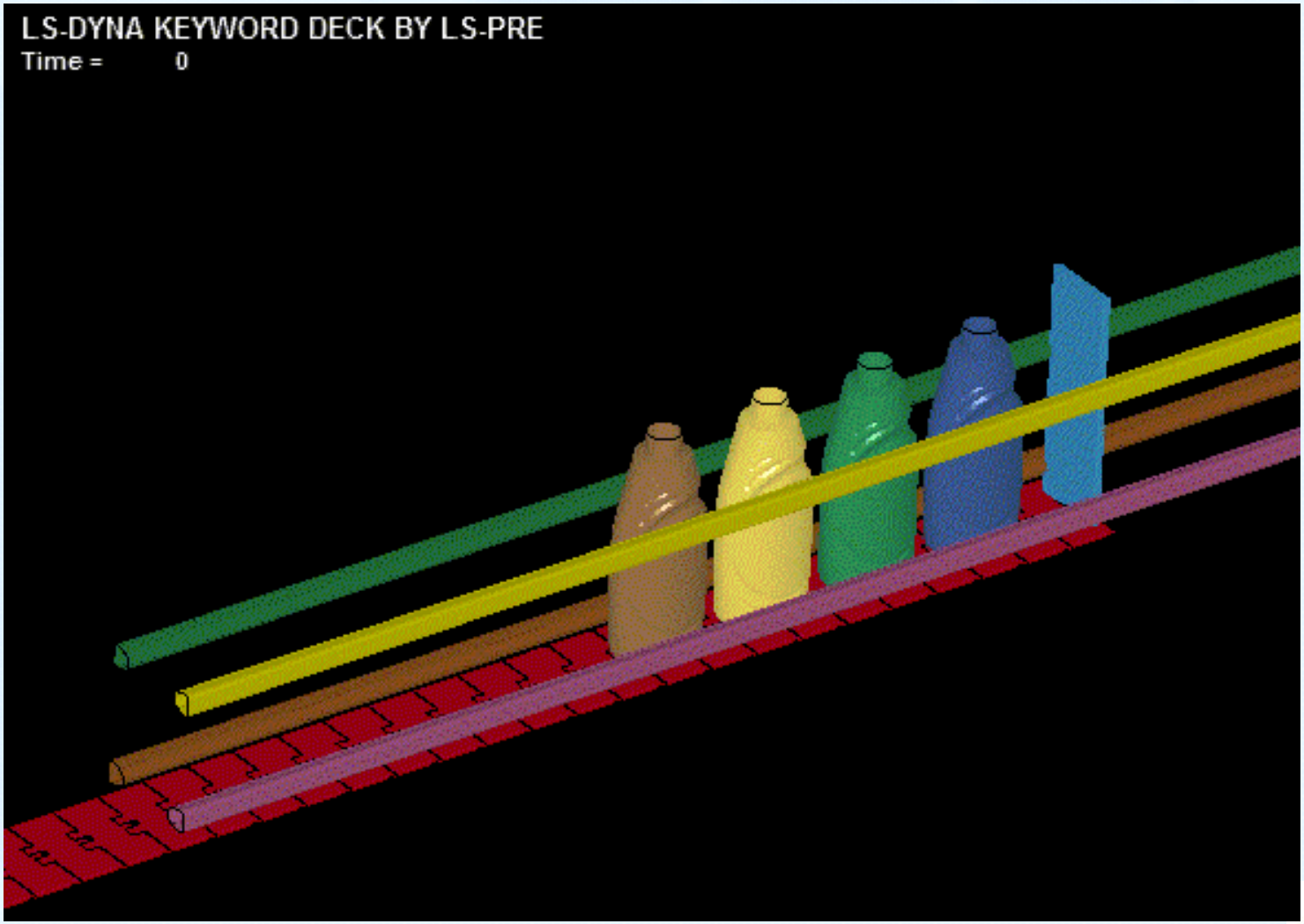
Virtual Race Track



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Fluids / Thermal

- **Computational Fluid Dynamics (CFD):**
  - Free Surface Flow
  - Contained Turbulent Flow
  - Multi-Phase Flows
  - Creeping & Low Reynold's Number Flows
  - Non-Newtonian & Visco-Elastic Material Properties
  - Flow in Porous Media

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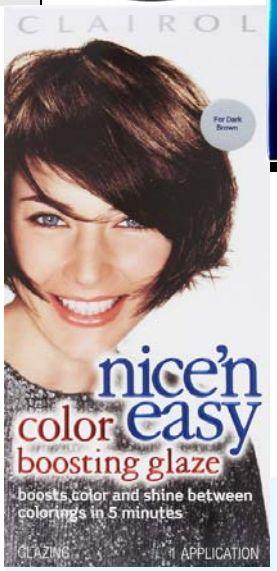
Mixing liquids:



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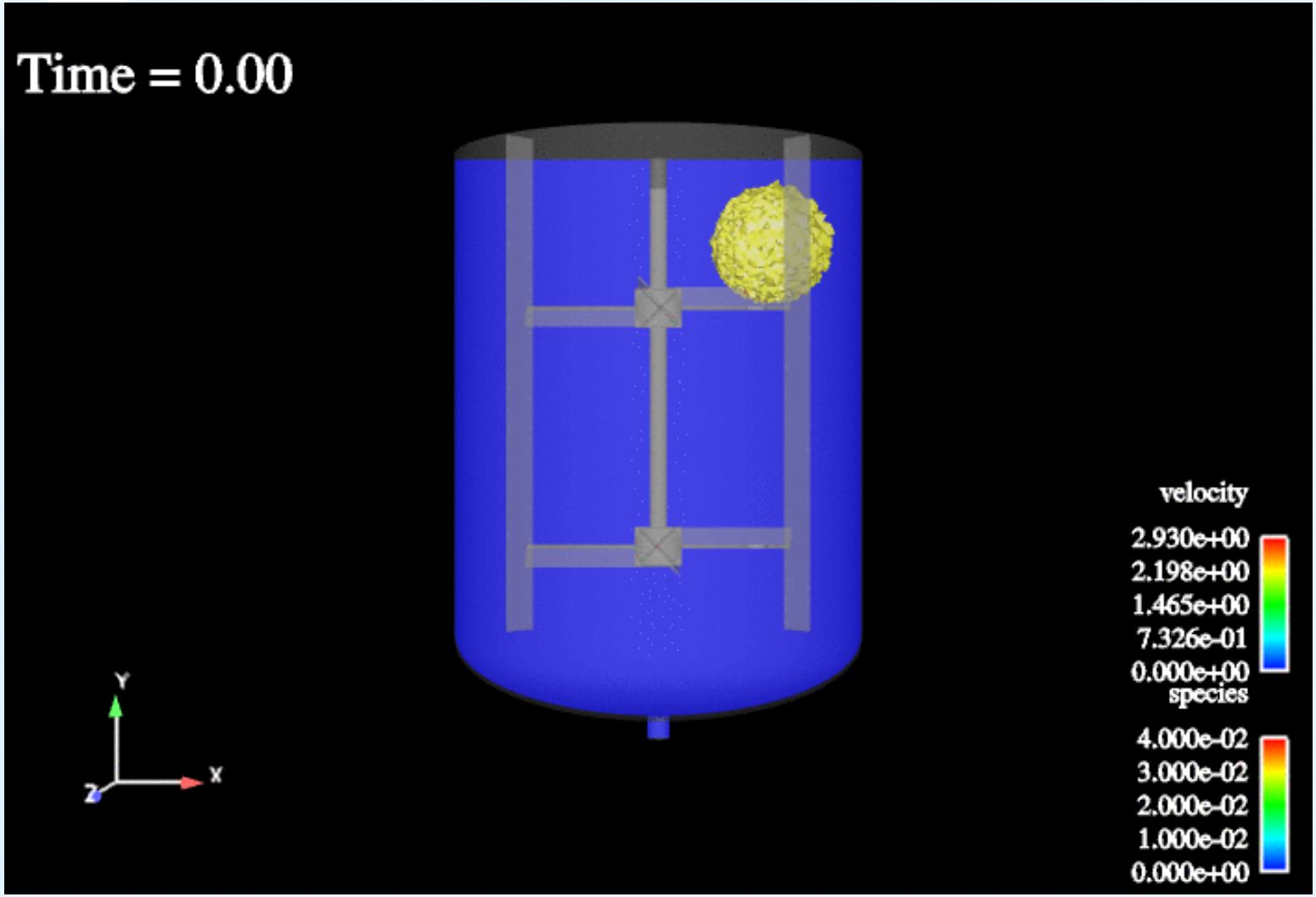
Mixing Dense Viscous Fluids



