Complex Engineered Systems at Procter & Gamble

September 5, 2012

Tom Lange Director, Modeling & Simulation Corporate R&D

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Investors Know P&G …

- Large, Global, & Successful Consumer Goods Company
  - Sales: $83.7 Billion FY June 30th, 2012
  - Net Earnings: $10.8 Billion
  - 4.2 billion Consumers purchase a P&G product about 40 Billion Times a year.
- We consistently build lasting shareholder value

  Founded in 1837…Celebrating our 175th
  - P&G has paid Dividends without Interruption since 1890
    - (one of only 9 publically traded companies to have done this)
  - 56 consecutive years of Increasing Dividend Payments
    - (6 companies to have done this)
  - $ 88 billion of cash returned to shareholders of 10 years
    - (90% of reported net earnings)
  - Market Cap ~ 189 billion COB 8/28/2012
- We Innovate to Grow:
  - Invested over $2 Billion/yr in R&D…in 2012

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P&G *Consumers* … Know Us by Brands

Beauty & Grooming

Health & Well-Being

Household Care

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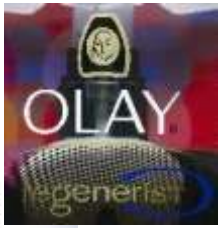
25 Billion $ Brands



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Why Brands?

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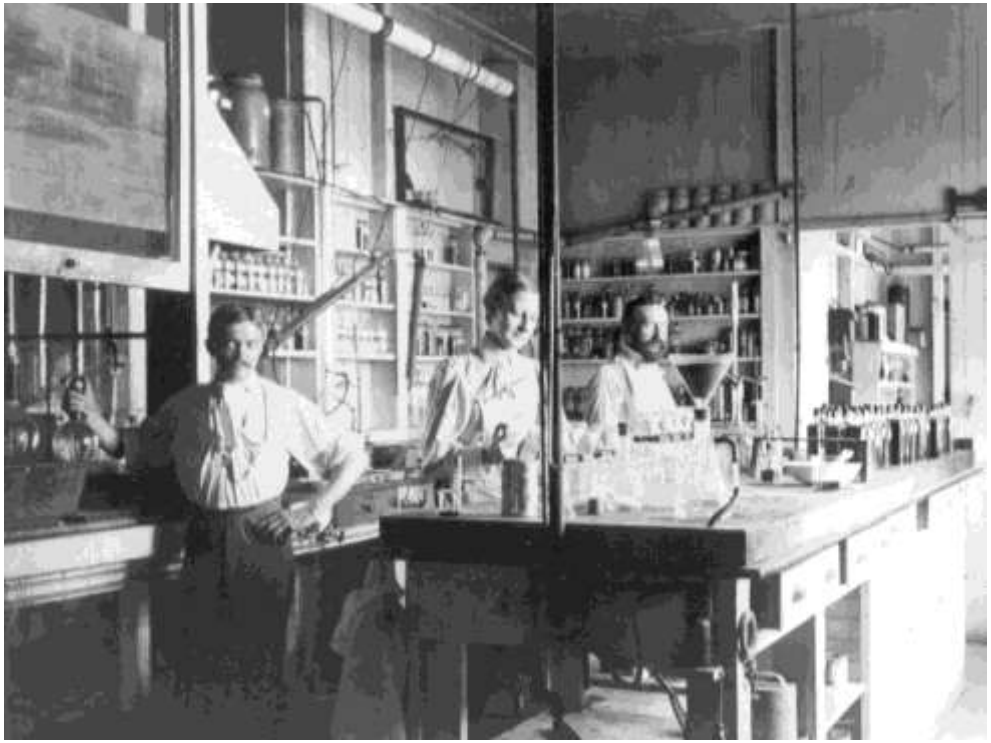
The Two Moments of Truth

‘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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Why the *"rocket science"*?

For such everyday things?

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Challenges of Making Everyday things…

Contradictions & Scale

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Product Contradictions…

- **Products must *perform* …**

- ***Performance* … is driven by Fundamental Science & Engineering <u>Contradictions</u>.**

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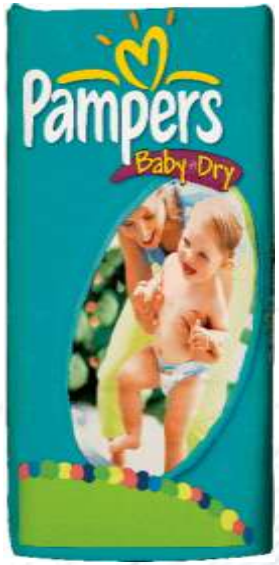
Innovation & Contradictions…

Materials …

- strong but soft
- stretch not break,
- breath but contain,
- break…not tear.



Packages …

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

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More Contradictions…

Formulations …

- protect fabrics … but remove stains.
- Be compact, but used easily.

Liquids …

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

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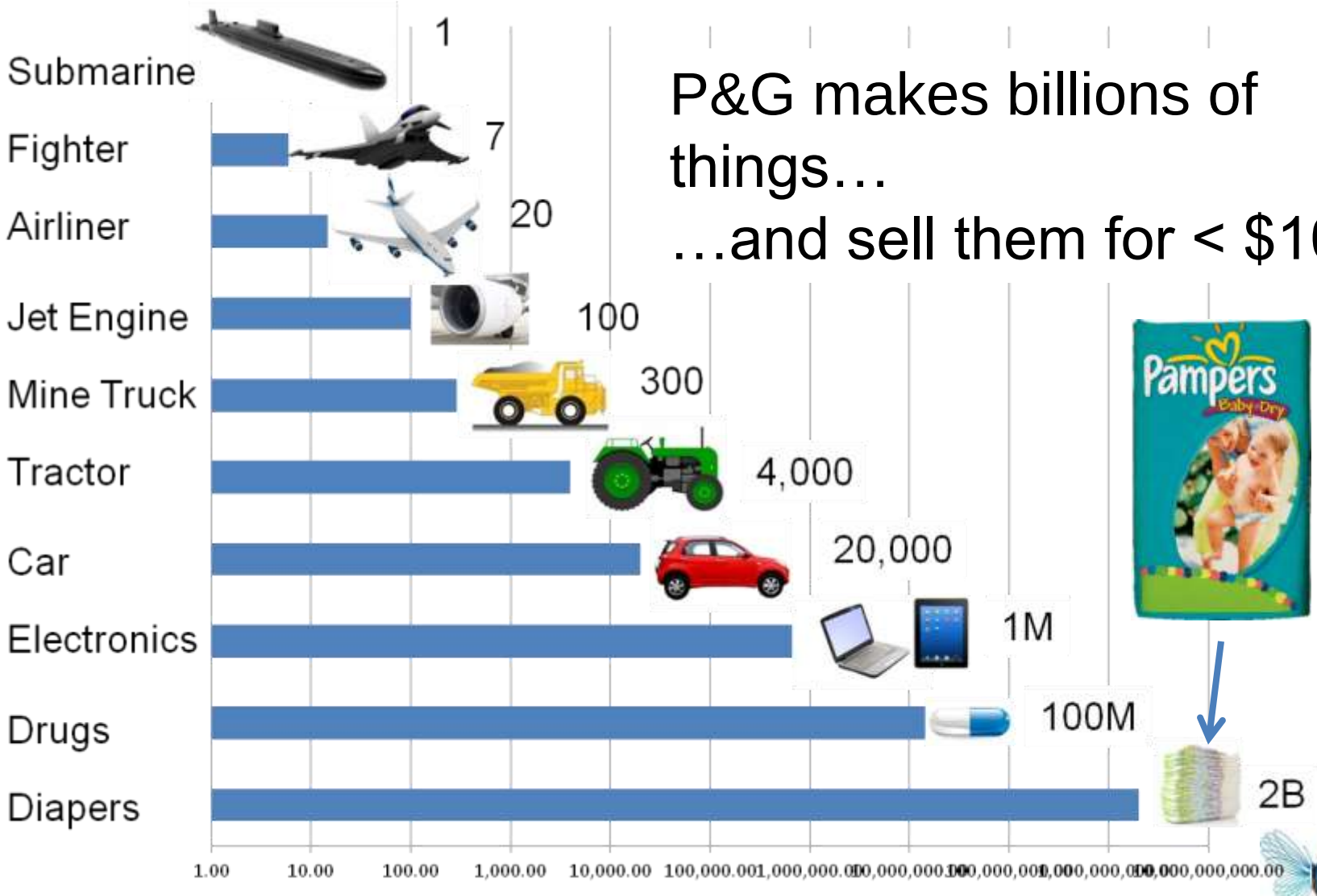
Scale: How to Sell $1B



P&G makes billions of things…
…and sell them for < $10

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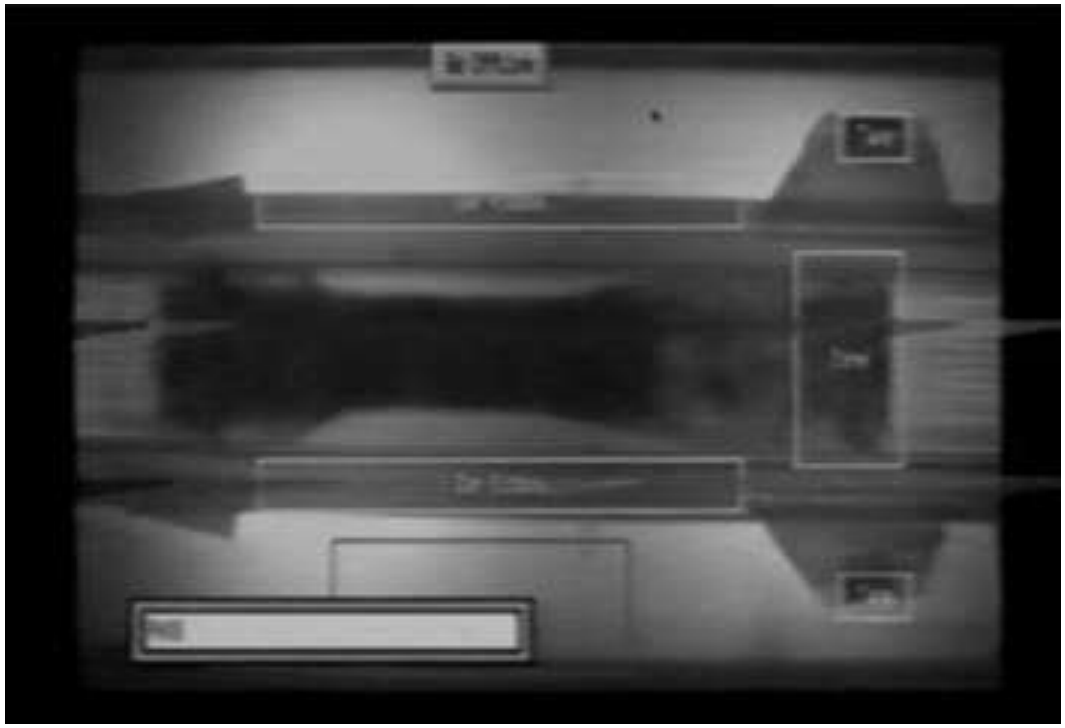
Make a Billion Diapers…

How many Pampers do we make in the blink of an eye?



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Innovation Cycle

Design it

Build it

•Fly it

•Crash it

•Fix it

"Learning" Loop

Outcomes

- **Costs too much:**
  - **-One-time-use Equipment**
  - **-Testing Infrastructure**
- **Takes too long:**
  - **-Cycles of Prototypes**
  - **-Development is Sequential**

Products are <u>not</u> innovative:

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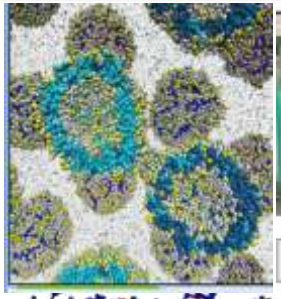
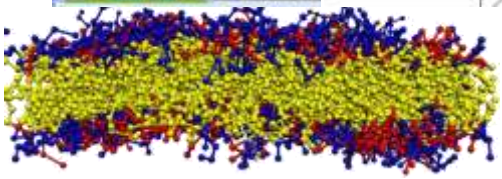
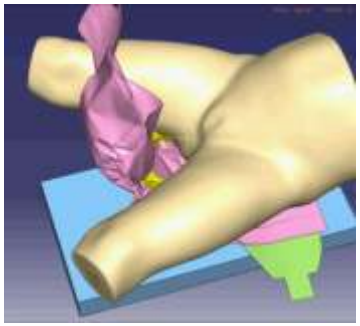
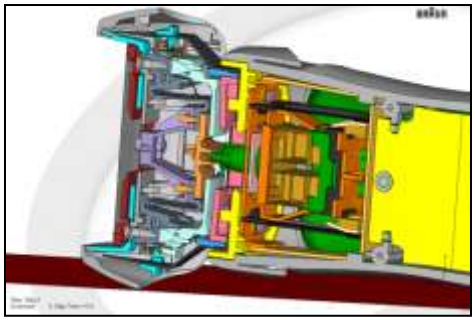
…Atoms to the Enterprise

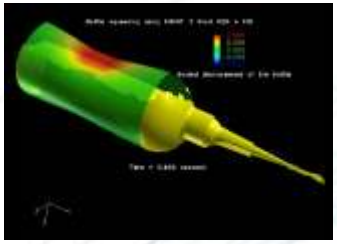
Product/ Materials/ Device/ Package



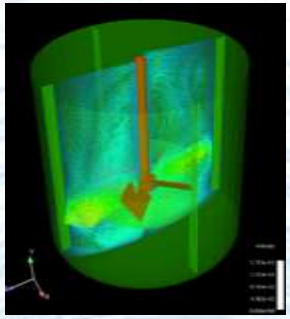


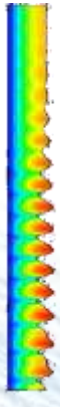


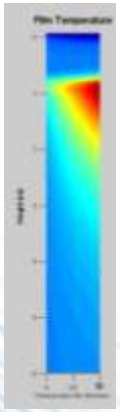


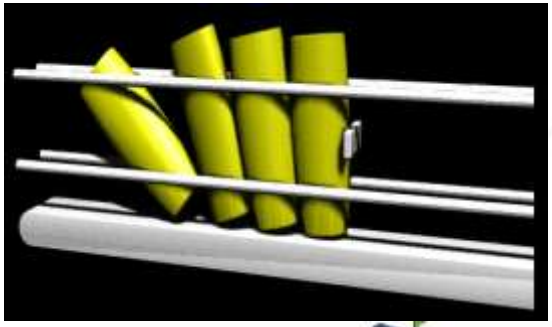


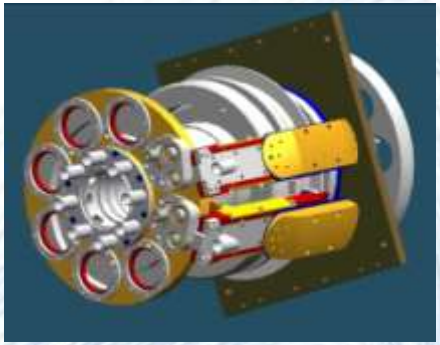
Process

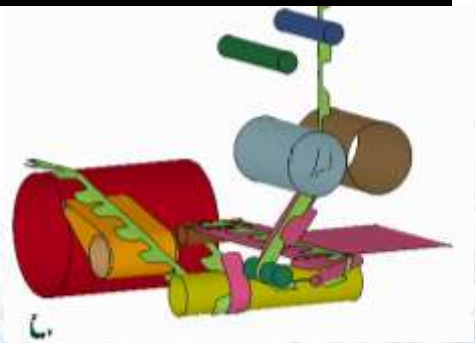




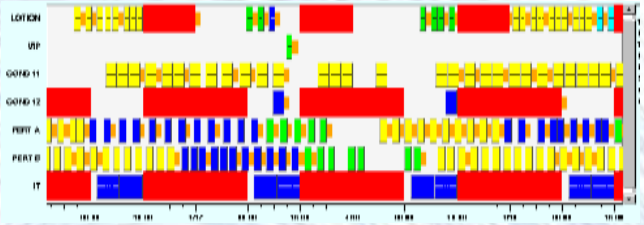








Production Plan & Schedule, Reliability



Converting & Machines

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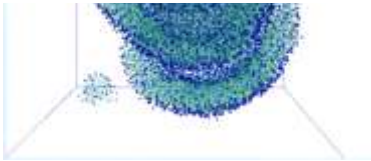
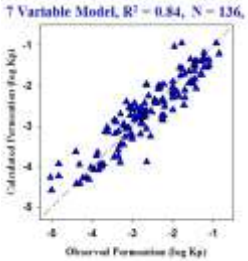
Computational Chemistry Disciplines

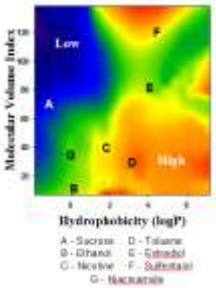
Computational Chemistry

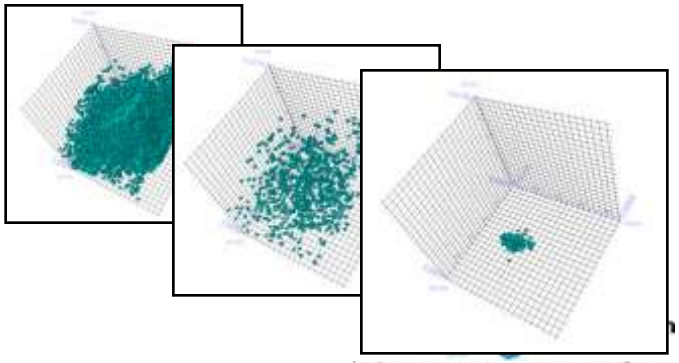
Meso-scale Methods



QSAR/QSPR







Virtual Library Synthesis
Nearest Neighbor Searches

Computational Chemistry

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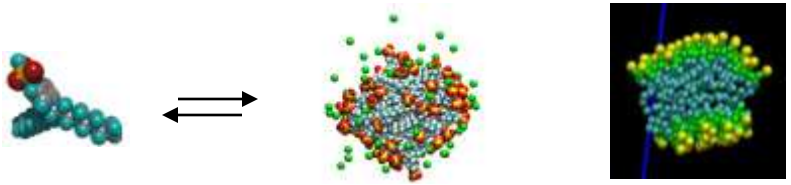
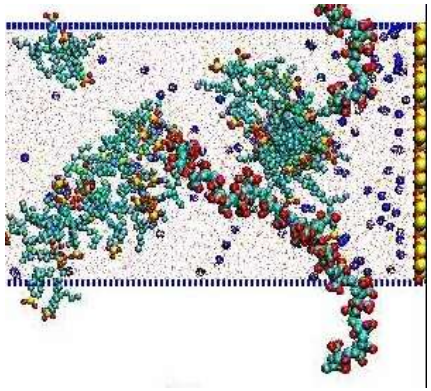
Performance Areas of Interest

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



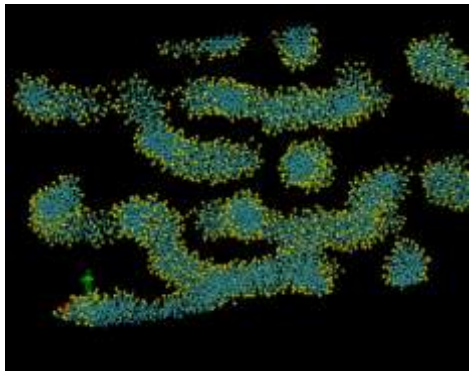
Spherical or lamellar (bilayer)

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

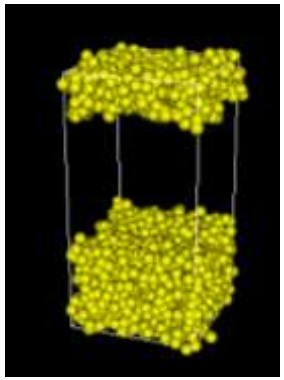


Surfactant at a clay surface

- 'Soil' Removal
  - Emulsification
  - Solubilization



cylindrical micelles



oil-water interfaces

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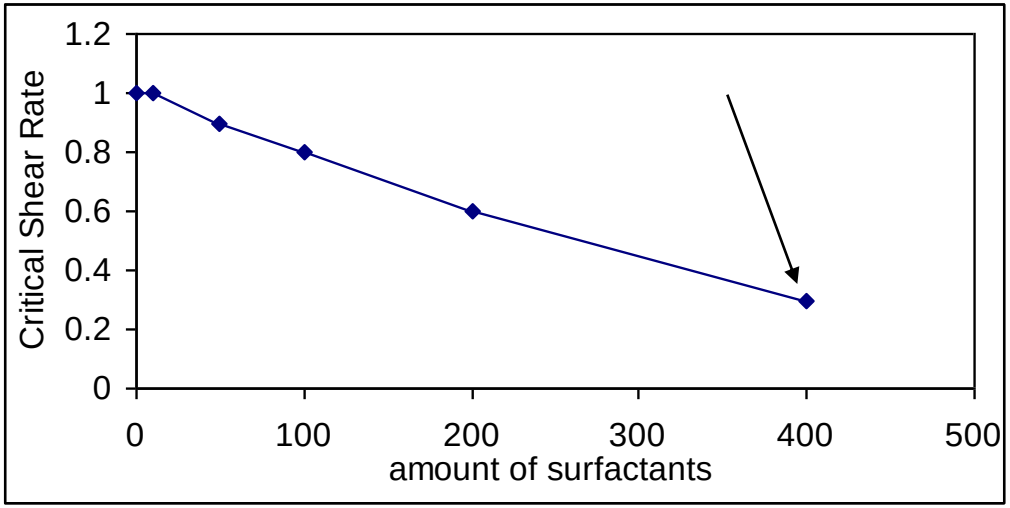
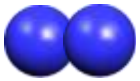
‘DPD’ Simulated Effect of Surfactant on ‘Detergency’



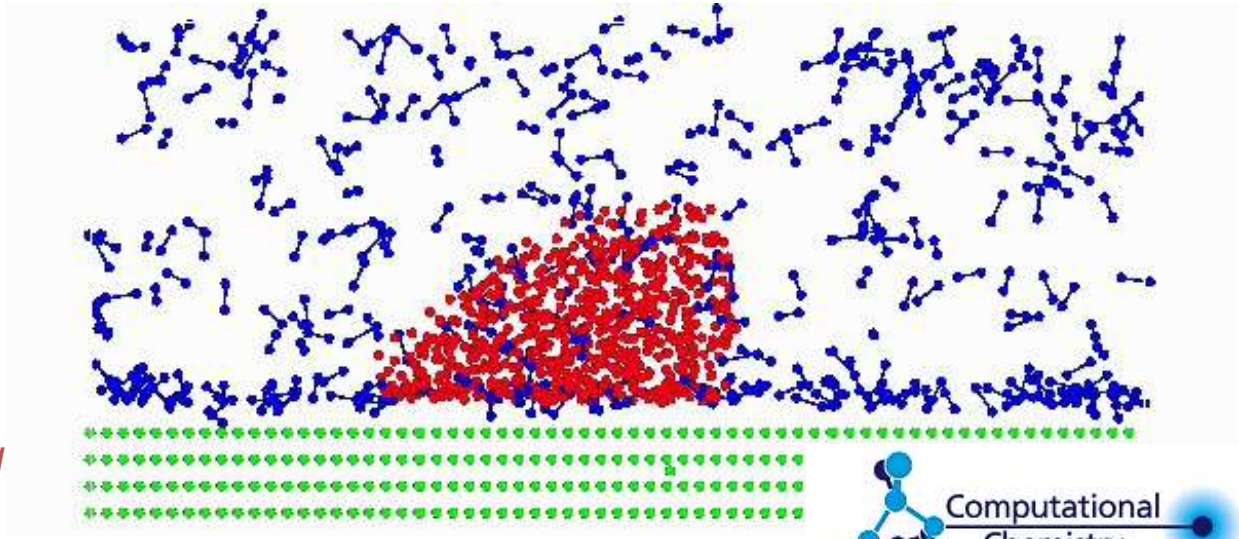
Shear Rate to Remove Oil Droplet



H-T surfactants

Oil bead

Solid bead



removal of a 90º contact ang droplet with 400 Surfactants

Computational Chemistry

CADMol

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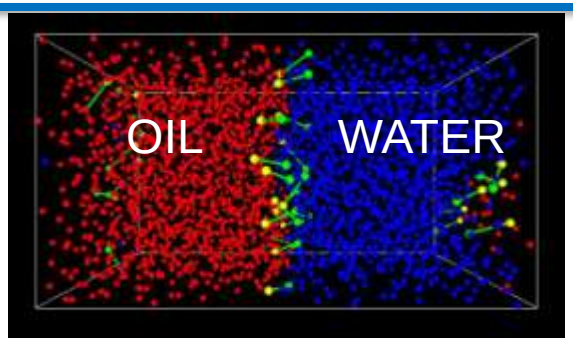
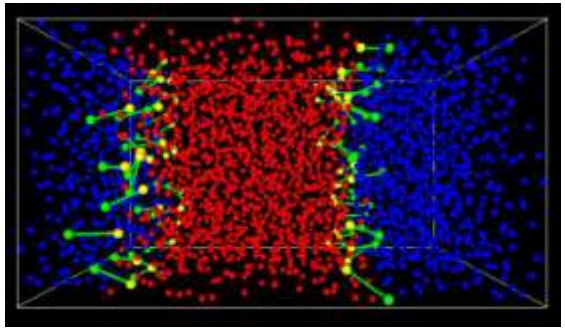
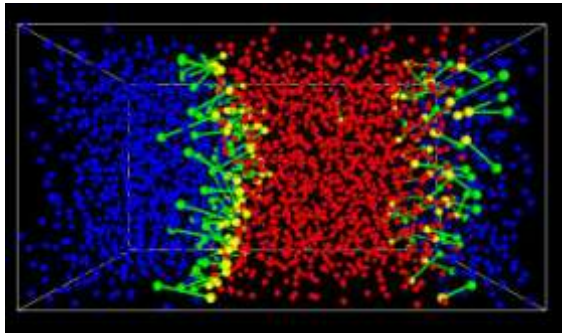
Mesoscale of Interfaces



(a) 1% surfactant

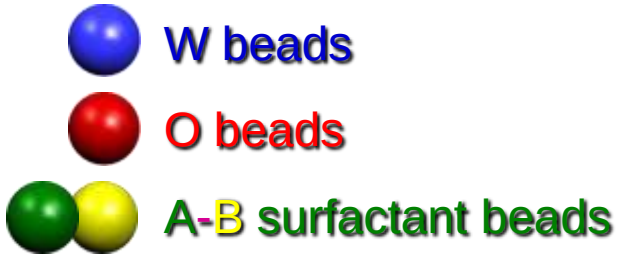


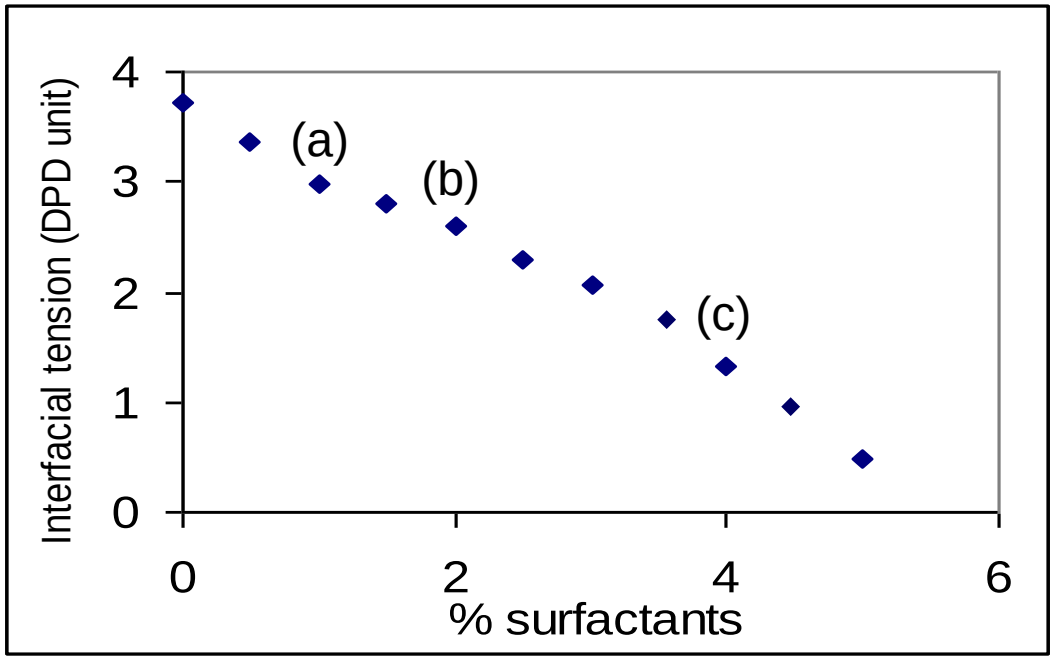
(b) 2% surfactant



(c) 4% surfactant

For Water/Oil/Surfactant system:





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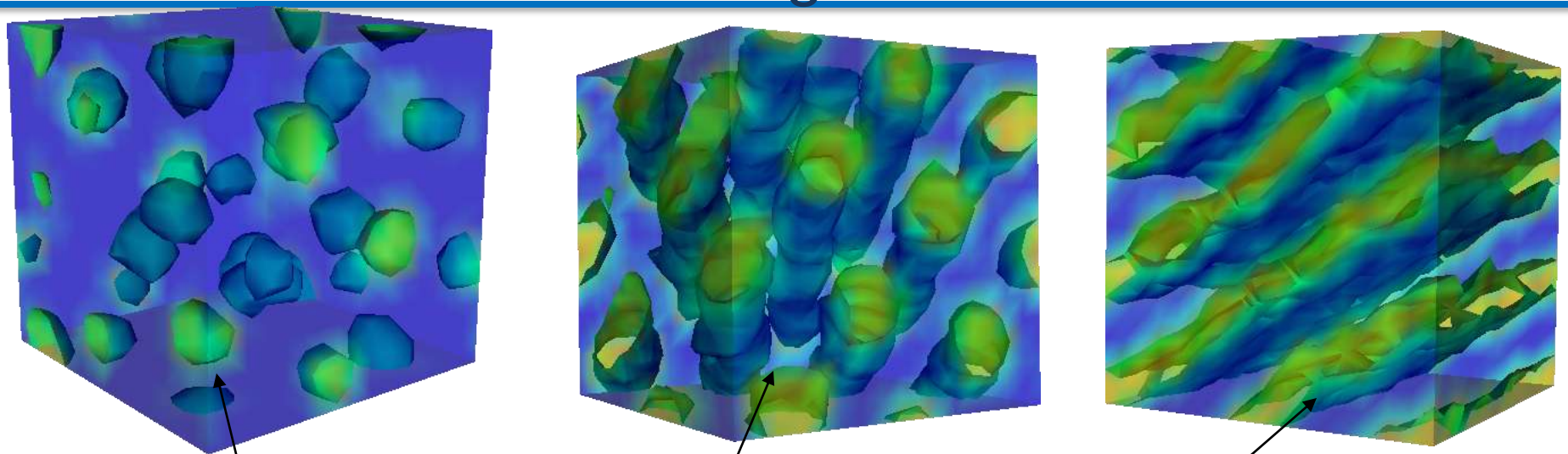
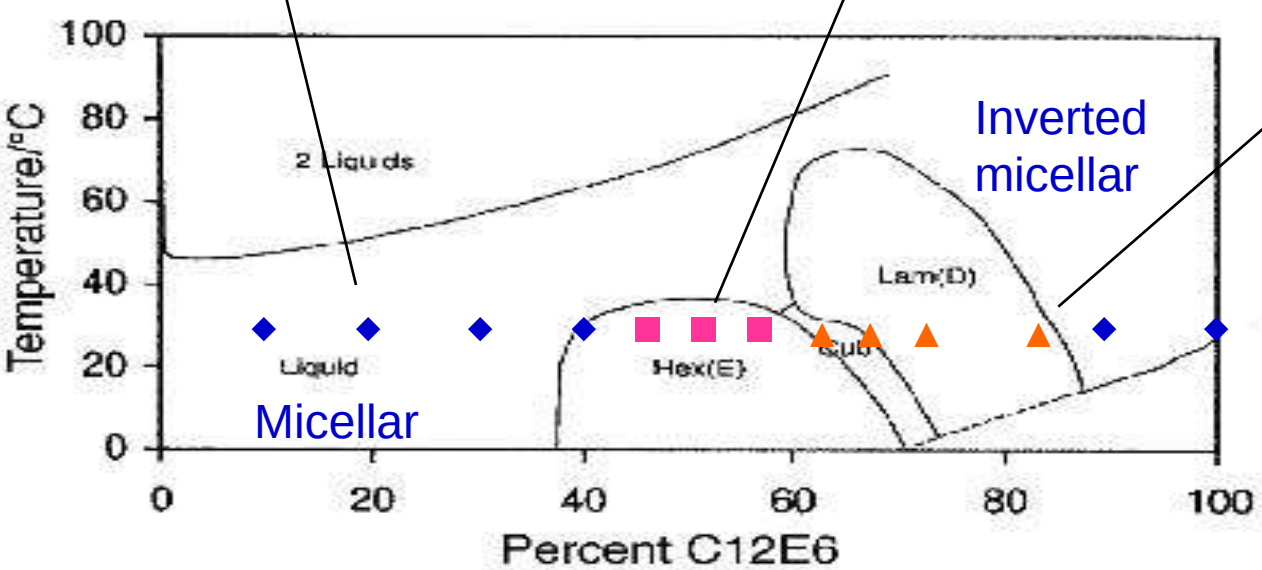
Mesoscale simulation of surfactant phase diagrams





Experimental phase diagram – B. Laughlin

- isotropic
- hexagonal
- lamellar

12000 beads in total:

- Water
- A-B surfactant

Computational Chemistry
CADMol

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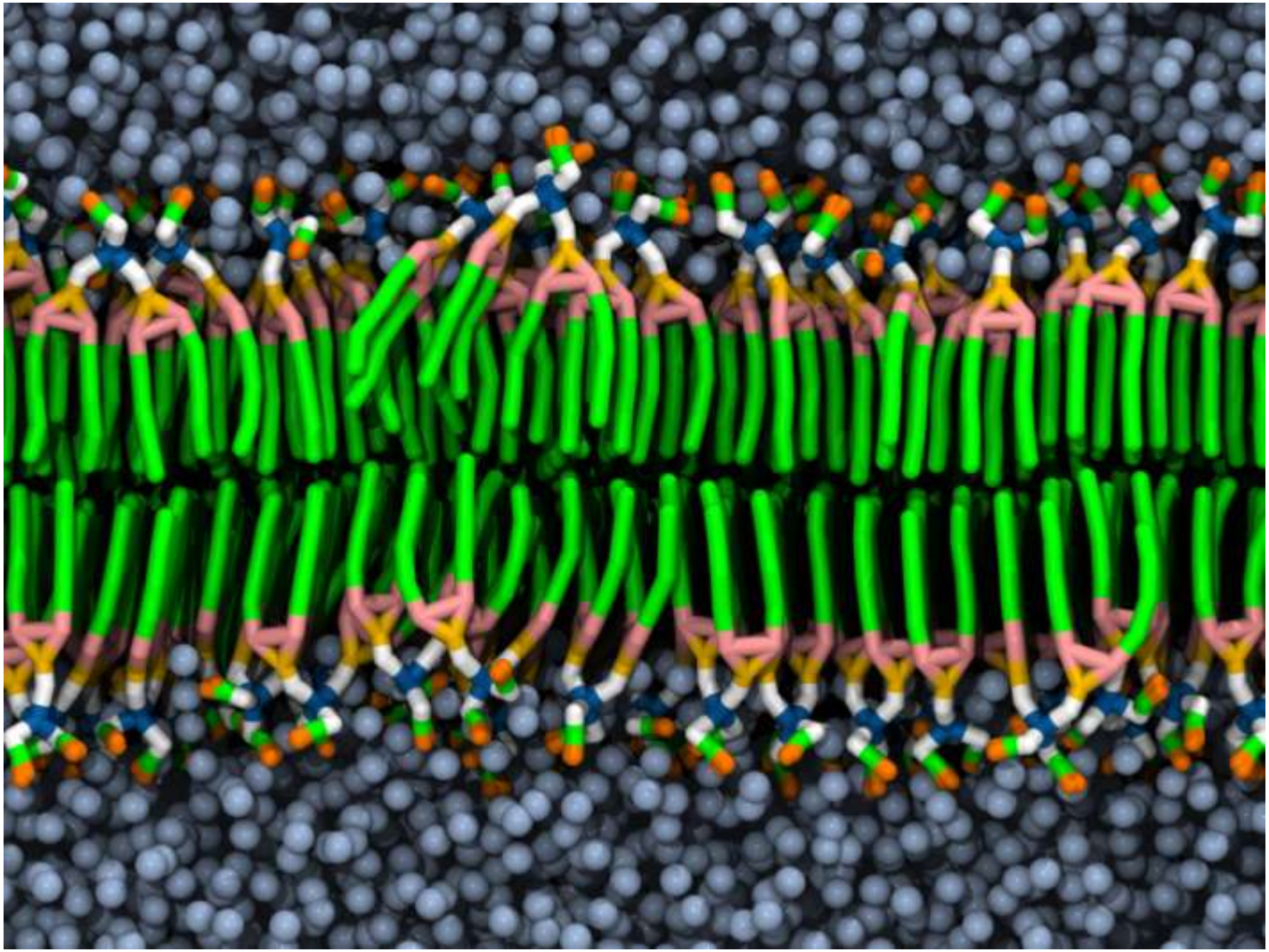
Bi-Layer Formation