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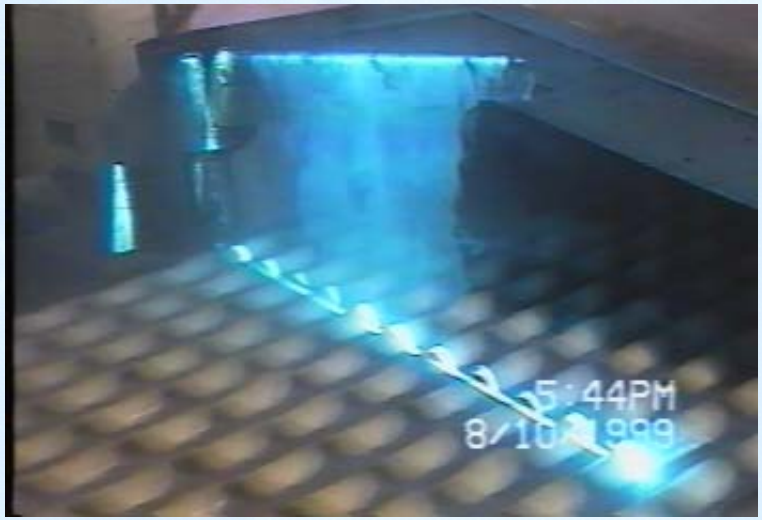
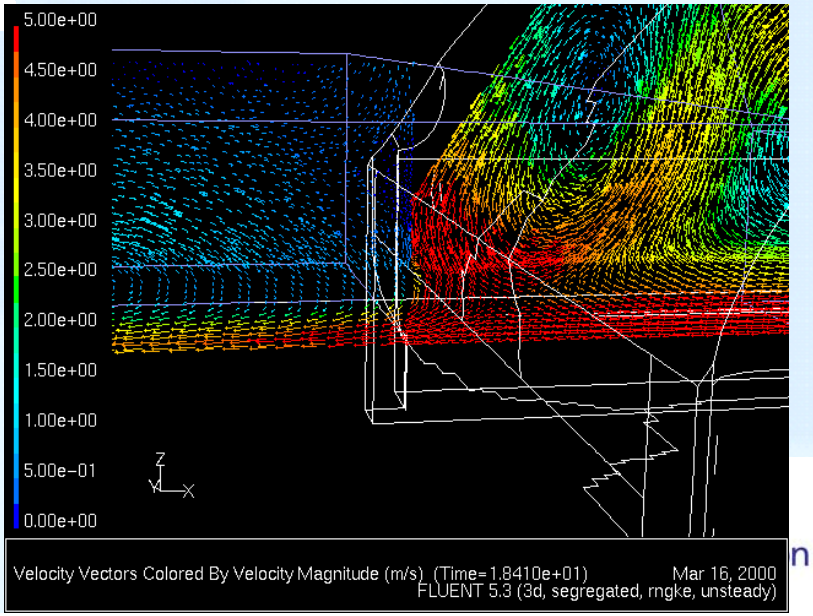
Make a 10^9 Pringles?



How long does it Take to make a **Billion** Pringles?



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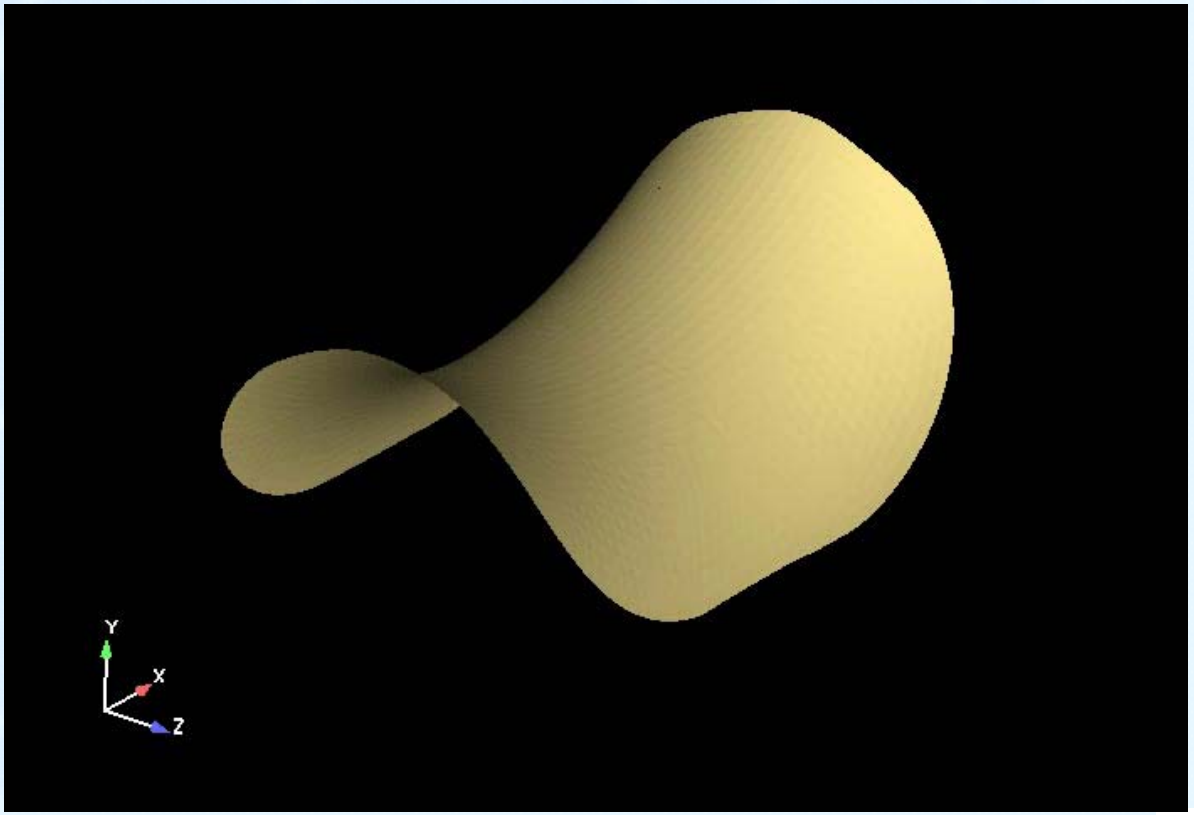
Make a Billion Pringles…

…Aerodynamics are Relevant



modeling & simulation

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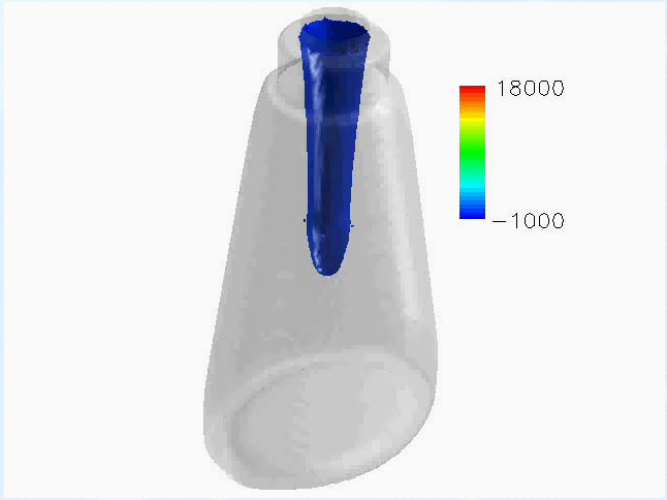
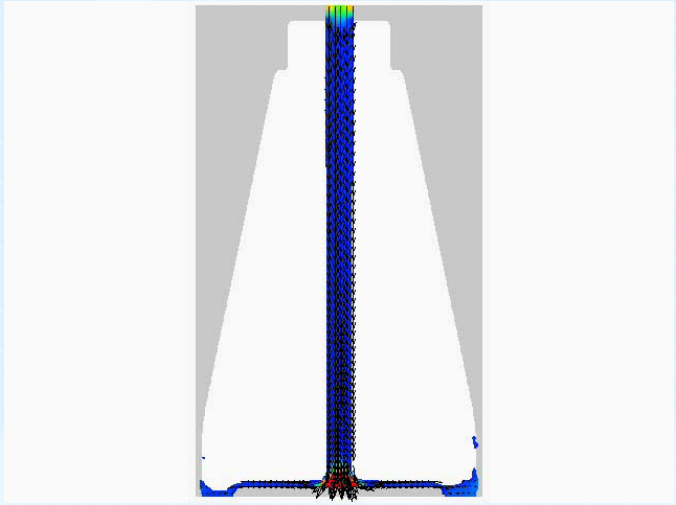
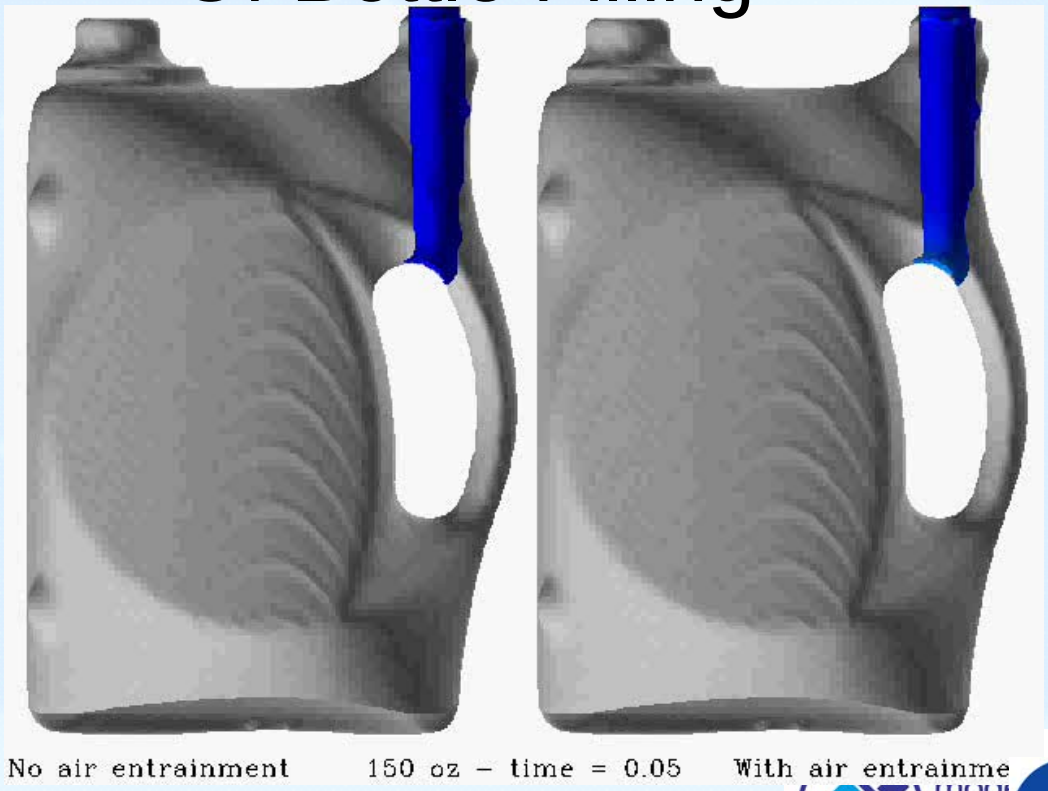
Virtual Filling