Michael Klein's Group,

Temple University

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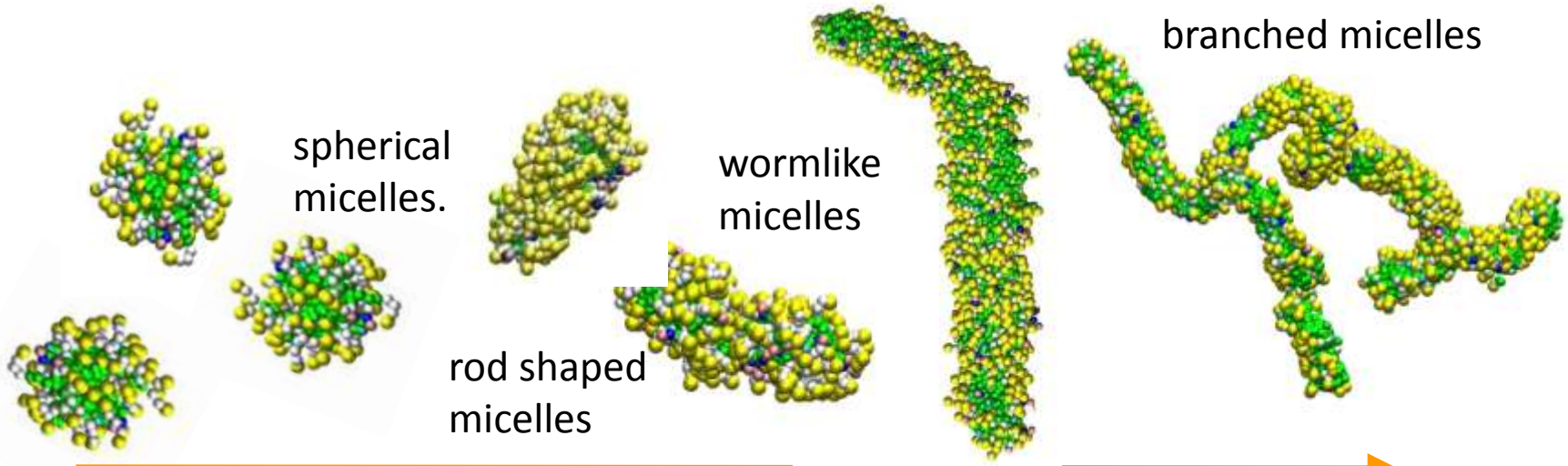
Understanding Body Wash Formulations – Micelles!

Why are some formulations thicker (e.g. rheologically)

at *different* concentrations?



concentration

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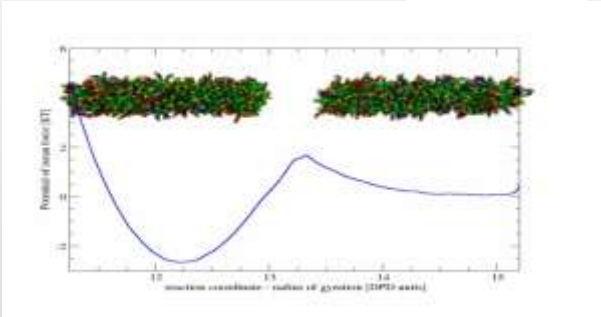
Micellar Properties in Formulations

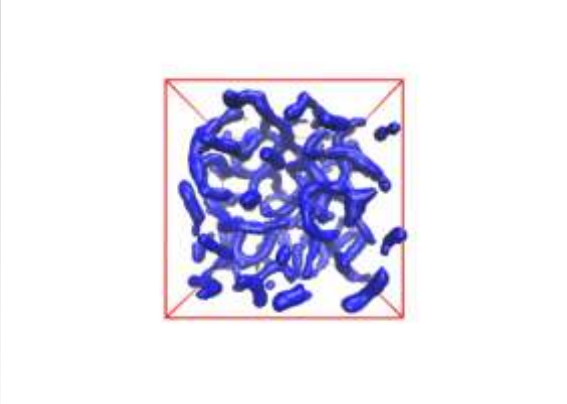
Ingredients

Molecular simulations

e.g. simulation of micelle scission

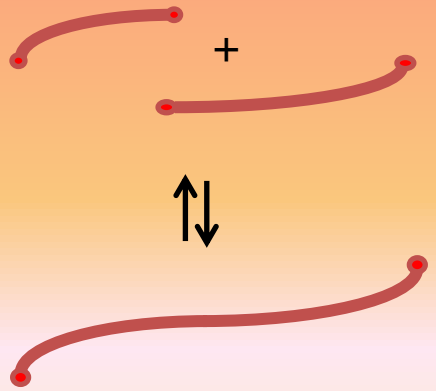


e.g. exploration of formulation microstructure and viscosity



Micellar properties

e.g. micelle scission energy predicts length of micelles

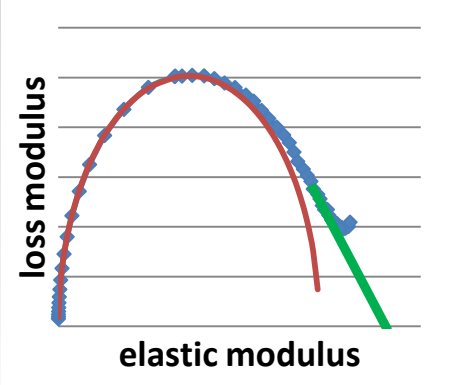


Neutron scattering

to probe micellar scale

Rheological characterization and modeling

e.g. modeling of characteristic relaxation times



Formulated product properties

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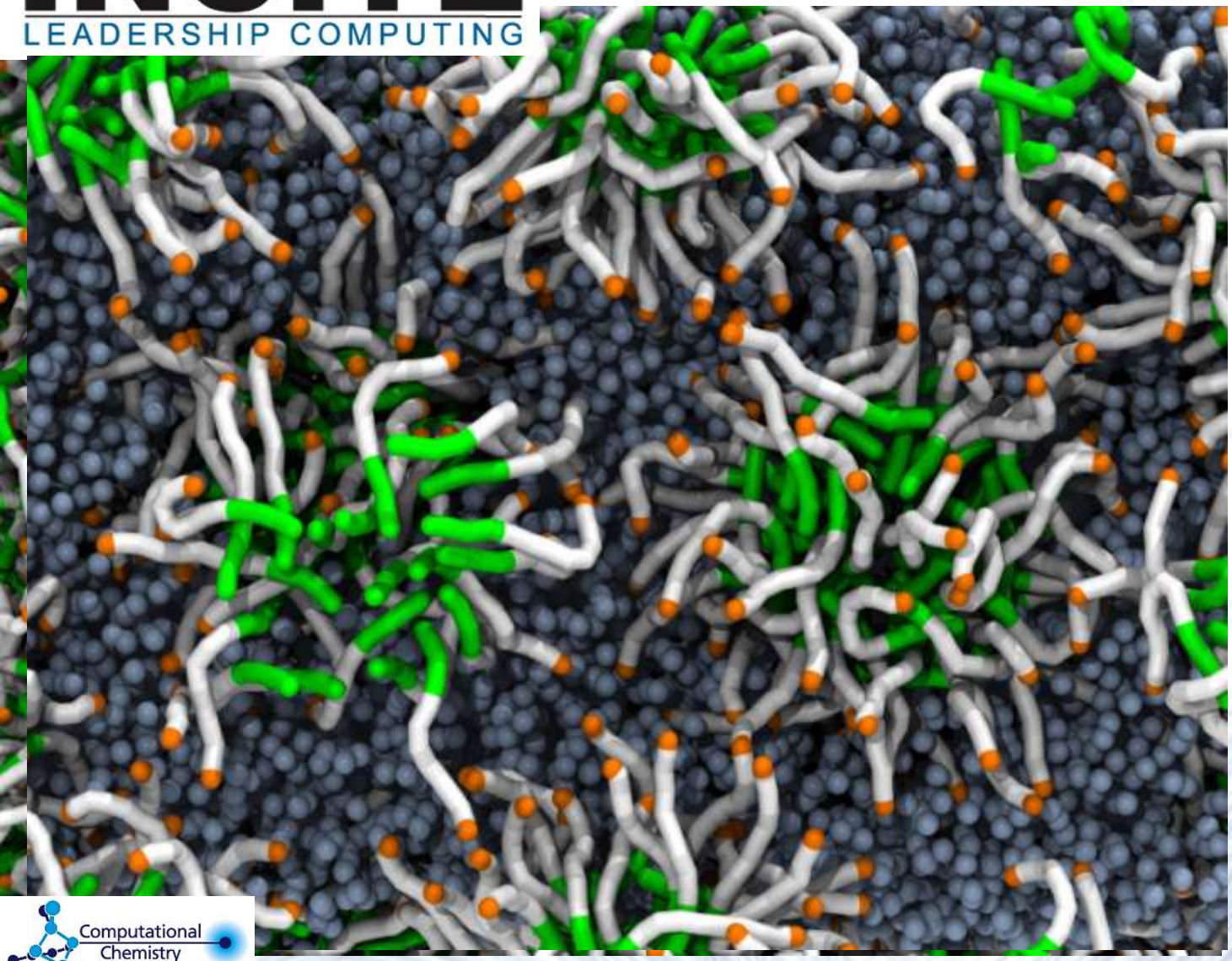
U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

OAK RIDGE NATIONAL LABORATORY
Managed by UT-Battelle for the Department of Energy



Dr. Michael Klein, Temple University

"Coarse Grained Molecular Dynamics Studies of Vesicle Formation and Fusion"

Computational Chemistry
CADMol

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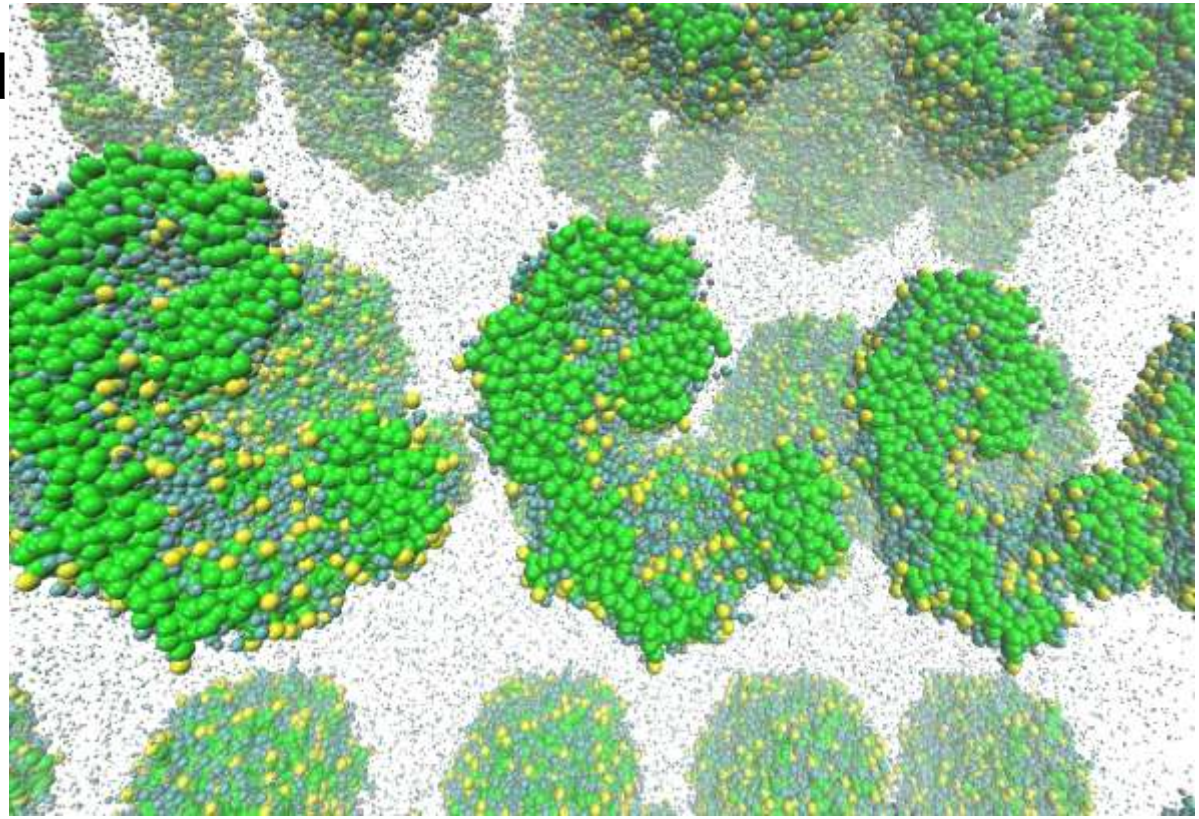
Spontaneous vesicle formation



10 Nano Meters

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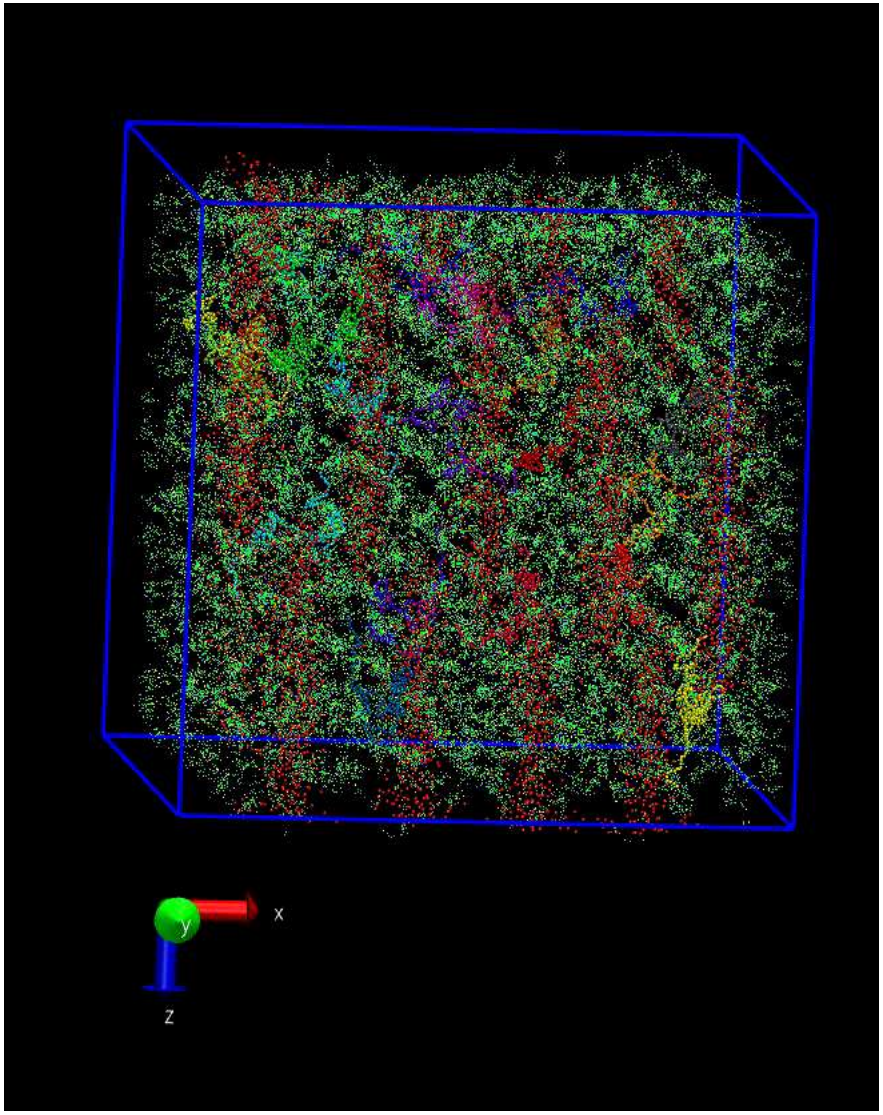
Complex Laundry Cleaning Mixtures



Large Simulation:

Vesicles, Polymers, LAS & Ca^{+} Interactions

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CAE Disciplines

CAE

computer aided engineering

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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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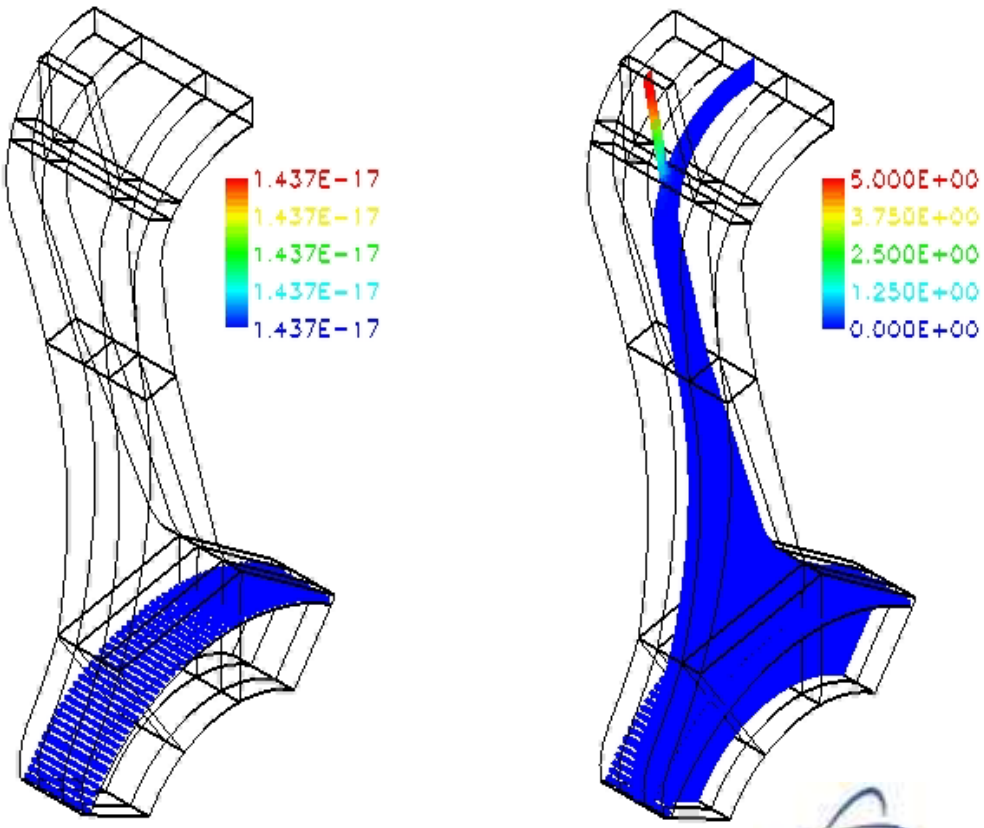
Fluids: Making Absorbent Diapers

Multi-Phase Turbulence… w/ Material Accumulation At the Boundaries



CFDlib w/ FLIP Markers
(Bucky Kashiwa)
@ Los Alamos National Labs

Los Alamos NATIONAL LABORATORY EST. 1943

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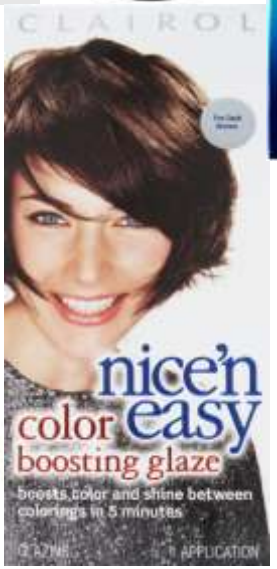
Mixing liquids:



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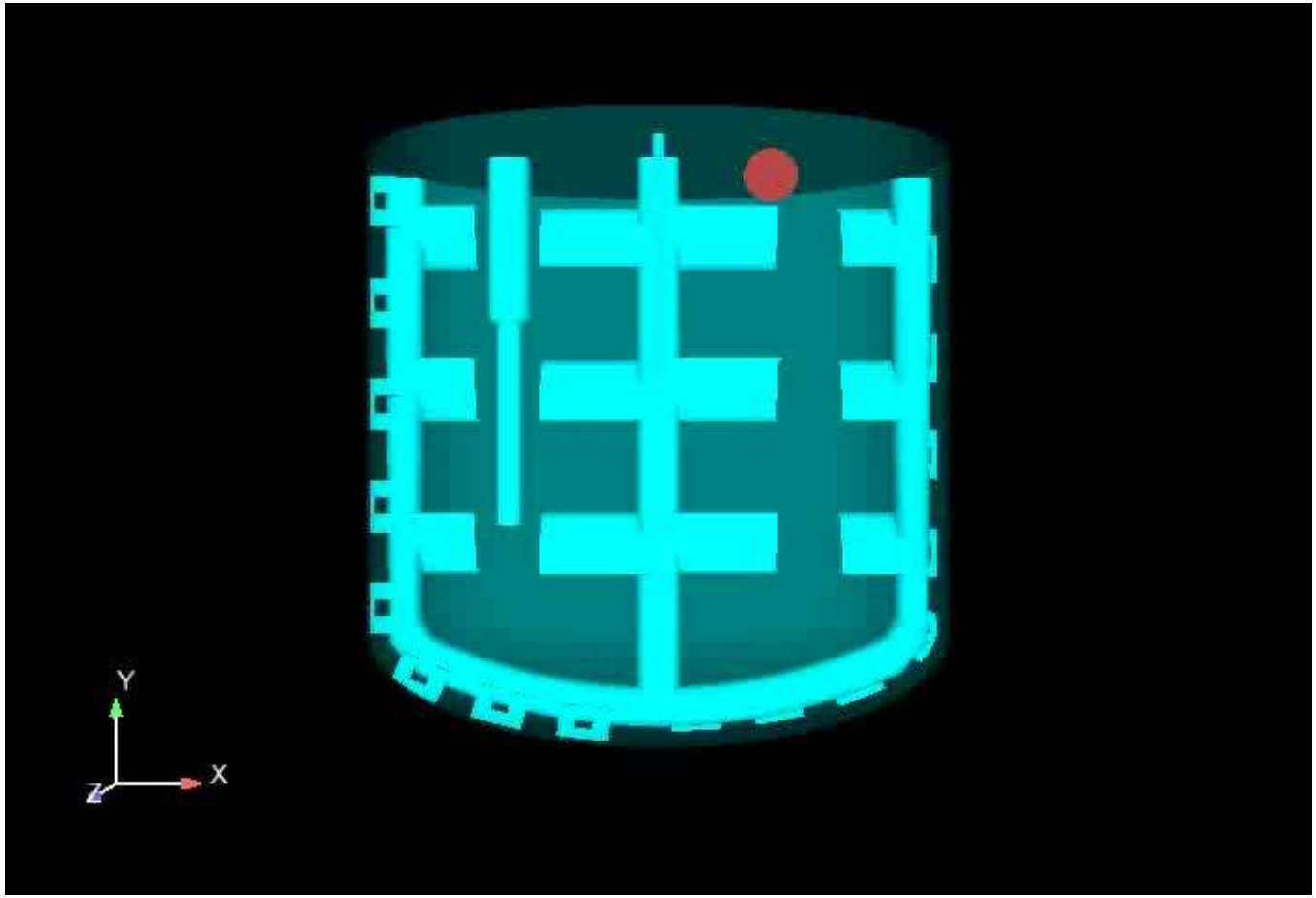
Mixing Non-Newtonian Fluids



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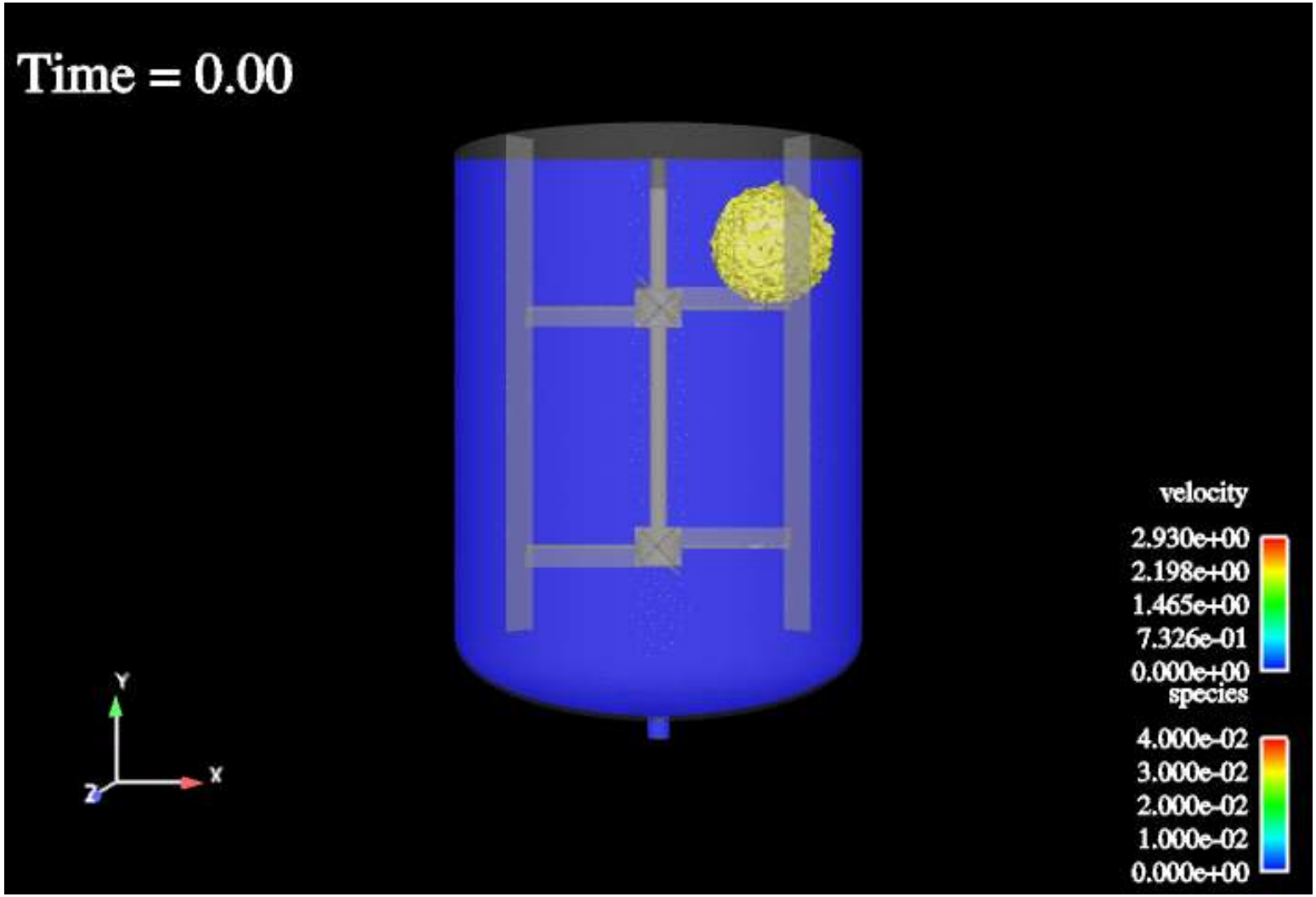
Mixing Dense Viscous Fluids



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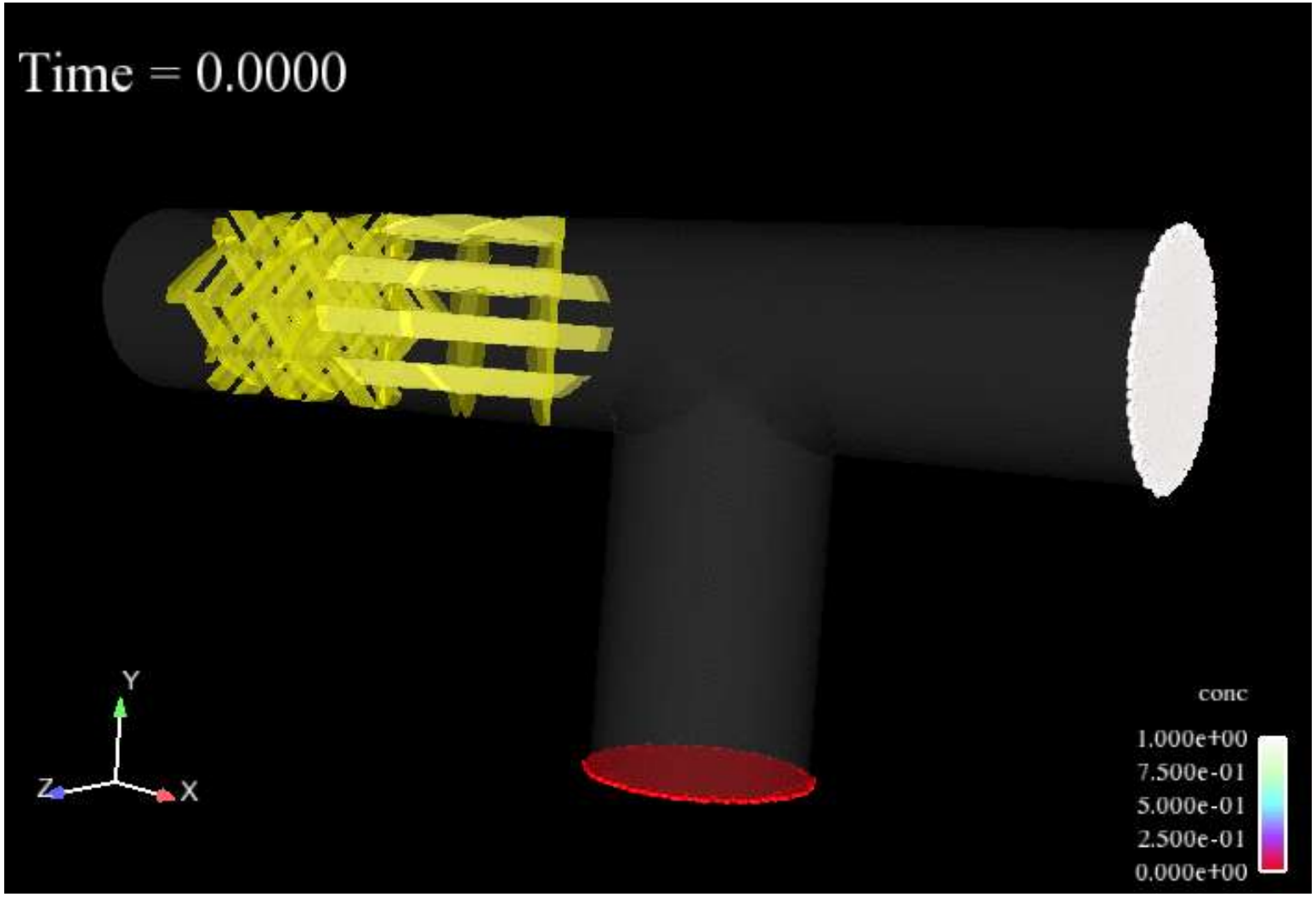
Static Mixer



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Filling at High Speed

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Paste Nozzle Flow = 1X

Coiling Flow

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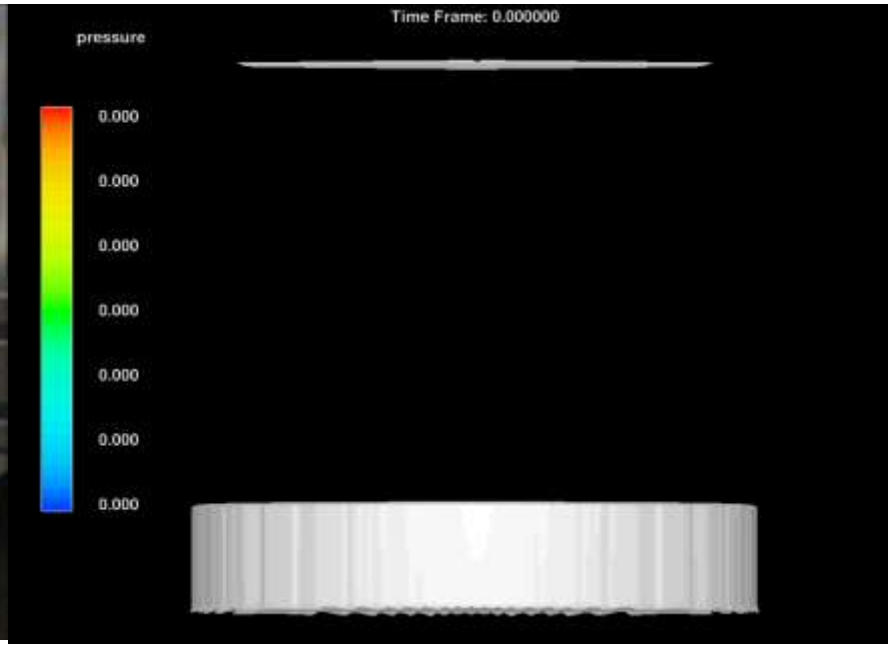
Paste Nozzle Flow = 6X to 10X Folding to Mounding Flow

Experiment

Simulation



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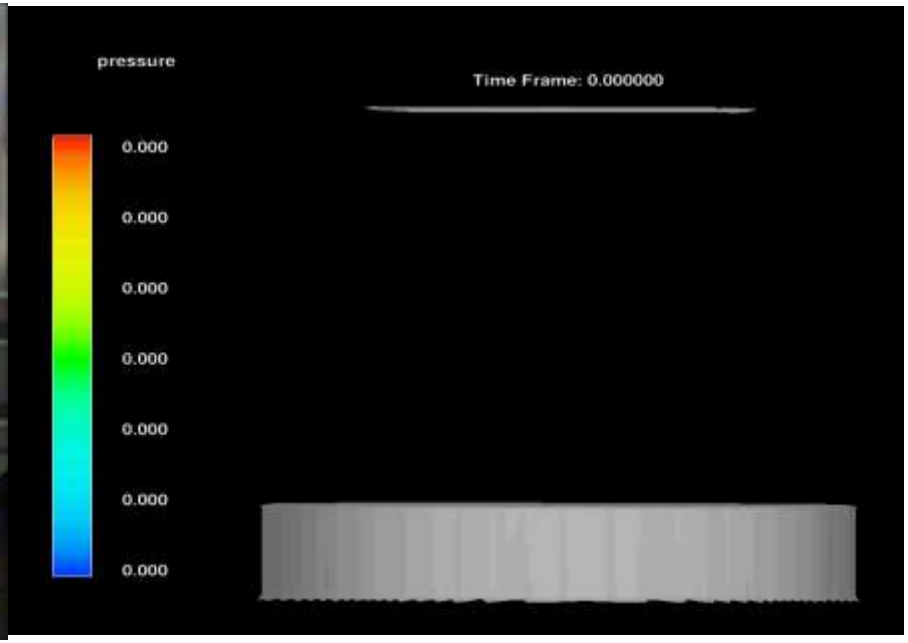
Paste Nozzle Flow = 66X to 171X Mounding to Steady Flow

Experiment

Simulation



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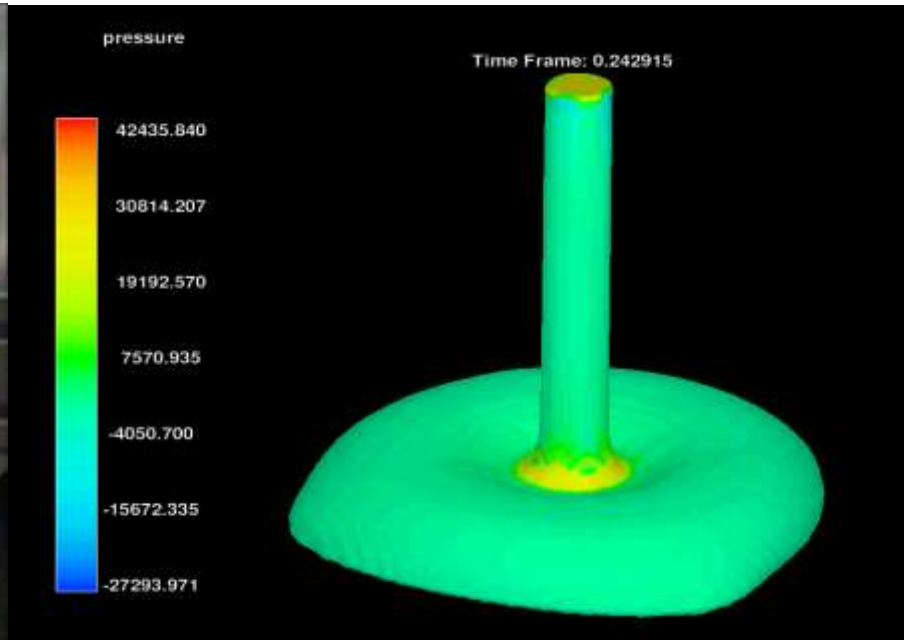
Paste Nozzle Flow = 170X to 210X Steady to Submerging Flow

Experiment

Simulation



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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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Behind Every Great Package…

…Is more than meets the eye!

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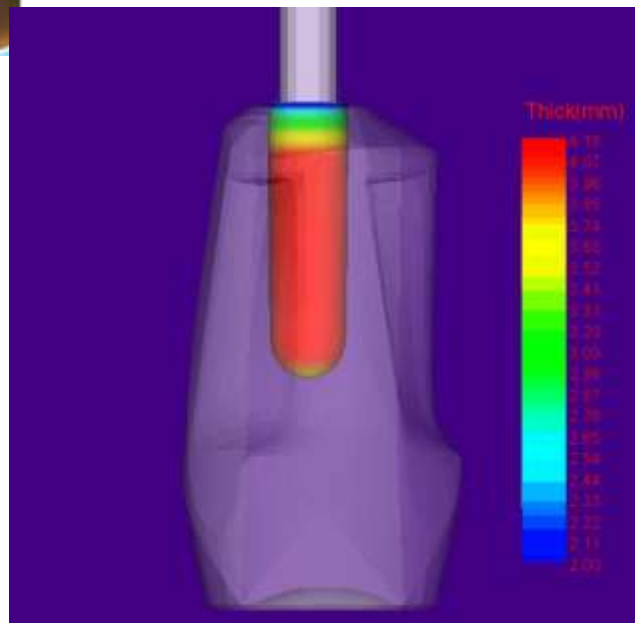
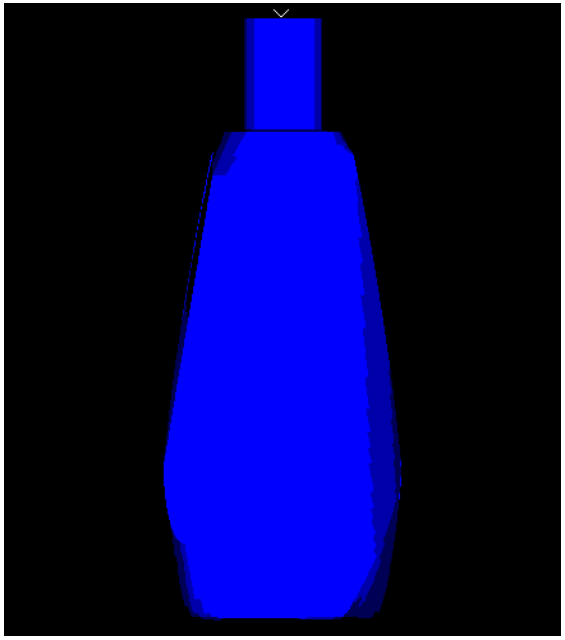
Bottle Weight Optimization

Wall Thickness Prediction



Injection Stretch Blow Molding

Top Load Stresses



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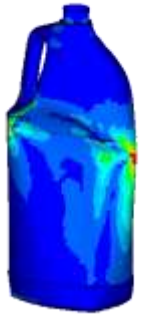
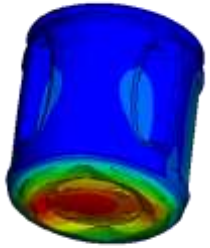
Load Cases

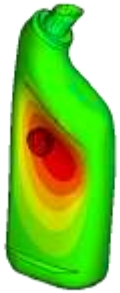
Top Load Empty



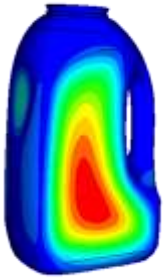
Pressure



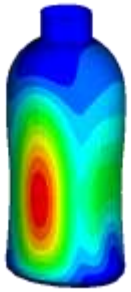
Squeeze



Top Load Filled



Vacuum



Hydrostatic

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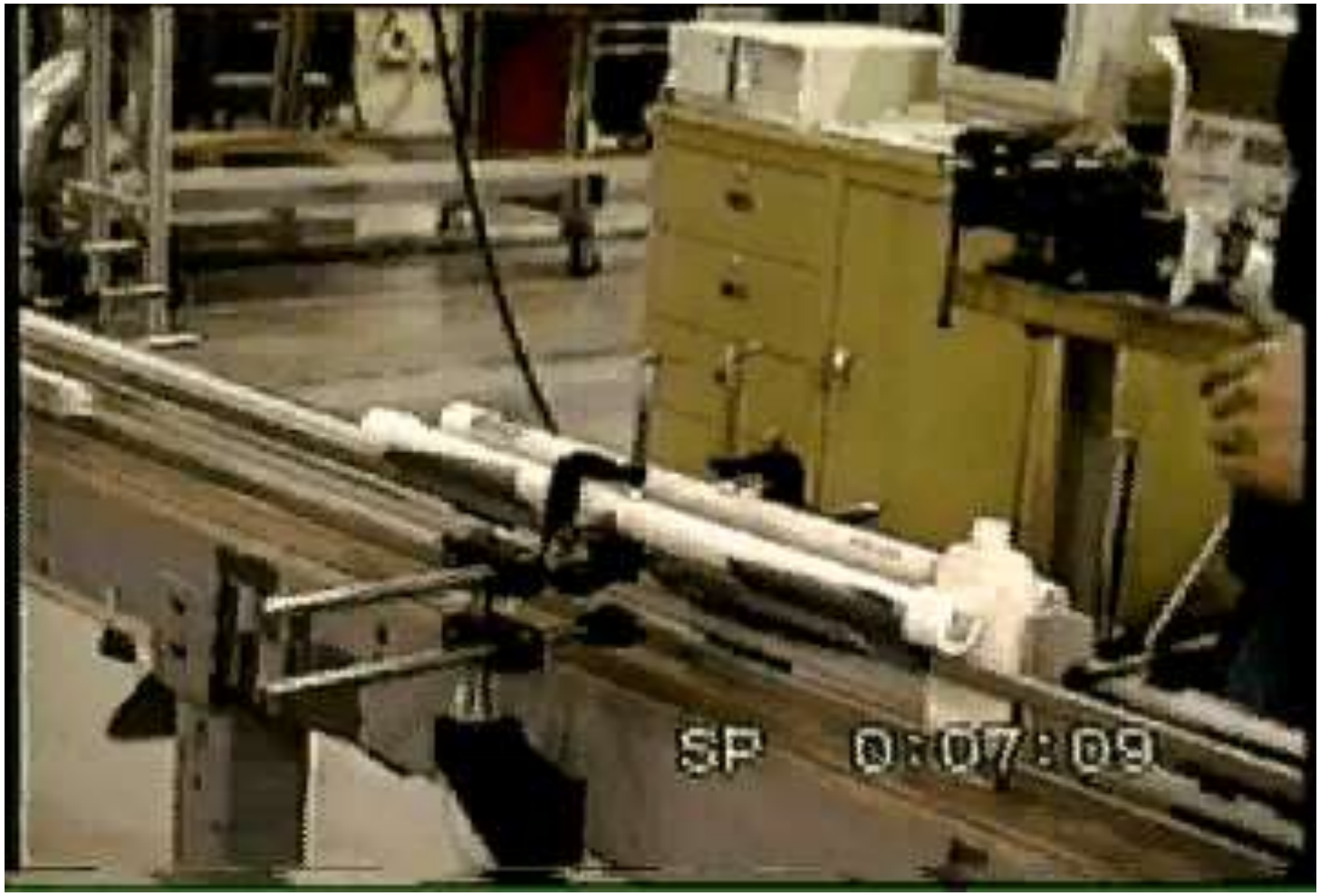
Can We Convey Bottles?



Bottle Race Track

'Circa 2000'

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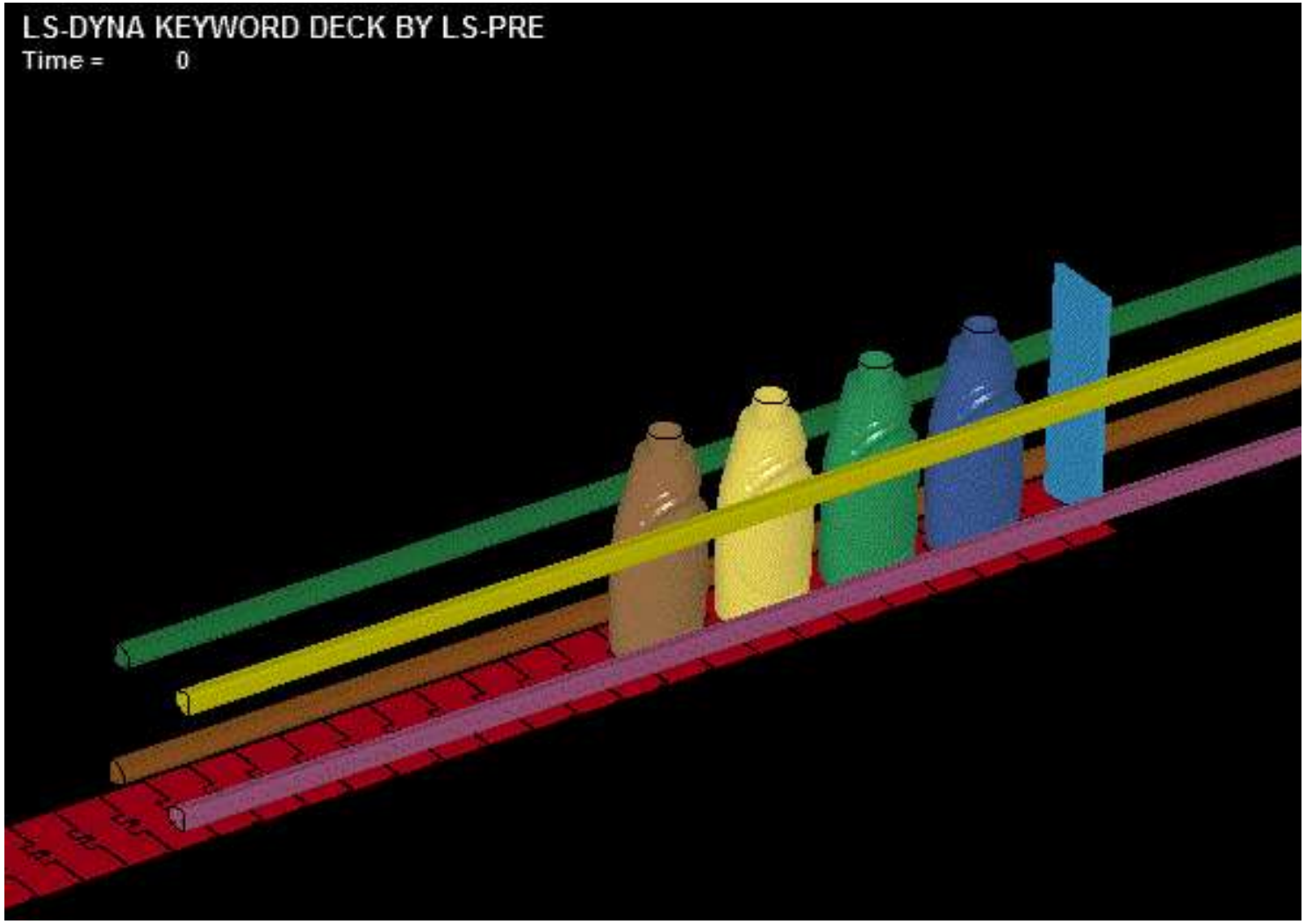
Virtual Race Track



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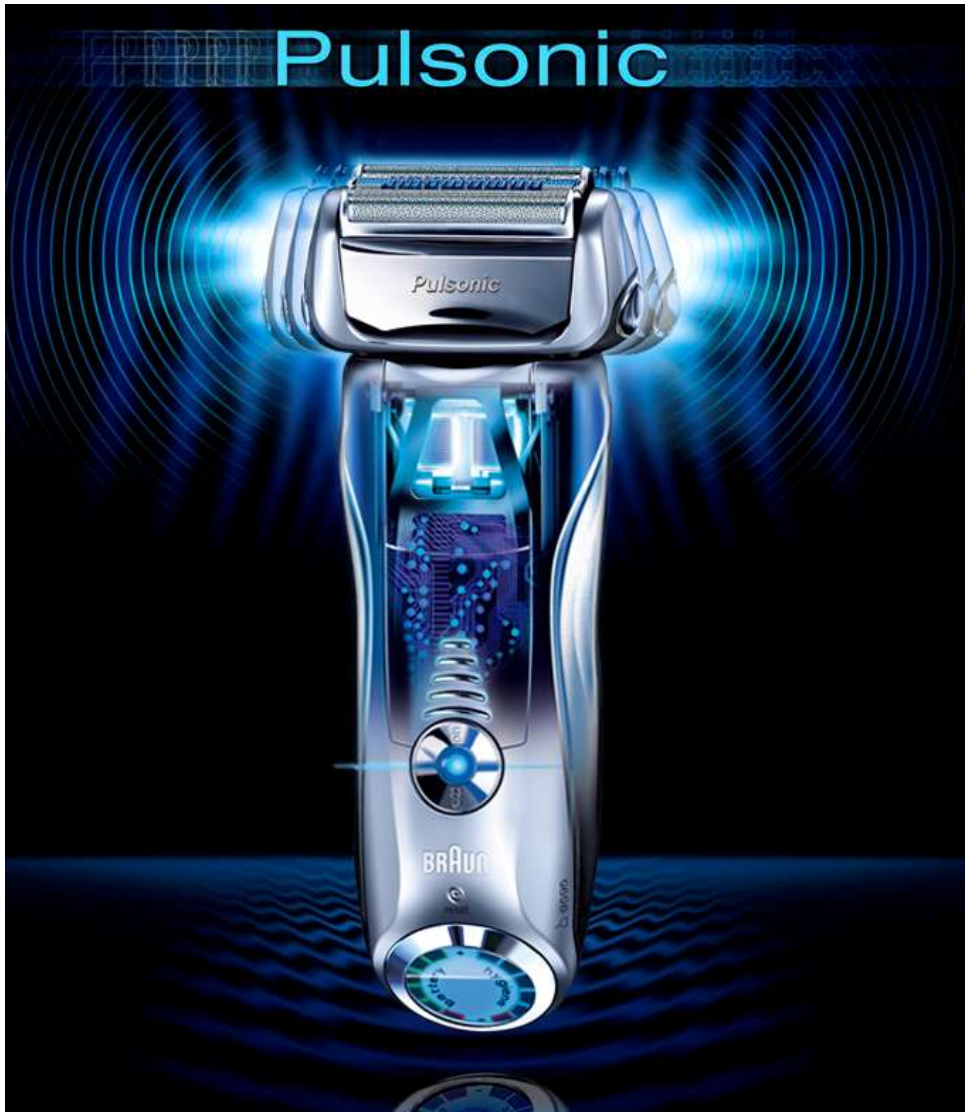
The new premium shaver …



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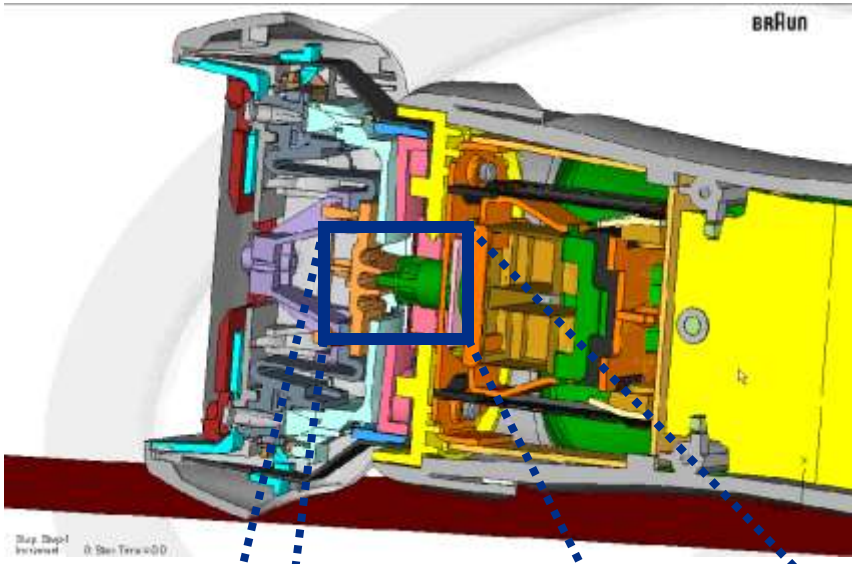
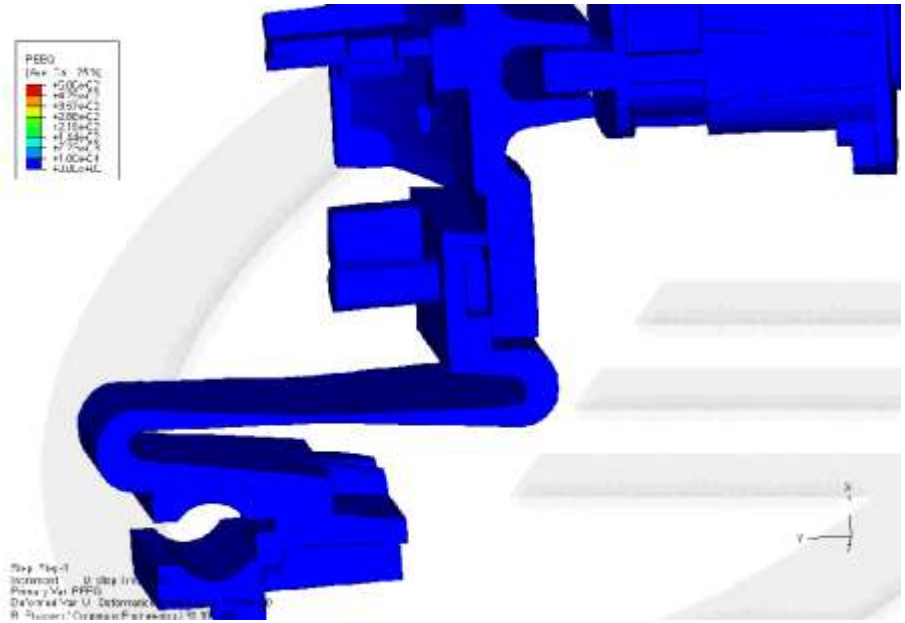
Bathroom Floor Drop





Lots of Small Parts...