Air Entrainment
During Process
Of Bottle Filling



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What are the areas of Challenge & Research?

Multi_Physics…

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Liquid Bottle Drop

What
You
Don't In
WalMart

Or
Your
Laundry
Room!

modeling
& simulation

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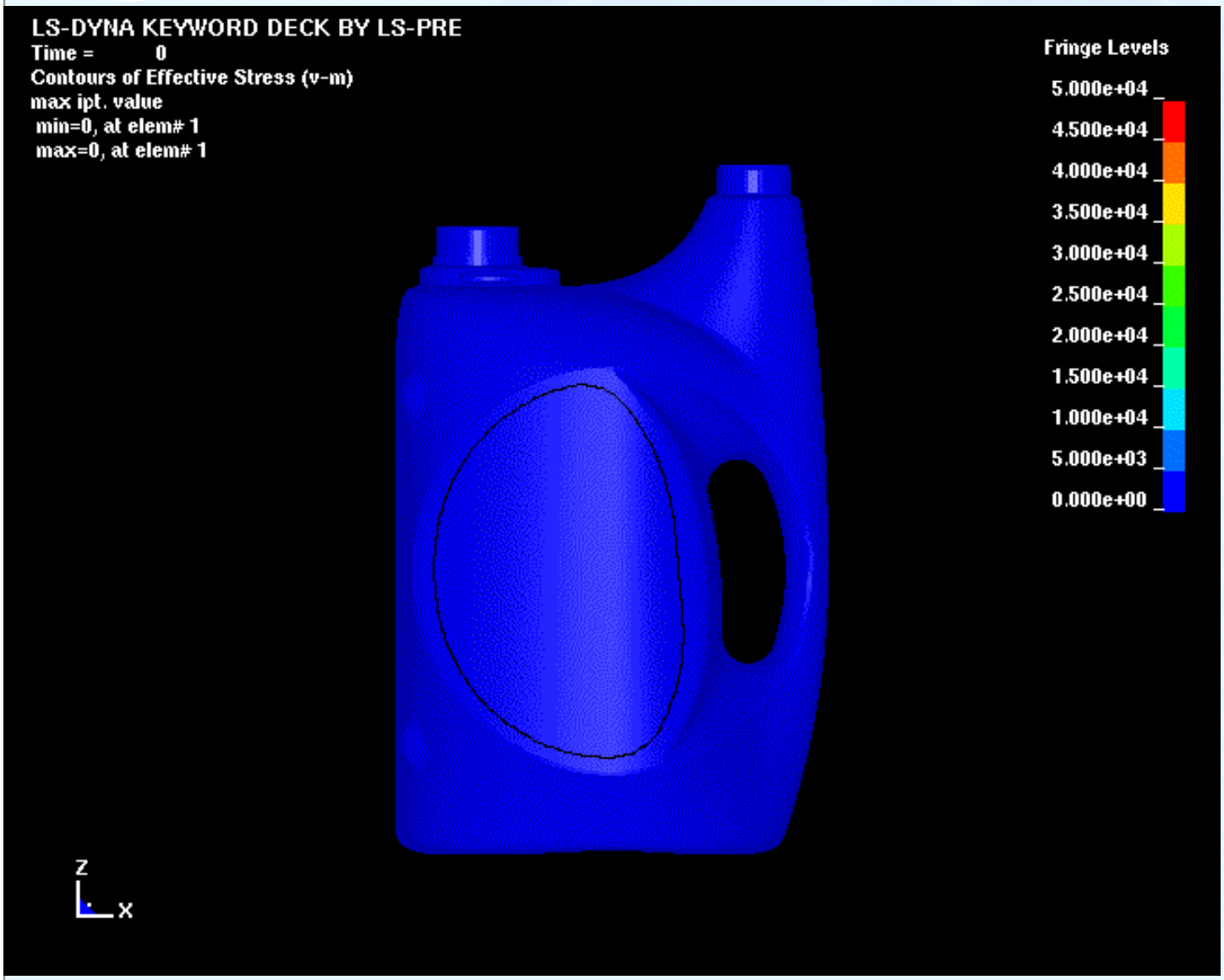
FSI Simulation



Material Properties Are The Key To Predicting Reality!

modeling & simulation

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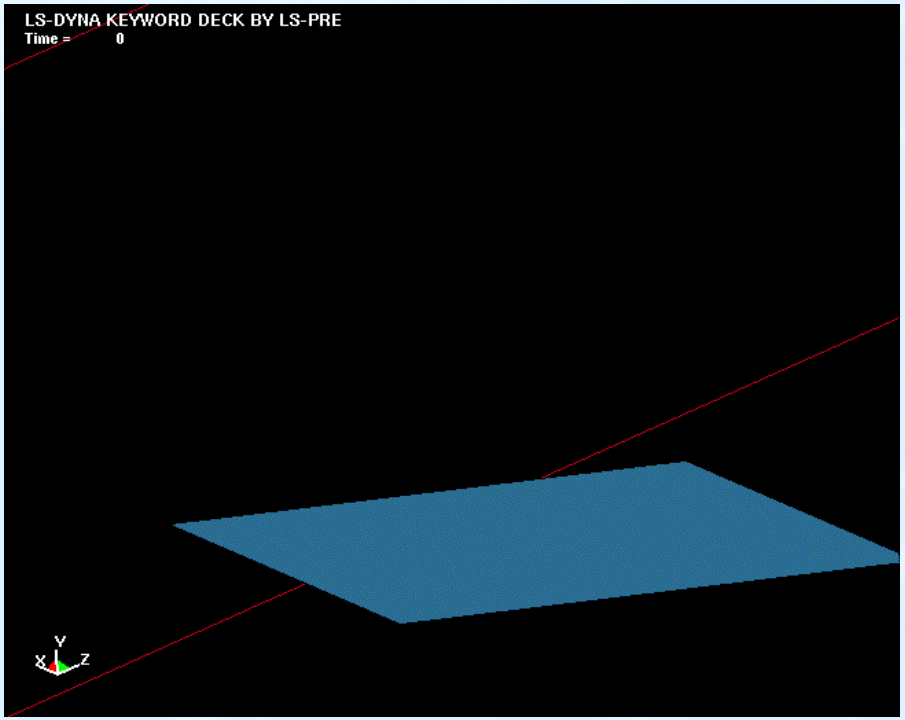
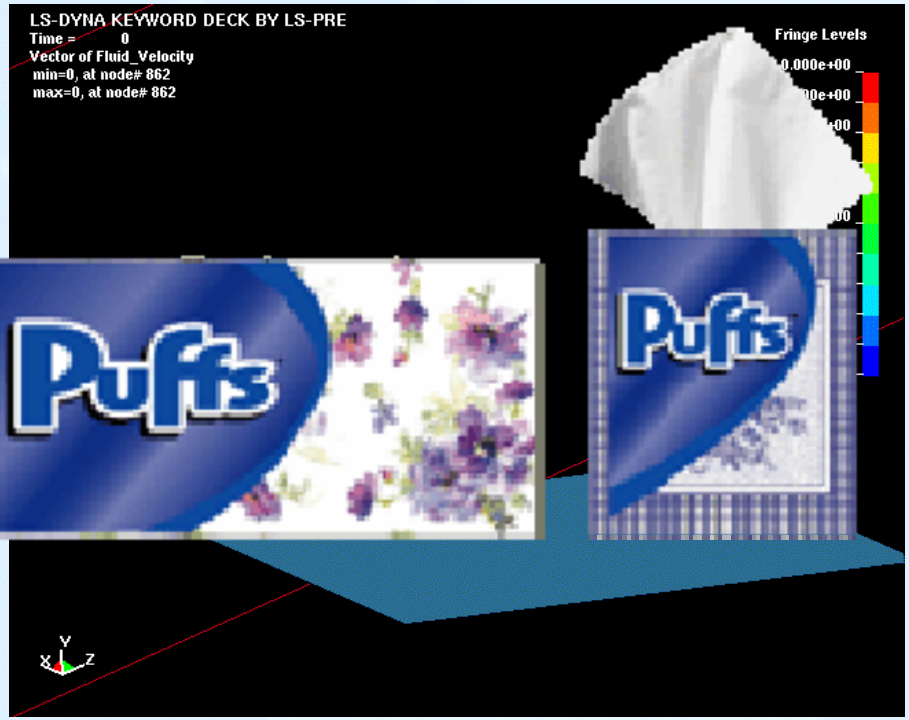
FSI: *Fluid Structure Interaction*