…Everyone must work!

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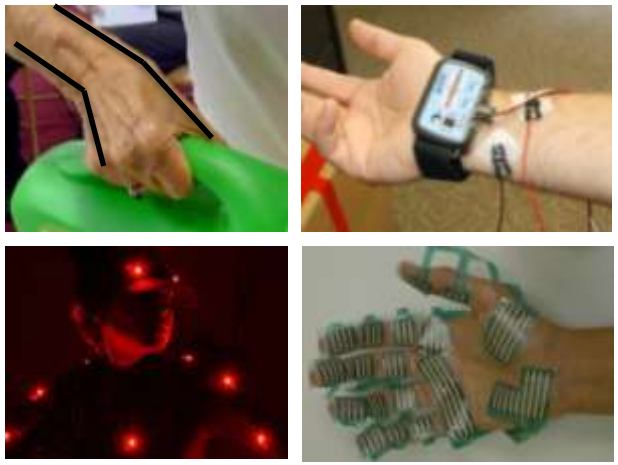
Hand Ergonomics

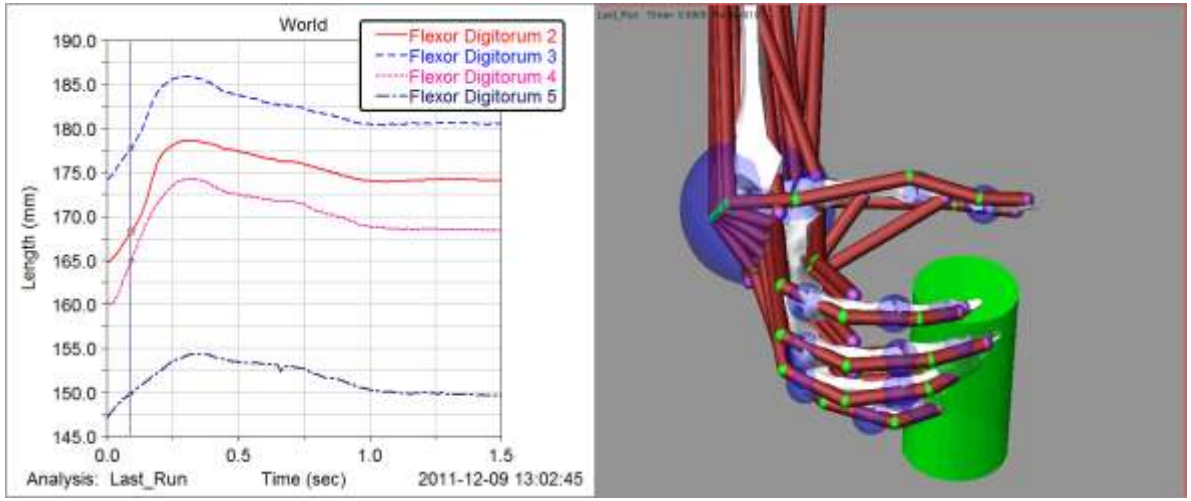
Experimental Measures

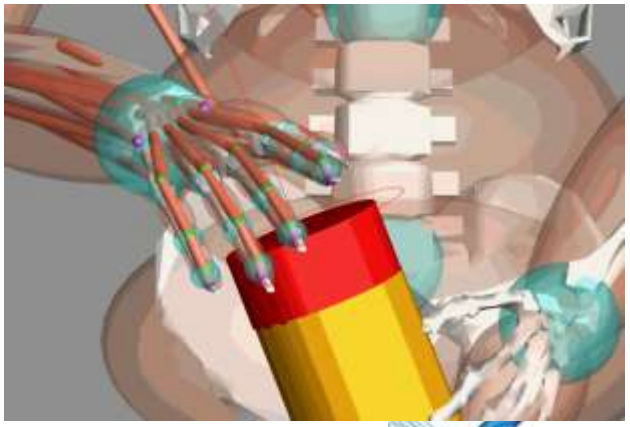
- **Goniometry (joint angles)**
- **EMG measures to measure muscle activity**
- **Motion capture and surface pressure measurements for direct hand interactions**



Kinematic Simulations

- Predict joint torques





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What are the areas of Challenge & Research?

Multi_Physics…

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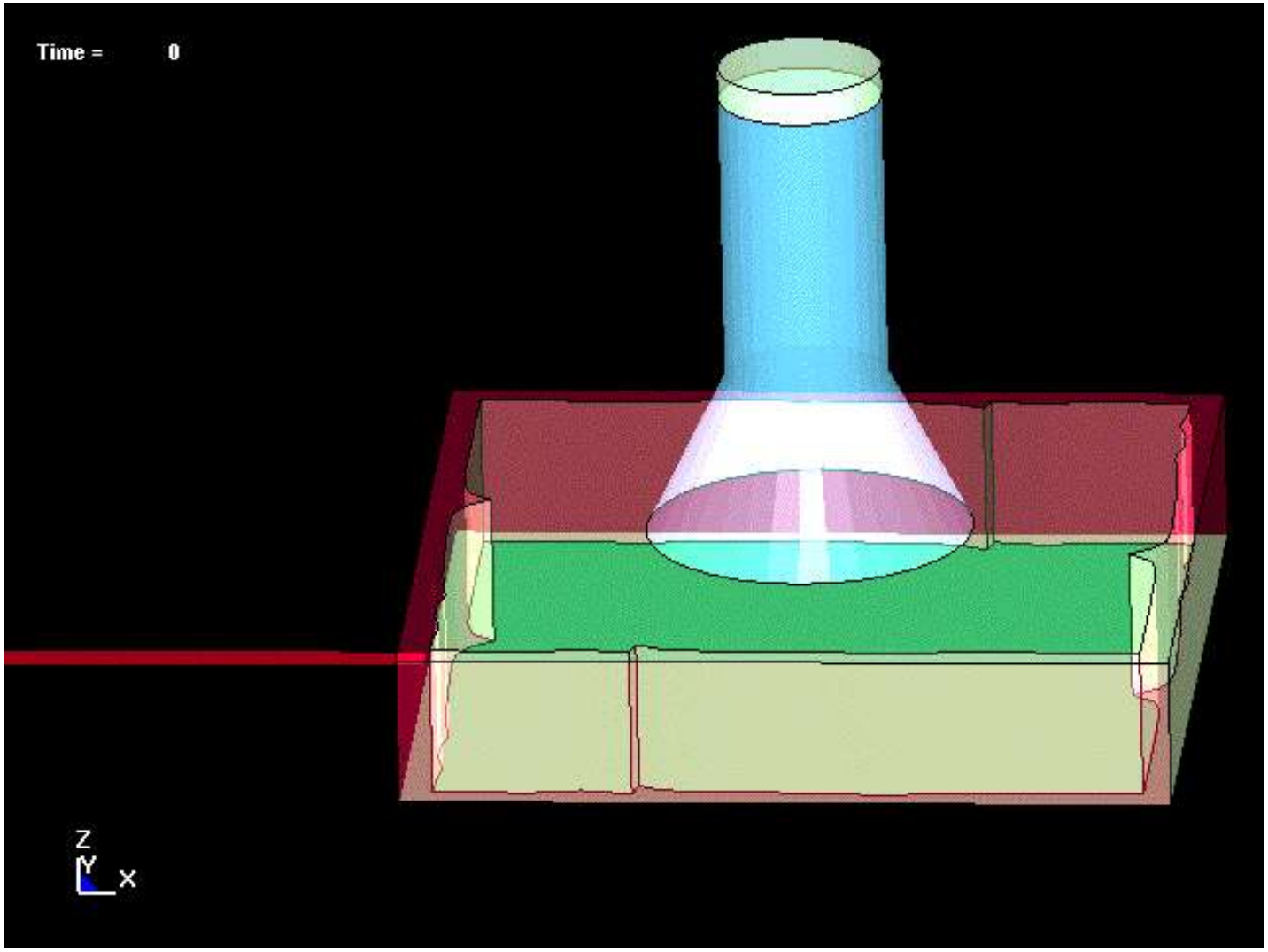
Vacuum Removal of Ribbons



Fluid-Structure Interaction (FSI)

w/ Non-turbulent Air

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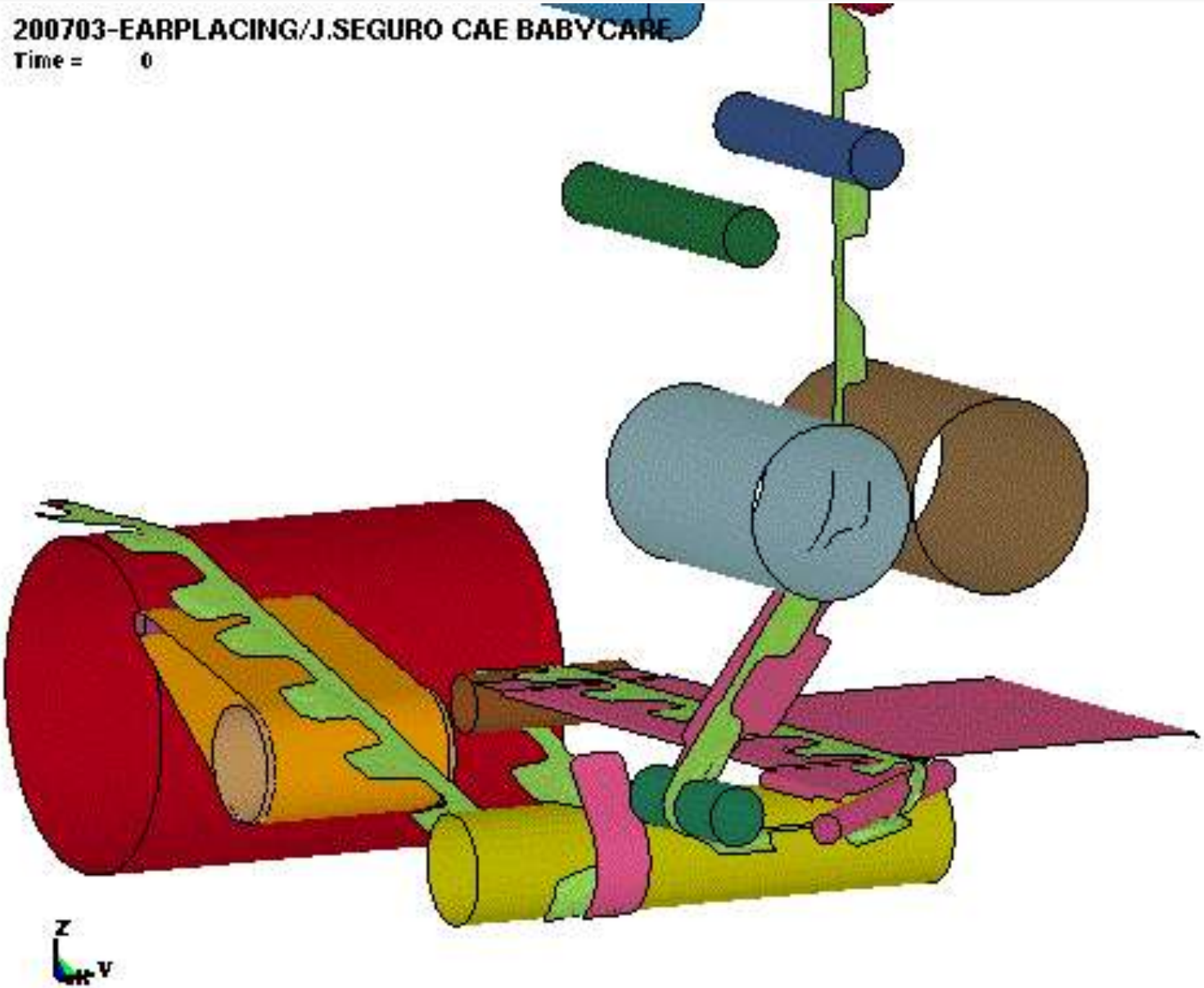
‘Flag & String’ FSI Problem



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Liquid Container Impact

What You Don't Want to Happen In Store Or Your Laundry Room!

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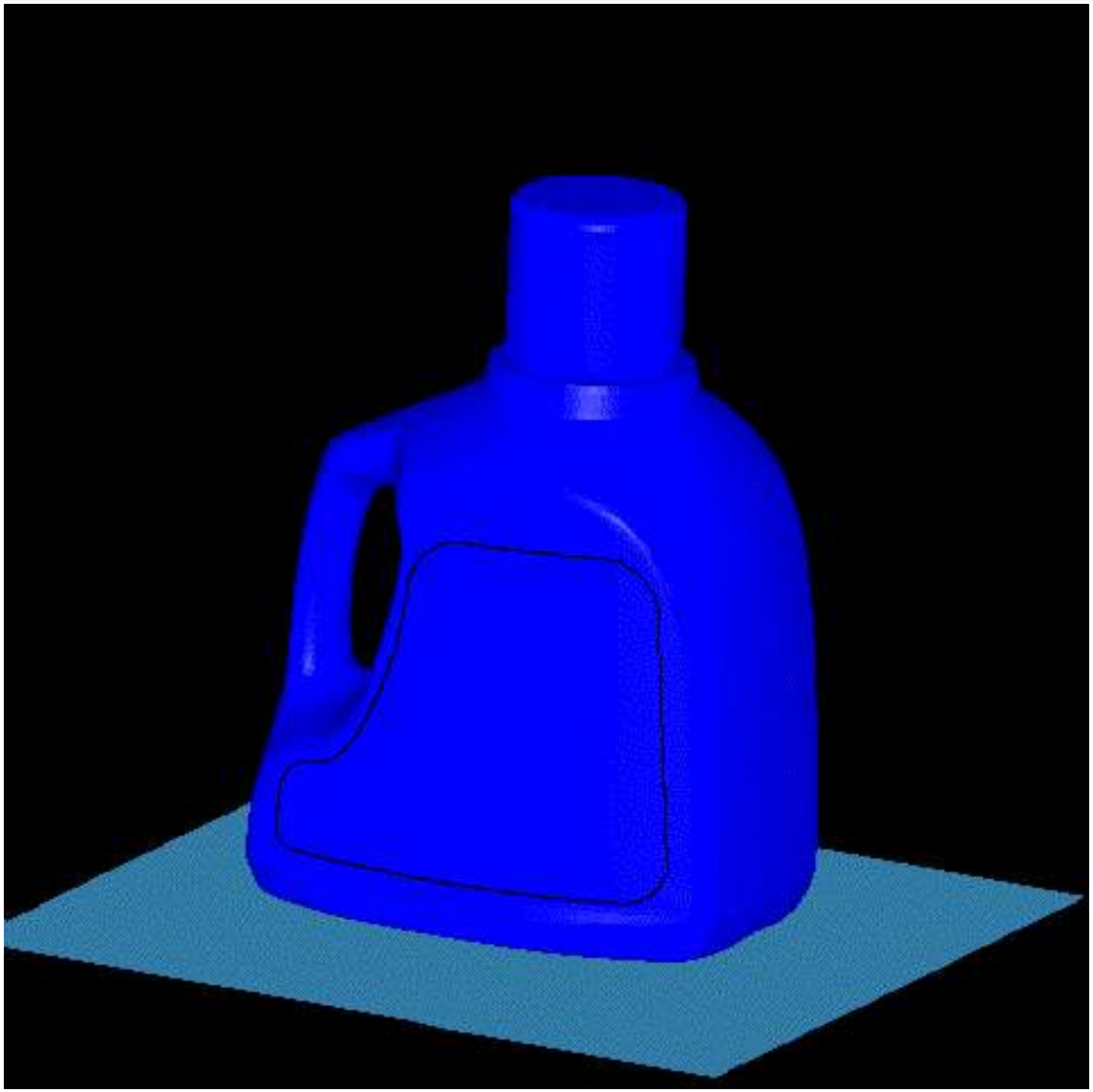
FSI Simulation



Material Properties Are The Key To Predicting Reality!

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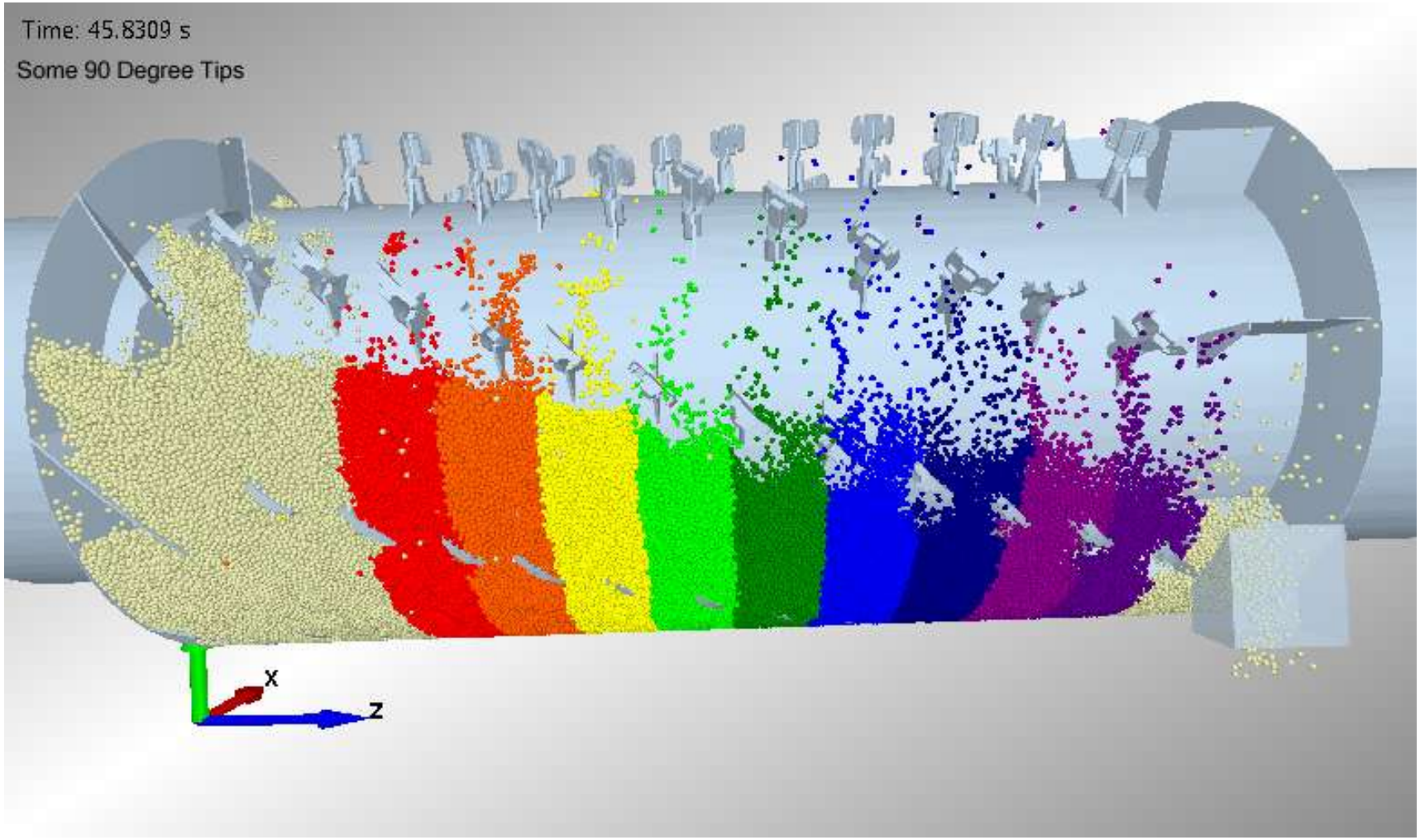
What is DEM
(Courtesy DEM-Solutions)



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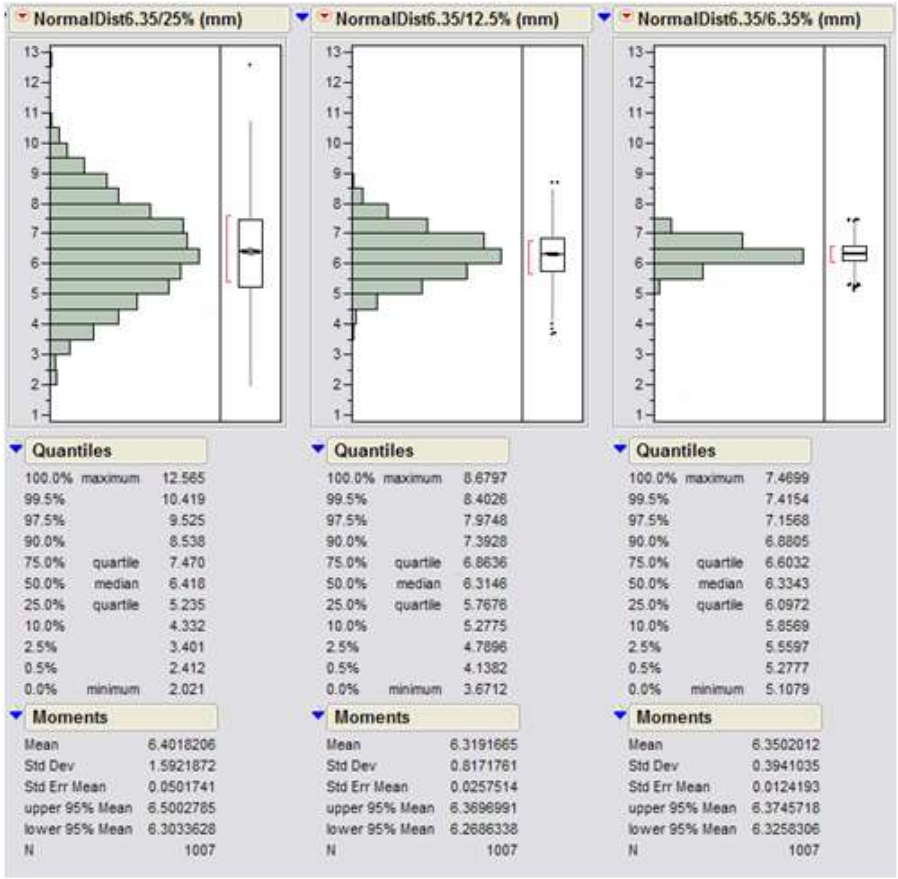
Glass Bead STD Study

- Standard Deviation (STD)



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Investigation using LSDyna

11,265 particles with both specific Shape distribution and specific Size distribution

The particles are treated as rigid and subjected to the force due to gravity.

It took 158 wall clock minutes, using 32 cpus to complete the 1.0 sec. solution with a 1e-05 sec timestep

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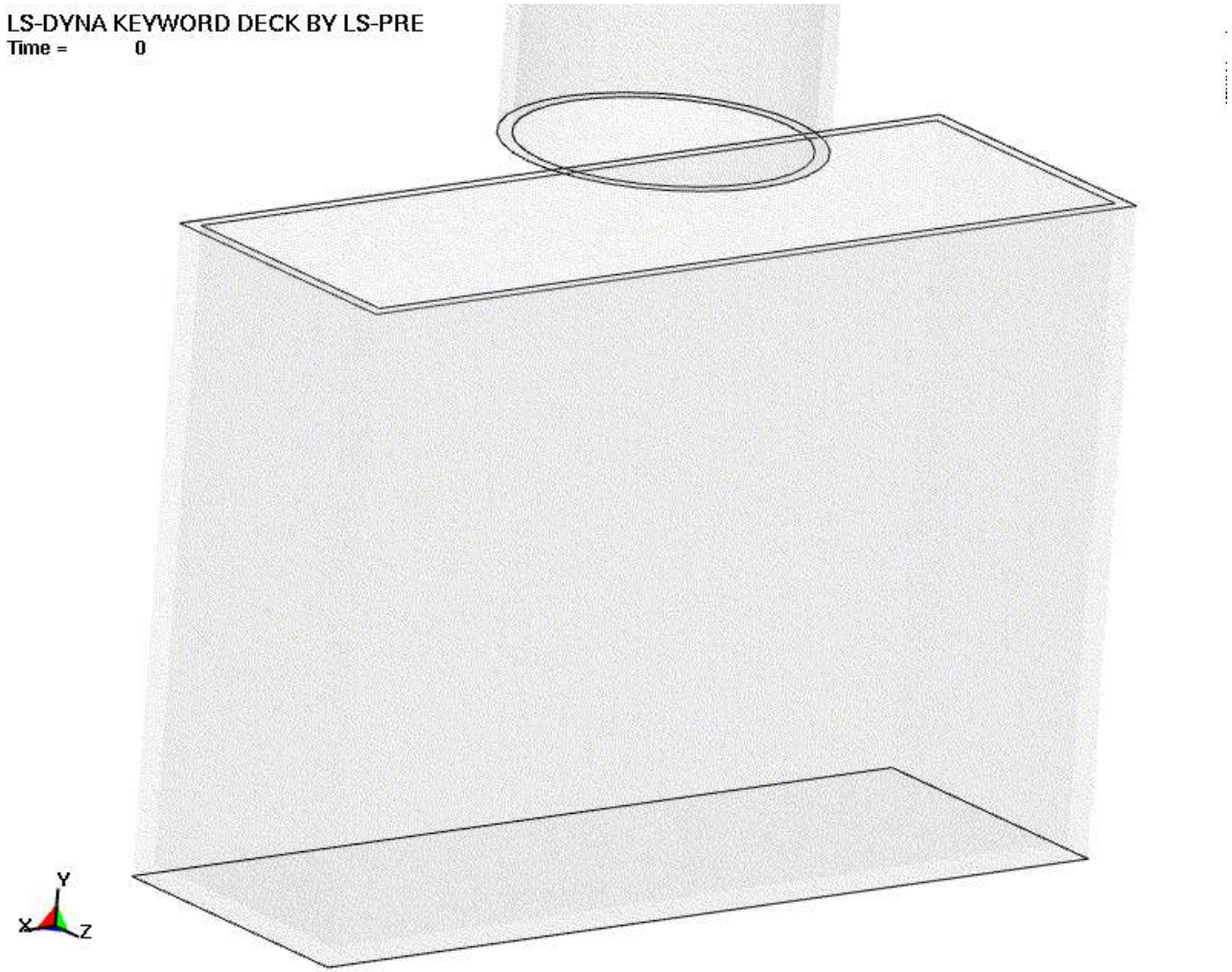

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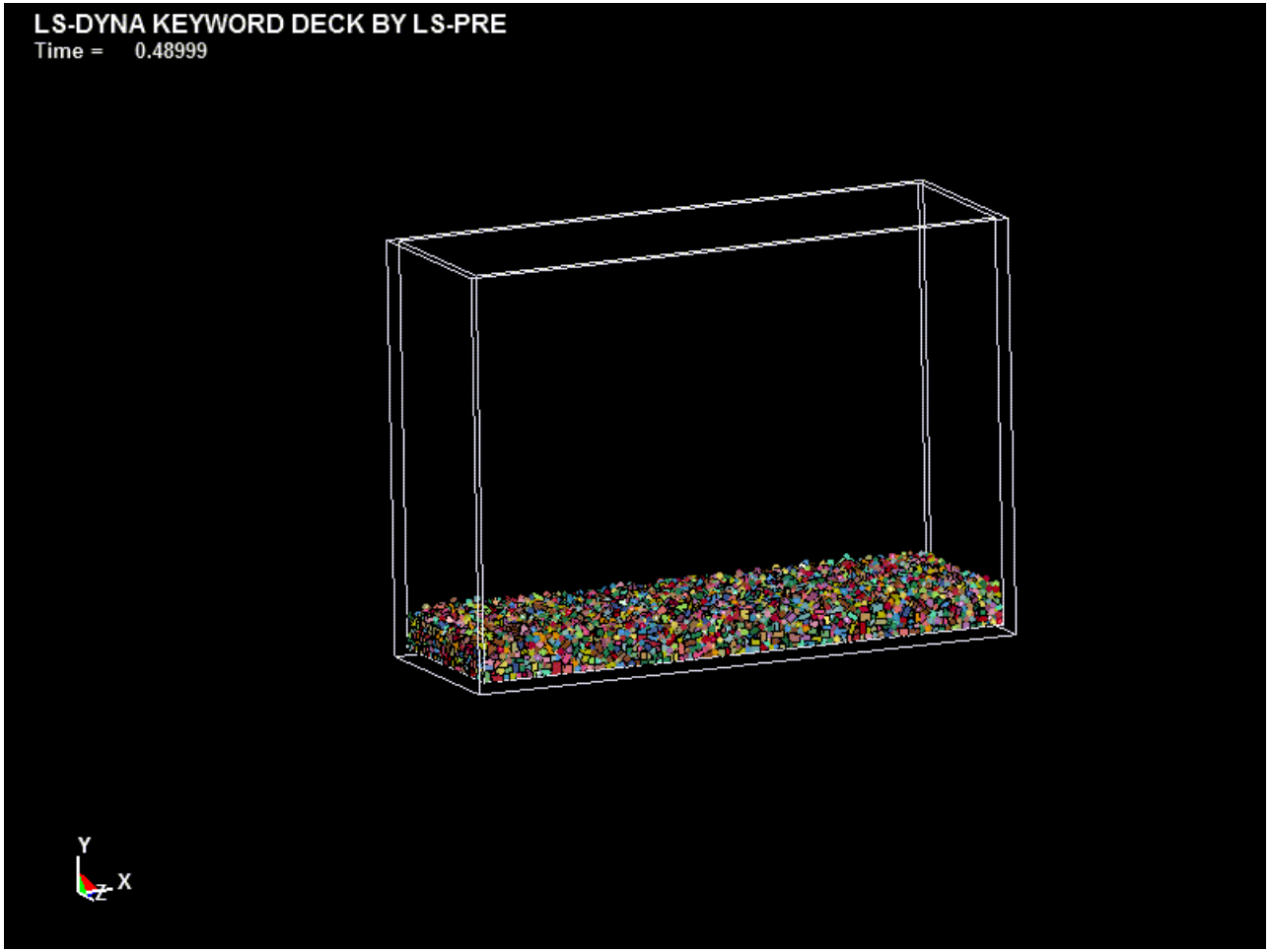
Rocking Box



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GAC microCT Simulation

- First usable microCT data July 10th limited to ~1000s particles

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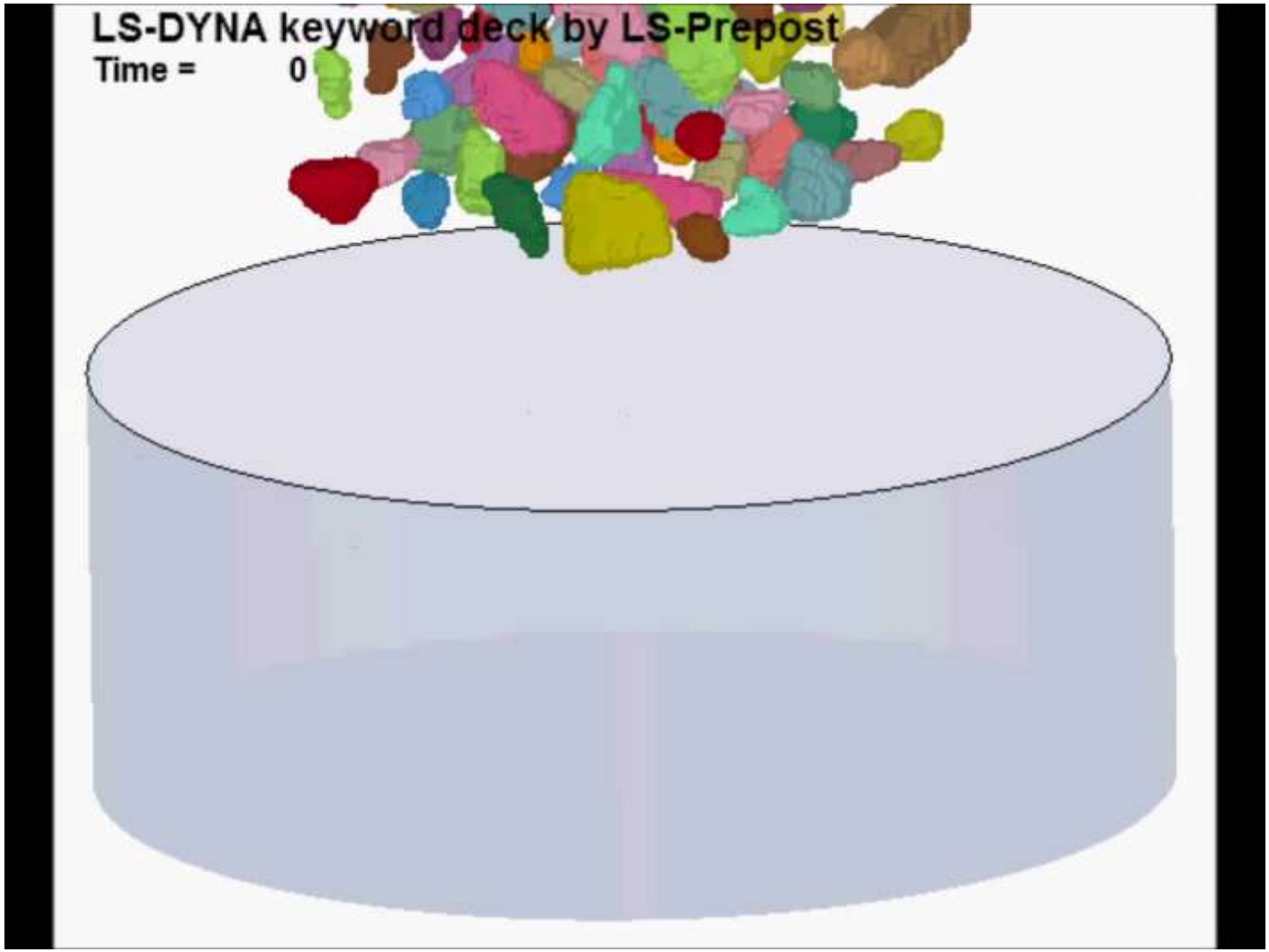
GAC microCT Simulation