Sheet Flutter



Sheet Flutter
w/flow Field

modeling & simulation

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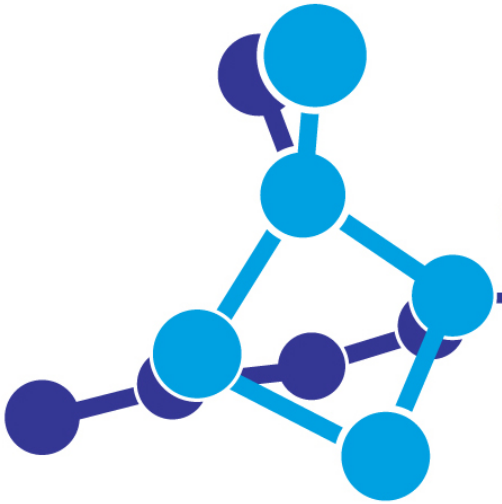
M&S 'Brands'



Computational Chemistry

modeling & simulation

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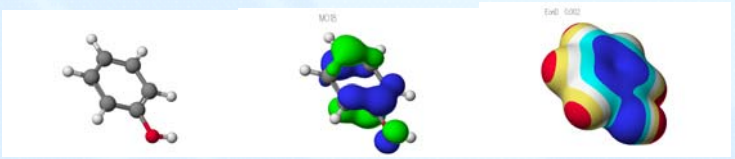
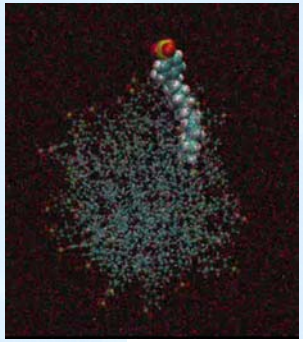
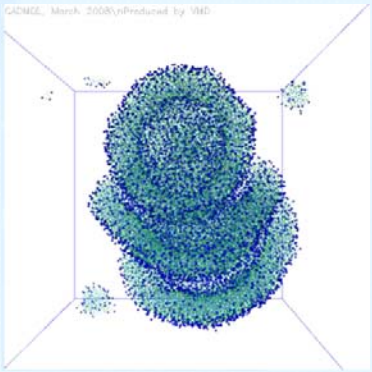
Computational Chemistry Disciplines

Atomistic & Quantum Methods

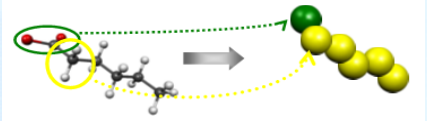


Molecular Dynamics

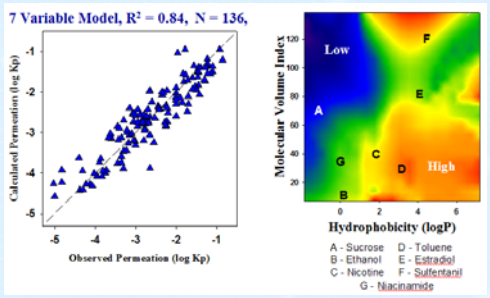




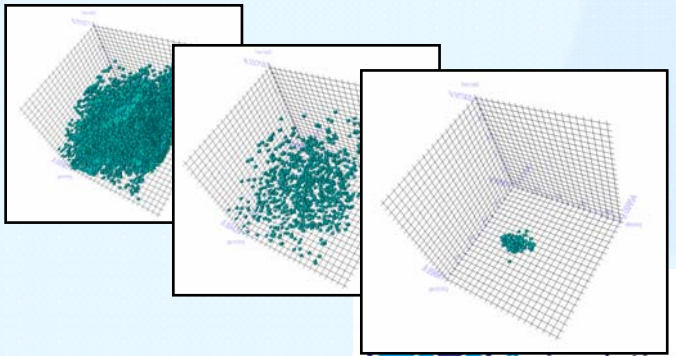
Meso-scale Methods



QSAR/QSPR



Virtual Library Synthesis
Nearest Neighbor Searches



& simulation

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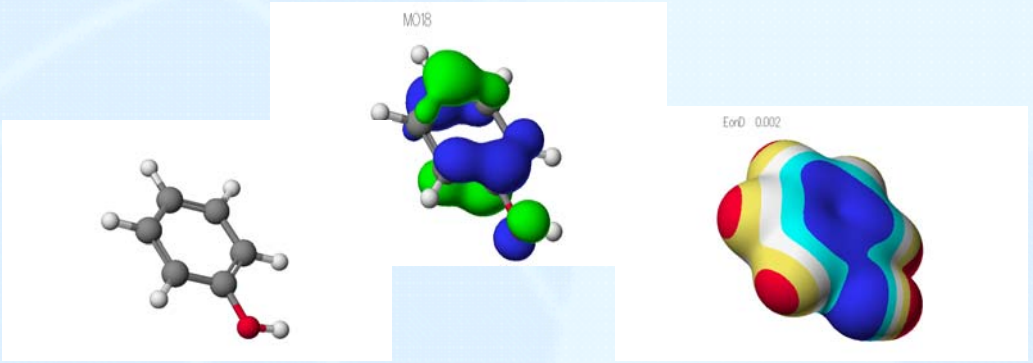
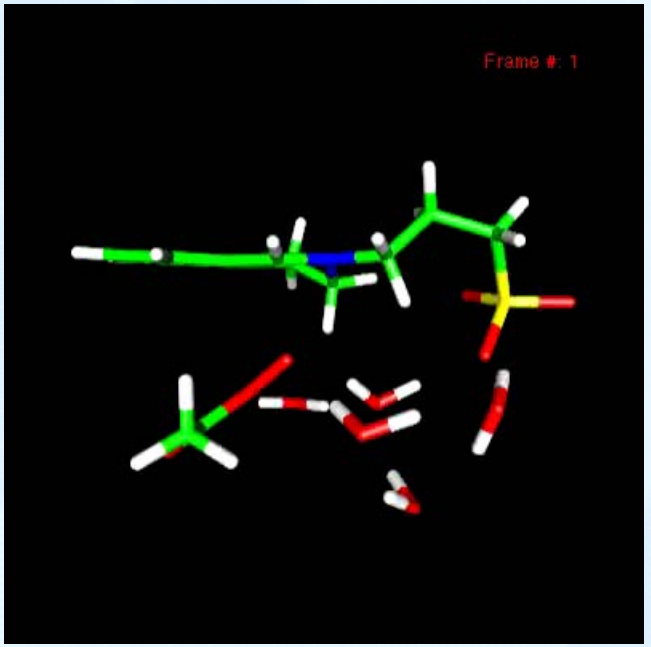
Quantum Chemistry

- **Electronic properties**
  - Reactivity
  - Structural details
  - Spectral properties



- **Femto-seconds, tens of atoms**

- **Challenges: simulating dynamic reactivity**
  (http://loki.na.pg.com:8080/~stein/tmp/every5.mpeg)
  - Hardware capacity
  - Theory (shortcuts) and software development



modeling & simulation

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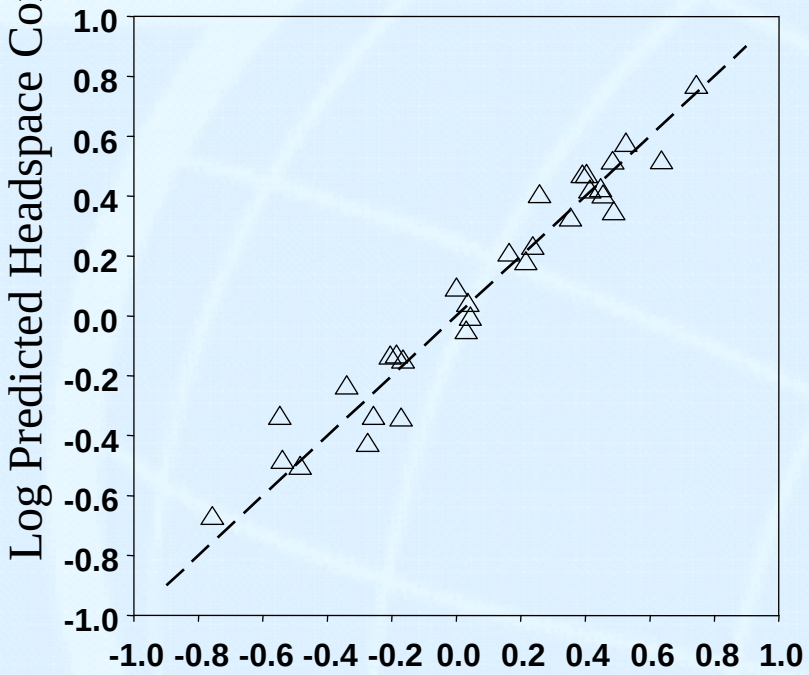
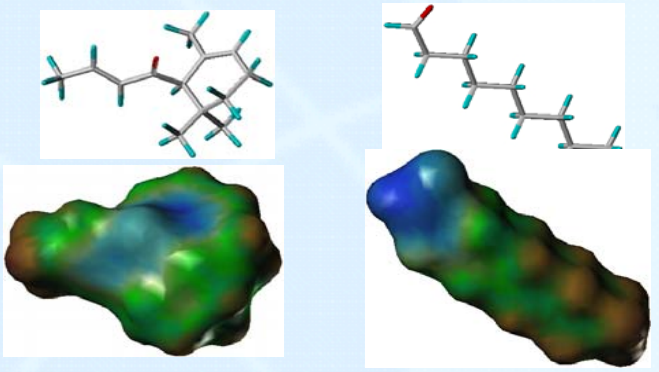
Perfume Residuality QSAR

5 Variable Model, $R^2 = 0.95$
N = 30



Modeling identified new technology which was not apparent from empirical testing

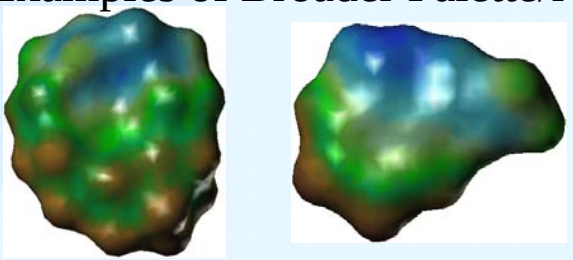
Good **Poor**



Damacenone Undecylenic Aldehyde

➢New Insights: Want Globular Structure with Partially Shielded Oxygen. Not Correlated with Reactivity and Aldehyde/Ketone not Required

➢Examples of Broader Palette/New IP



xxx olide Methyl xxxx

modeling & simulation

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Stability of Complex Fluids

Increasing Age

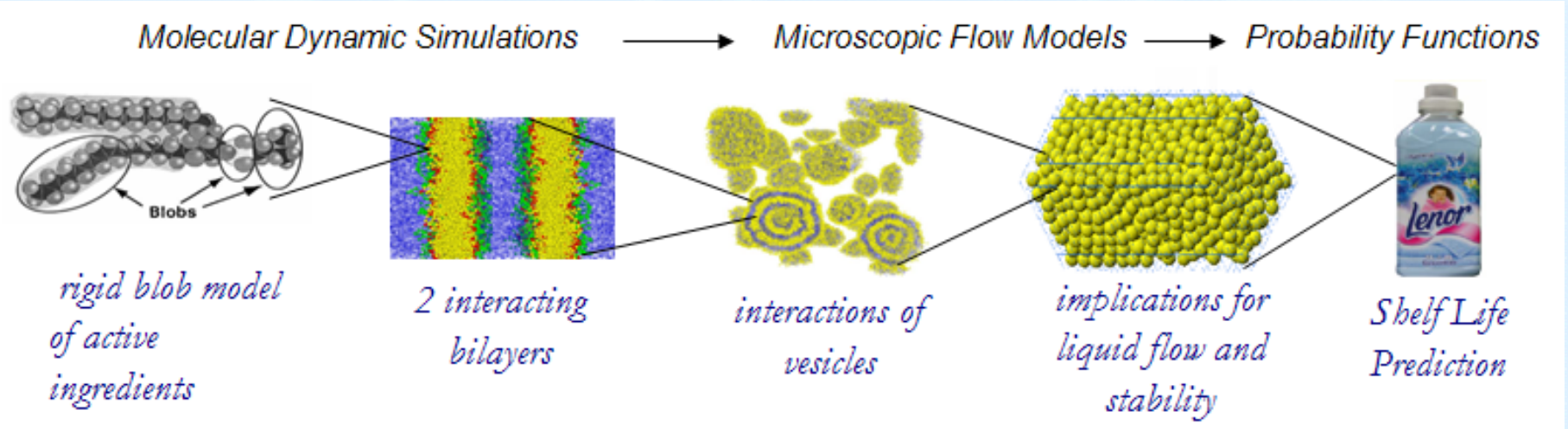
Increasing ‘Phase Separation’

Computational Chemistry

© 2008

modeling & simulation

Multi-Scale Problem: Predict Viscosity Stability



Nano-Meters

Nano-Secs

Centimeters

Months

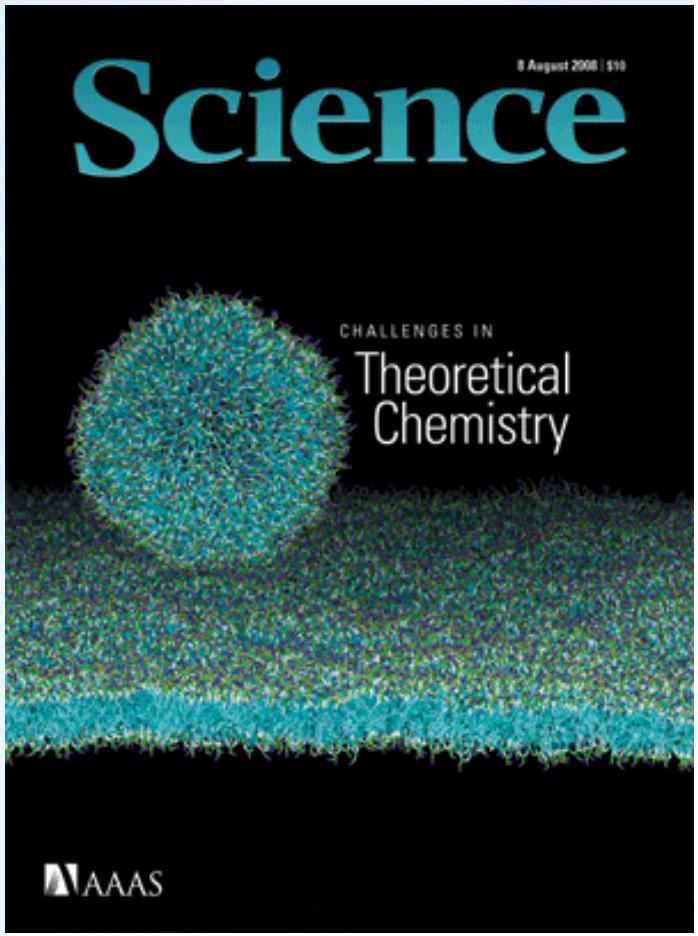
Computational Chemistry © 2008

modeling & simulation

Coarse-Grained Molecular Dynamics of Suds / Cleaning

Kelly Anderson,

Xibing He, Russell Devane,
Michael Klein (Upenn)



Phospholipid membrane…
interacting with a vesicle..

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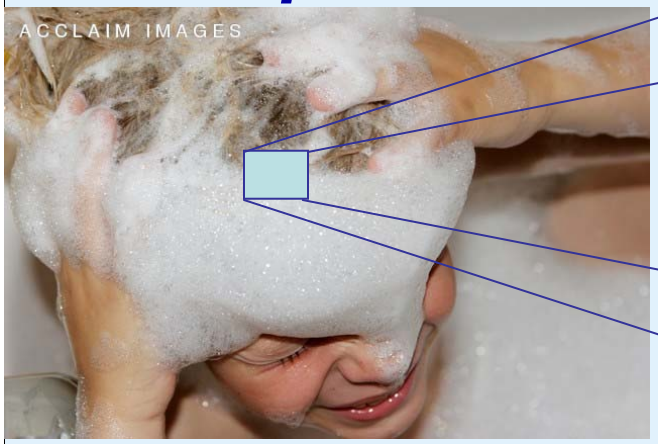
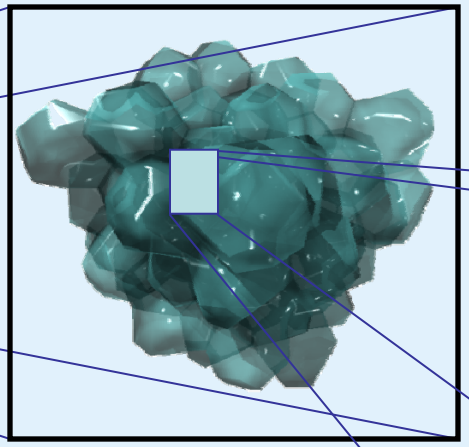
Multi-scale modeling of surfactant lather for shampoos