J. Kitching

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Fluid Flow

Water Inlet
Velocity BC

Water made
transparent

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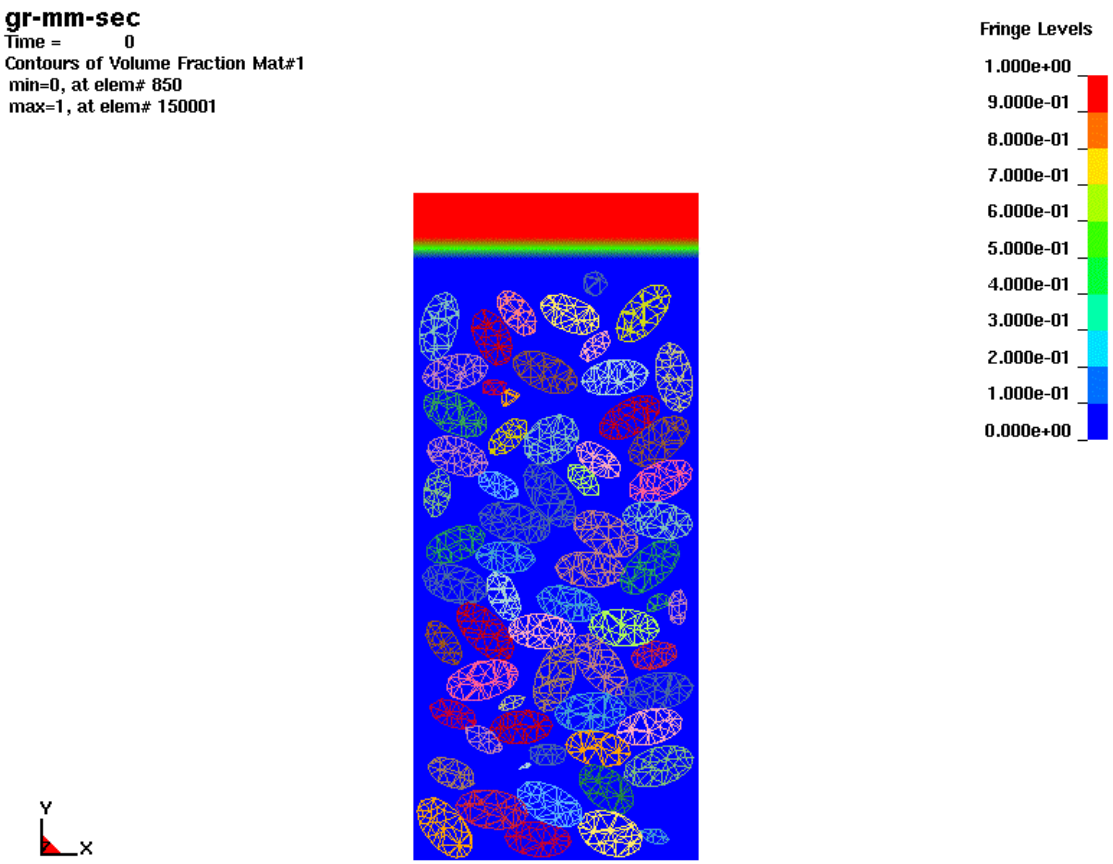
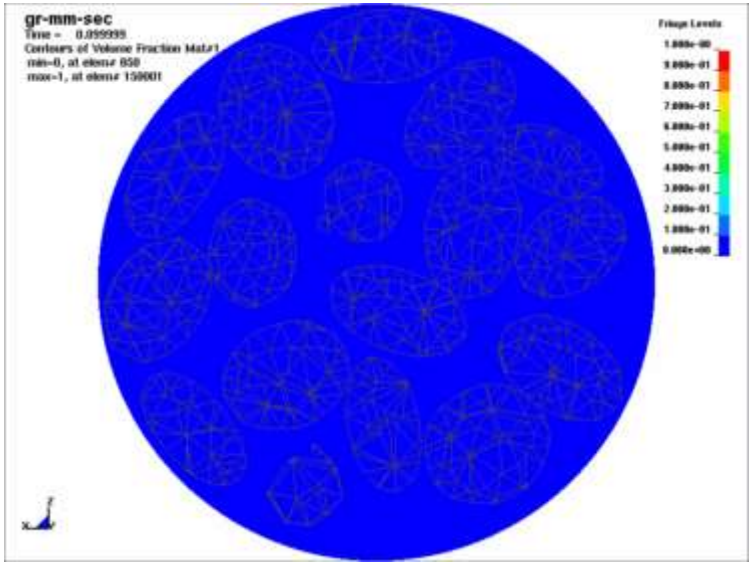
Fluid Flow Through Bed



SideView

Top View



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Some Management stuff

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Making $ with M&S

What if ? ,
Why not ?,
How much?.

Define Problem

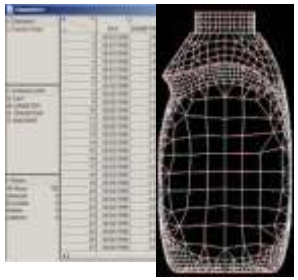
1. **Translate Business Challenge into Science question**

2. **Express Science in Equations**

$$\left(\sqrt{1+4\frac{\beta\rho}{\alpha^2\mu^2}\frac{\Delta p}{\Delta L}}\right)$$

Get Data

Consumer Ratings, Plant Reliability, Material Properties, Geometry etc.

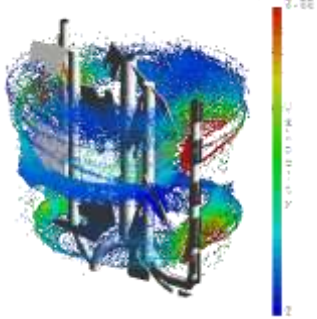


Solve Equations

1. **Solve Equations**
2. **Build Simulation**

Display & Communicate

Display results For non-expert understanding



Shape Decisions

Apply & Deploy:
-reframe the question
-guide the choices
-confirm the situation
-stop the project

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P&G Modeling & Simulation

Measure Business Contribution in the ‘Currency’ of Finance

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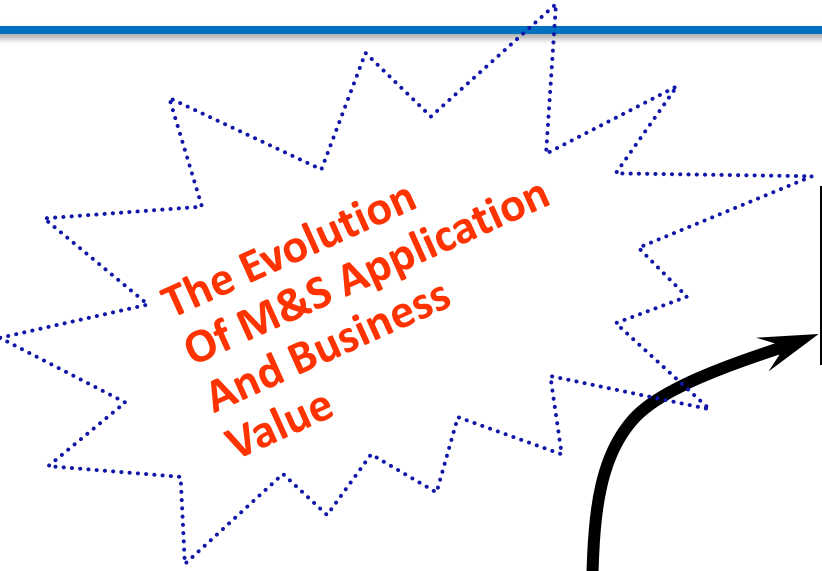
…How do we USE the Power!



"Analysis Led" Discovery → Defines the option space 'where' ***designs*** work…or don't work

"Virtual" Trial & Error → Predicts 'why' ***designs*** work…or don't work

(in systems that don't exist yet)

Pathology → Explains 'why' ***existing*** products & systems work…or don't work

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M&S Org. Strategy

P&G ***General Scientists & Engineers***, ***in BU's with mainstream career paths***, **are familiar with capabilities & contacts for help.**

Tier I

P&G ***Modeling Practitioners***, ***in BU's with main-stream career paths***, **are trained and capable of routine analysis. Do most routine analysis.**

1 for every 10 Scientist/ Engineer

Tier II

P&G ***M&S technologists***, ***mostly reside in the BU***, **do/lead bulk of M&S application & deployment.**

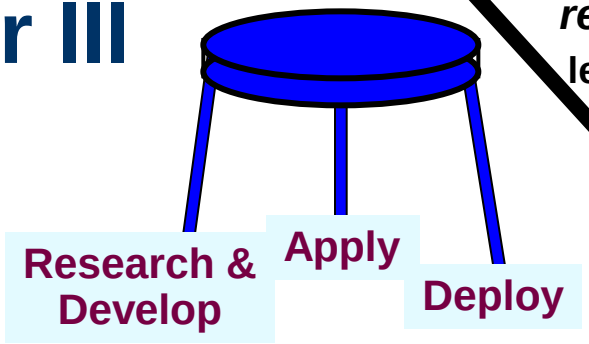
1 for every 6 Practitioner

Tier III

P&G ***M&S experts,*** ***most reside in Corporate***

lead M&S Research, Development, & Teaching

1 for every 3 Technologist



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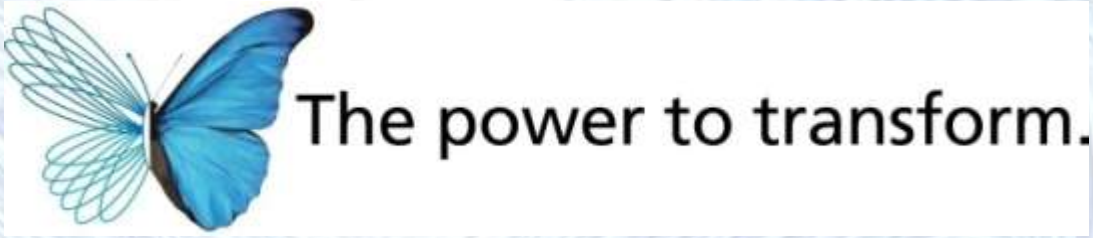
Themes for the Future



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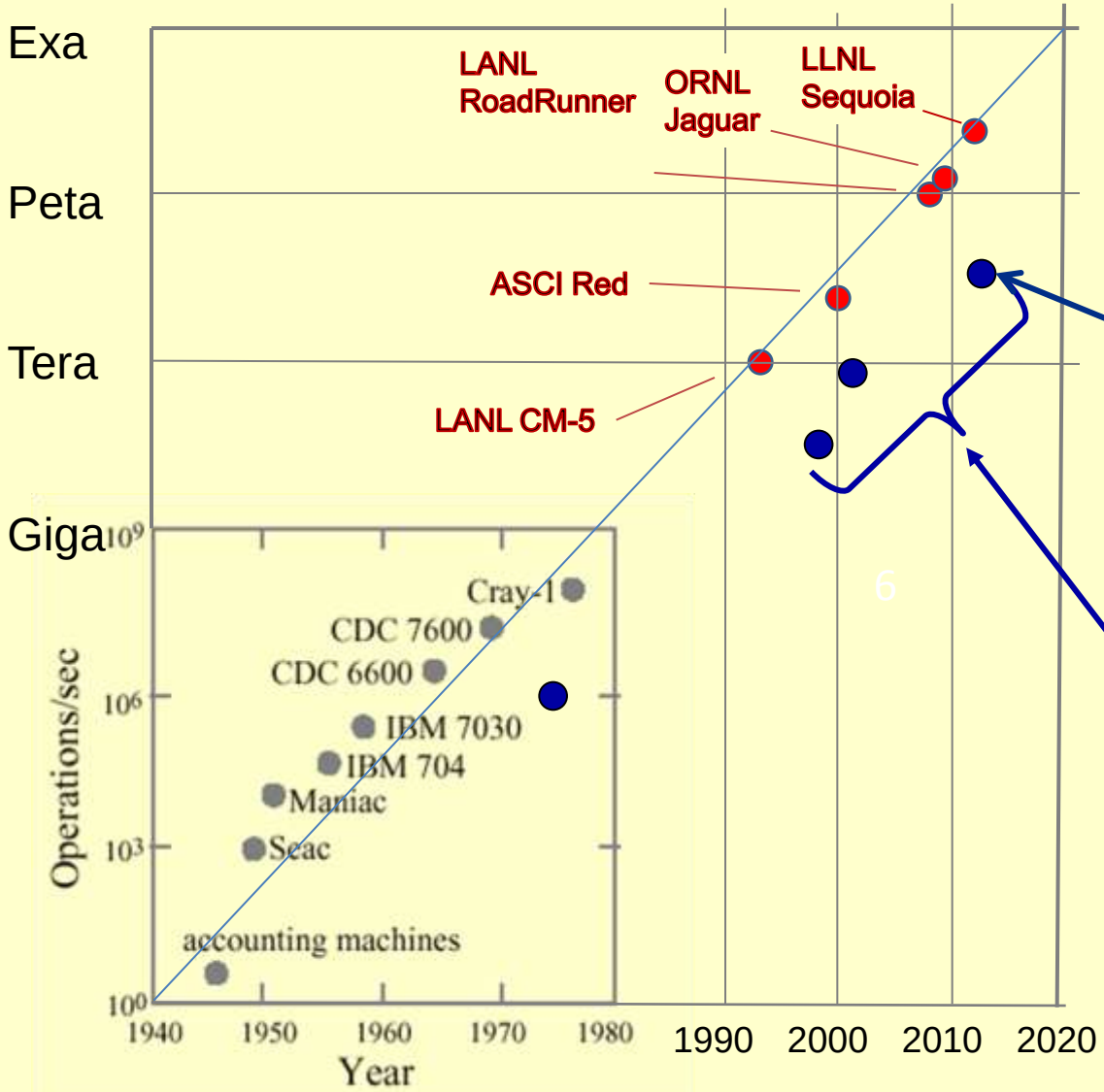
History of HPC…at DOE & P&G



U.S. DOE 'Leadership' Class Machines

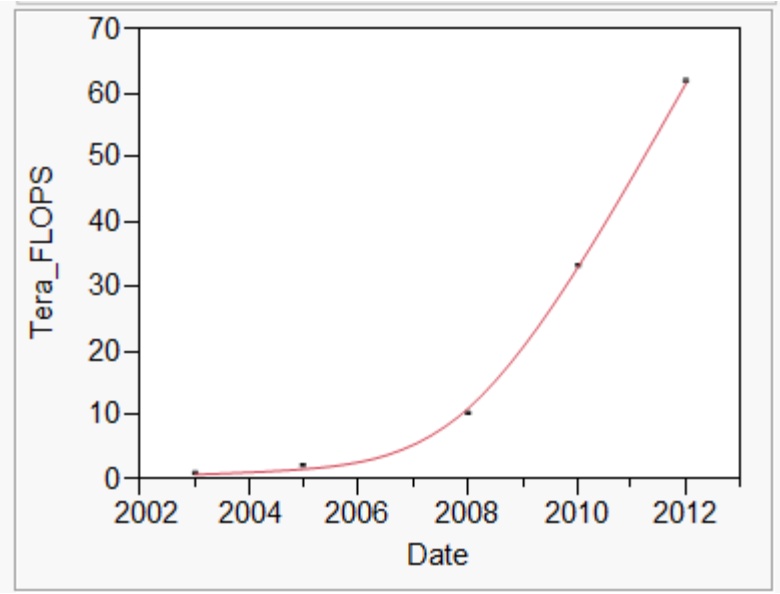
62 Tflops …499th IF we applied

P&G's 1st, 2nd, & 3rd Generation Super Computers

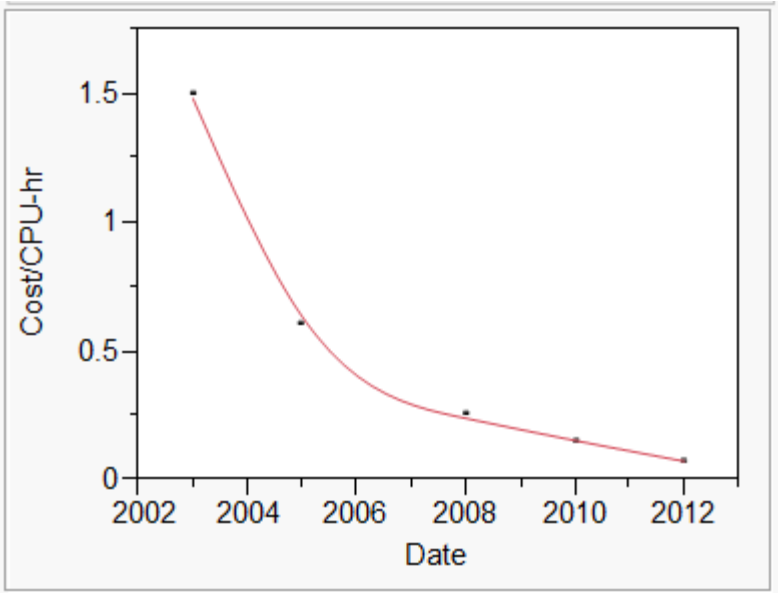
Source: Norman Johnson – T3 LANL… Circa 2000

P&G Decades History of HPC

Computer Power (FLOPS)



Hardware Cost $/CPU-hr



Software Costs have 2x to 3x over the same period!

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Another ‘Bet’ I would place…

Replace:

Slow and Expensive
Physical Learning Cycles

With:

Faster, Smaller Experiments; Virtual
Models & Simulations

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How?

Replacing ‘Physical’ learning … with ‘Virtual’…

Requires a relentless pursuit of …

REALISM

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Realism Requires fidelity and Reach…

- Tackle 'Bigger' more complex Problems more Completely
  - (e.g. multi-physics… broaden temporal & spatial scales)
- Solve Larger equation sets…
  - (Billion Elements, Billion Atoms/Molecules…etc.)
- Do parametric studies vs. point estimate Calculations
  - (Stochastic parameter inputs, Ensemble Averages)
- 'Turbo Tax' Analysis…Shape more Decisions with more 'Amateur' Analysts
  - (Automate for Practitioners, what requires an expert today)

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Must have Top Management ***Public*** Support

M&S must be a win for THEIR jobs…
their stakeholders, board members
etc.

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NOVEMBER 2011

McKinsey Quarterly

Inside P&G's digital revolution

CEO Robert McDonald wants to make the consumer goods giant the world's most technologically enabled company. Here's how.

Digitizing innovation

We're even digitizing the creation of molecules. For example, in the research and development for our new dishwashing liquid, we used modeling to predict how moisture would excite various fragrance molecules so that throughout the dishwashing process you get the right fragrance notes at the right time. We did that all virtually.

The digital workforce

"We needed people with backgrounds in computer modeling & simulation."

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Take Away This….

- ‘Cash in’ Moore’s Law:
  - Replace slow & expensive learning with smaller, faster & Virtual
  - The Relentless Pursuit of Realism…Higher Fidelity.
- Moore’s law Continues…Parallel
  - Software is the Key, who is working on it?
  - Solvers must Spatially & Temporally scale.
- Analysis ‘Democratizes’
  - HPC & M&S skills: Base for all Engineers & Scientists.
  - Simulation Data Management will Emerge.

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