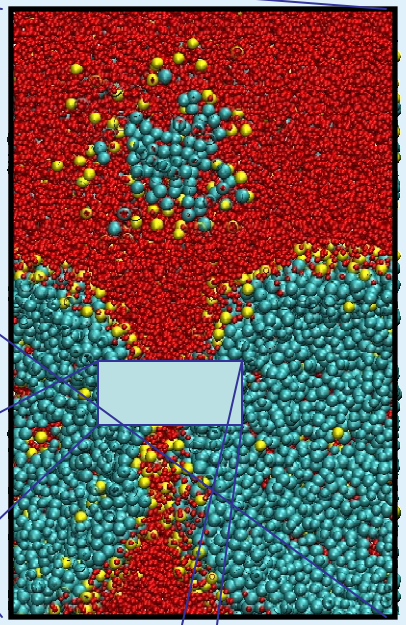


centimeters / seconds

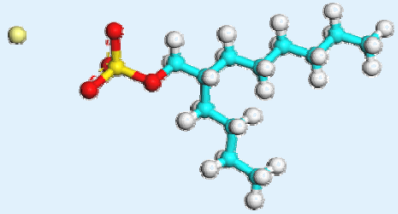


millimeters / milliseconds

micrometers / microseconds

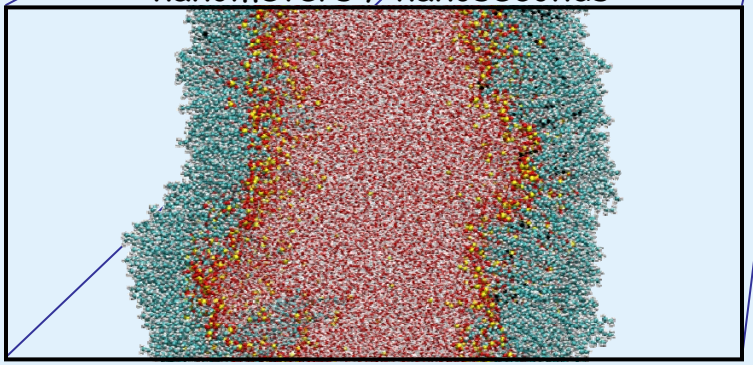


Color codes for Mesoscale / Atomistic simulations:
Aqua; Surfactant tail
Yellow; Surfactant head
Red; Water or Oxygen



New surfactants designed for consumer preference

nanometers / nanoseconds

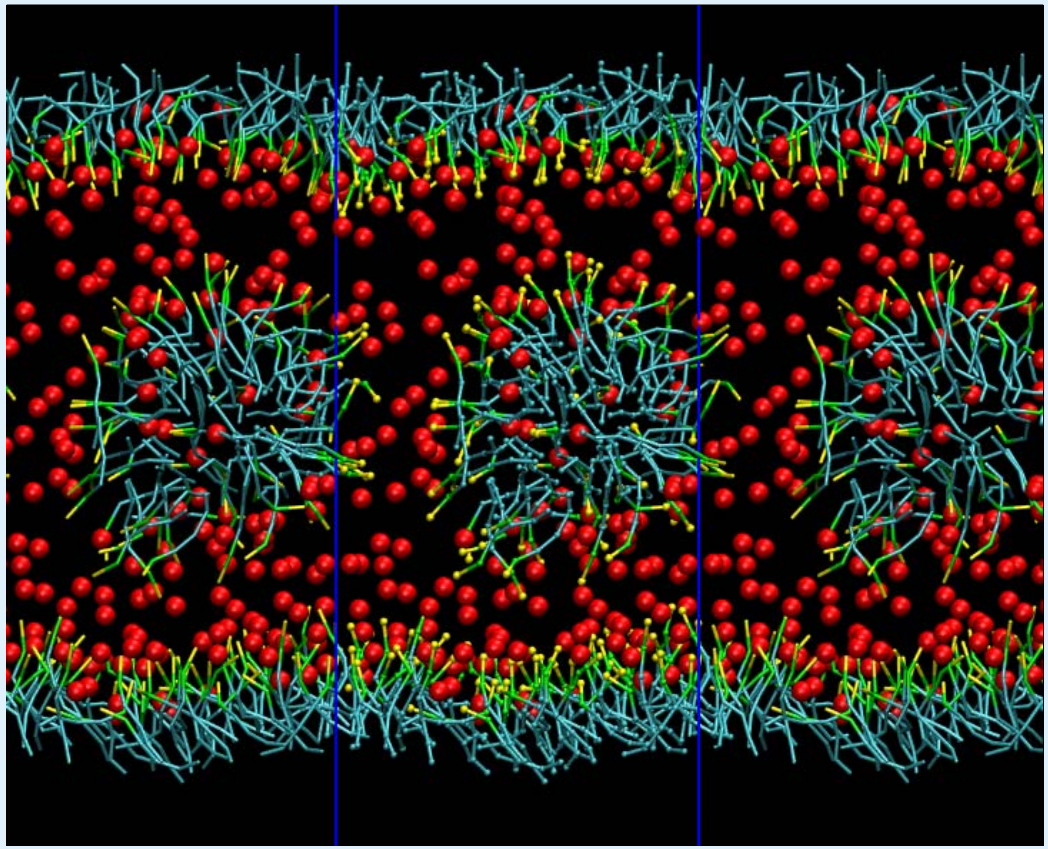


Predicting equilibrium surface structure

Vacuum

Water

Vacuum

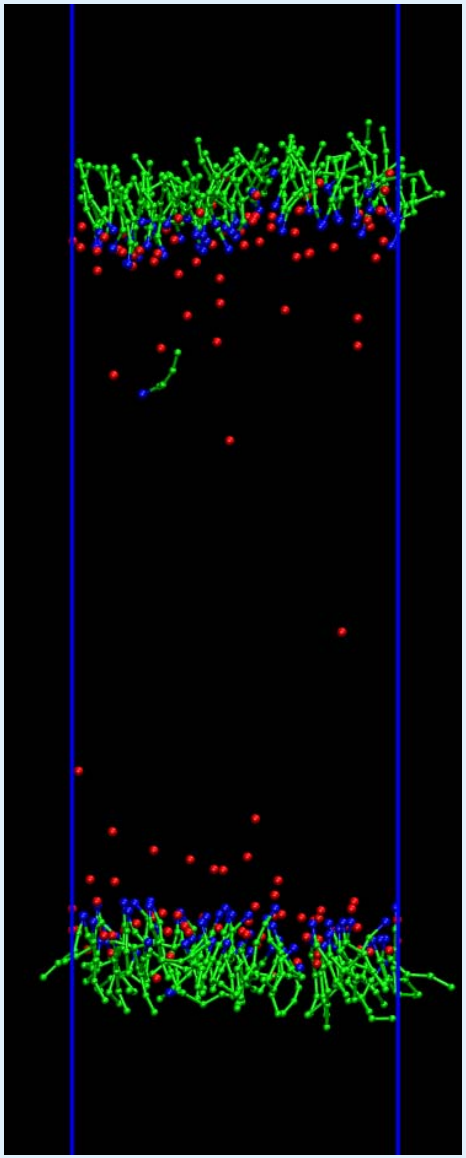


AES
(SLES)

Sodium
Laura
Ether
Sulfate

Blue beads represent alkane chains, green beads represent Ether groups, yellow bead represent sulfate groups and red Spheres represent sodium ions. Water has been removed For clarity.

Predicting equilibrium surface properties

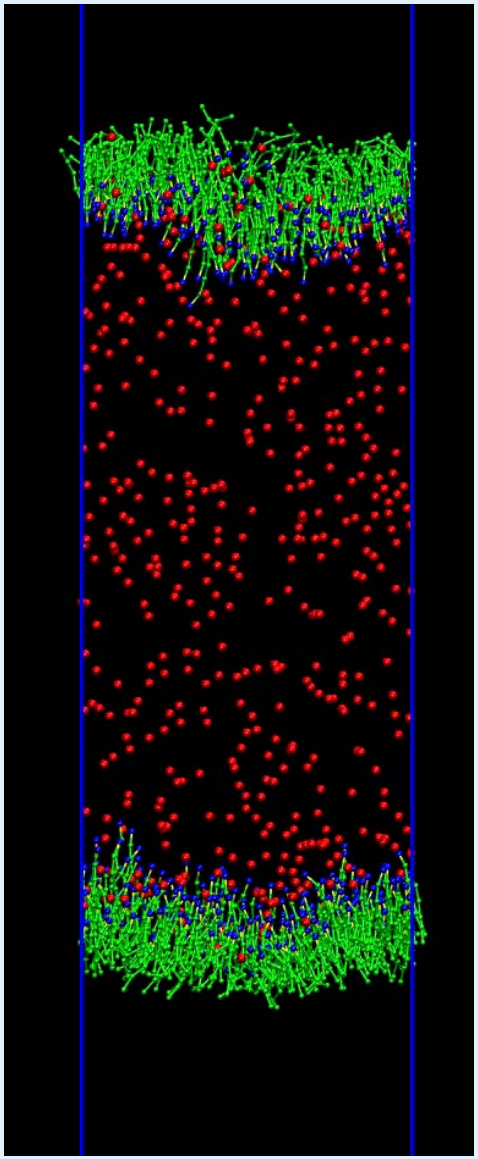


Initial:
Surface Area / Molecule = 45 Å^2

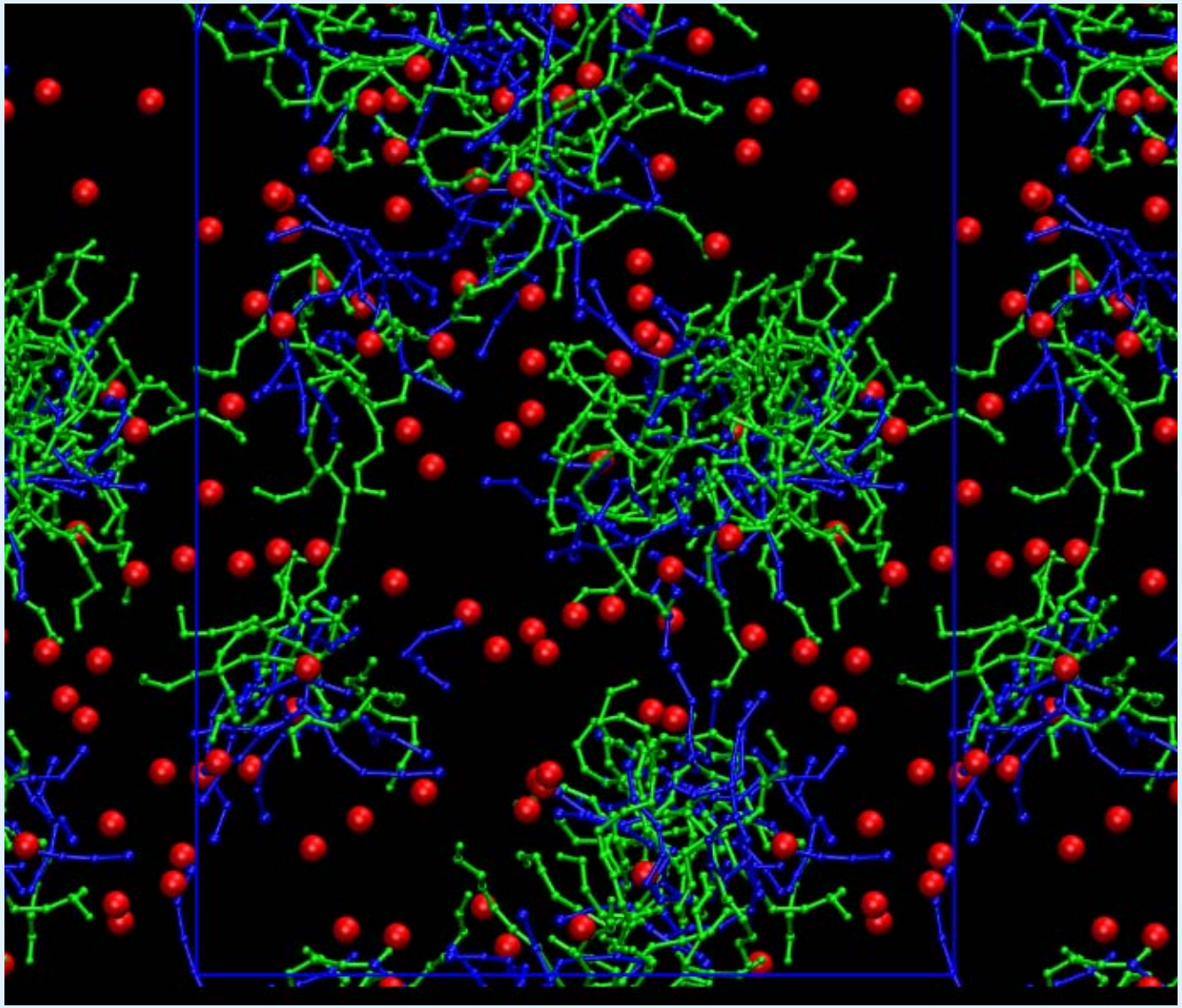
Final:
Surface Tension = 43 mN/m

Initial:
Surface Area / Moldecule= 22 Å^2

Final:
SA/M= 46 Å^2
ST= 45 mN/m



Predicting how mixtures of surfactants behave



PEG C12E6 Phase Transition

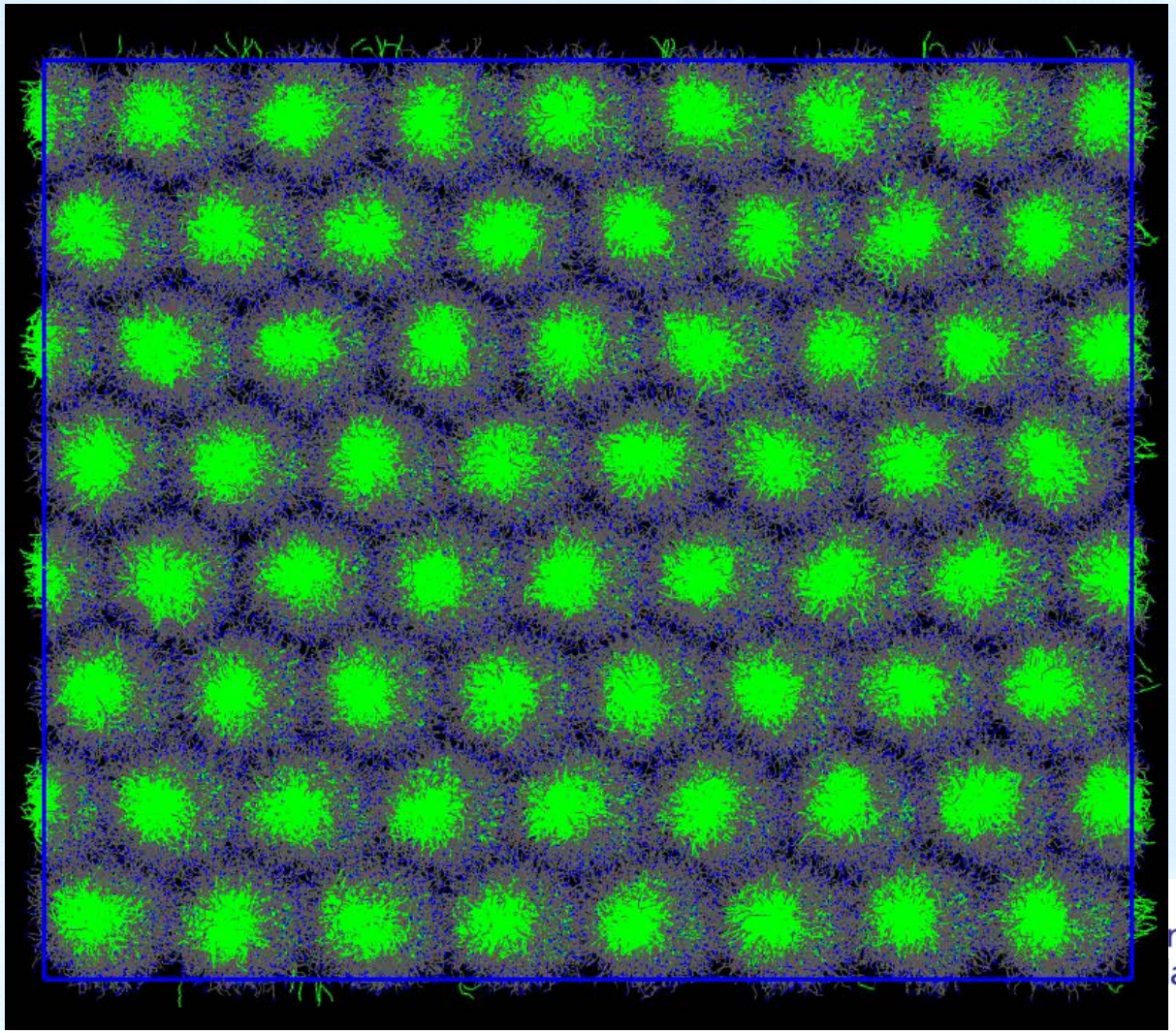
807,360 CG beads
61696 PEG molecules

Start 50 wt% PEG
(Hexagonal phase)

↓ Dehydrate

80 wt% PEG
(Lamellar)

465 ns



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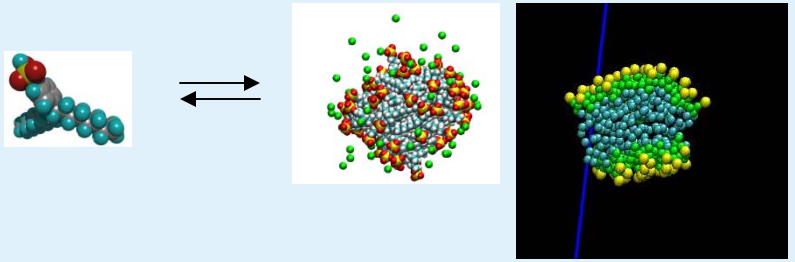
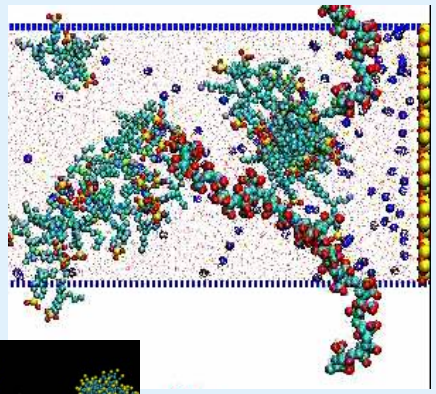
The Grand Cleaning Model

- Micellization:
  - Calcium effects, size, CMC
  - Polymer effects, size, CAC

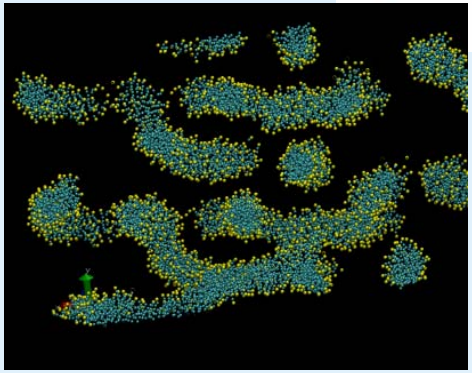


- Interfacial Effects:
  - Calcium effects
  - Polymer effects
  - Surfactant effects
  - Hydrodynamic effects

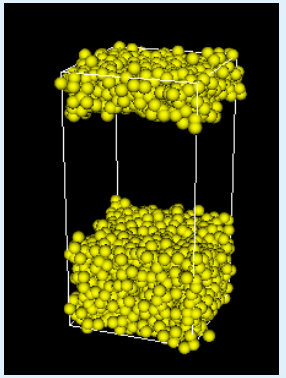


Polyacrylate and surfactant at a clay surface

- ‘Soil’ Removal
  - Emulsification
  - Solubilization

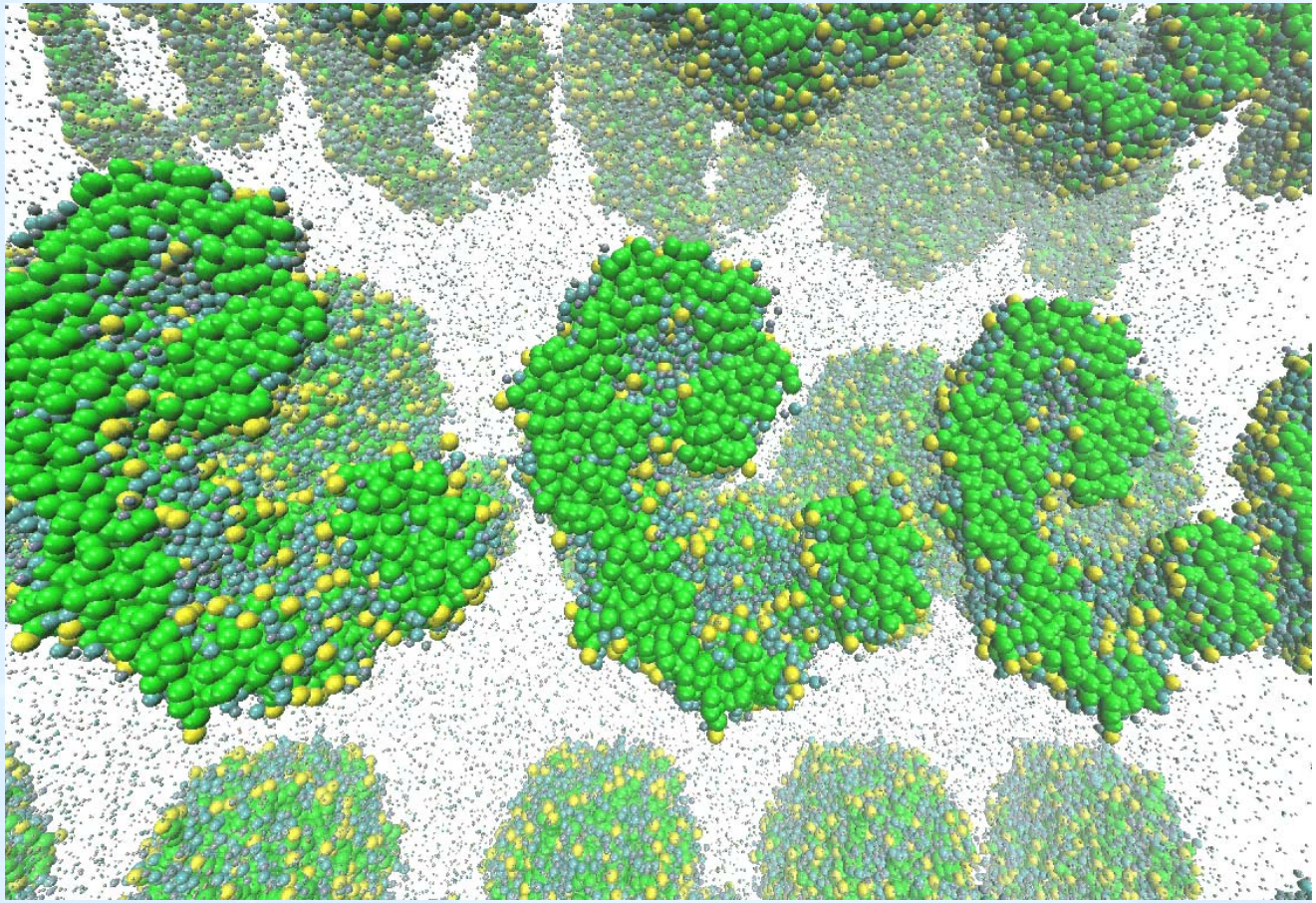


cylindrical micelles



oil-water interfaces

Spontaneous vesicle formation



10 nm Vesicles…

Attempted fusion of two vesicles (cross section). Fusion is not spontaneous!

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The High Performance Computing 'opportunity'

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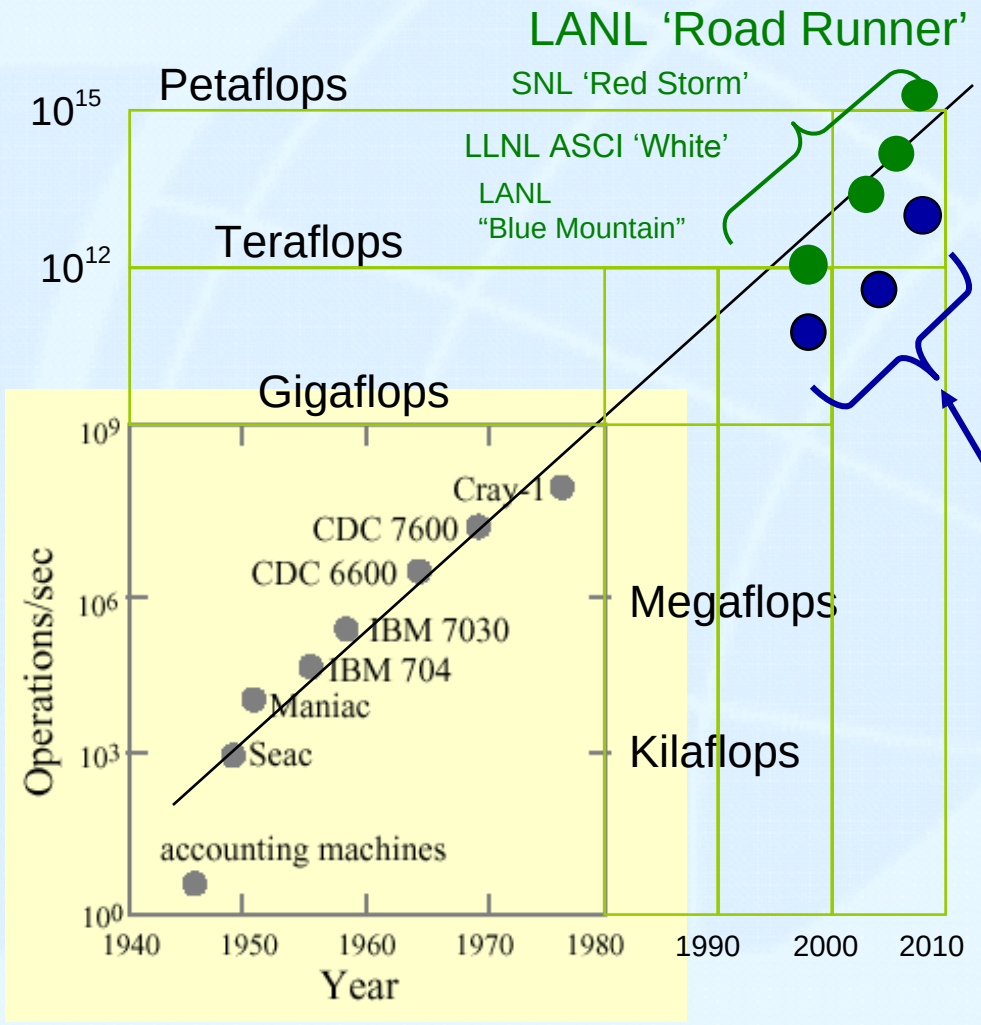
'Moore's Law'

Computing Hardware Performance



U.S. DOE 'Leadership' Class Machines

P&G's 1st, 2nd, & 3rd Generations

modeling & simulation

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Computing Costs $/CPU-hr

- In 2001…Computing (hardware only) cost P&G ~$1.50 per CPU-hr
- In 2008…P&G computing costs (Hdwr, support, facilities…) are ~ $0.15 per Core-hr.
- 2012 Computing (hardware only) projecting to cost ~ $0.01-0.03 per Core-hr.

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Future of HPTC…

What are we going to Do with All that Power?

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How do we cash-in 'moore's Law?

modeling & simulation

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How do we cash-in ‘moore’s Law?

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Pursuing Realism???

- Solve ‘Bigger’ more complex Problems (Billion Elements, Billion Atoms/Molecules…etc.)
- do parametric studies vs. point estimates (Stochastic)
- Reach more analysts … Automating what it takes an expert to do today

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The Challenge?...

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The Challenges

- Application Software
  - Parallelism
    - Spatial AND
      - Is Temporal Decomposition Possible?
  - *FAST* Multi-physics Integration
  - The path from Basic Research to Commercial
- The DATA management issue…
- Education …
  - Engineering & Science Graduates that are ‘computational’ aware (BS/MS)

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