Advanced Scientific Computing Advisory Committee

Gaithersburg, MD
October 28, 2008
The Modeling & Simulation behind everyday Products

Tom Lange
Director, Procter & Gamble
Modeling & Simulation
Global Capability Organization R&D
...Founded in 1837

Started with STAR Candles

Introduced Ivory Soap In 1879

‘Cleaning’

P&G Is the 4th Oldest Entity of the Fortune 50

‘Lighting’

James Gamble
Soap Maker

William Procter
Candle Maker
...After a hundred years

CLEANING

1937
...By the time I was born

Clothes
CLEANing
House
Teeth & Hair
EATing
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.


- **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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Consumers Know Us by...

Beauty
Health Care
Fabric Care & Home Care
Baby Care & Family Care
Snacks, & Pet Care
Blades & Razors Duracell & Braun

P&G

300+ World Brands...
23 Billion $ Brands...

Beauty

Health Care

Fabric Care & Home Care

Baby Care & Family Care

Snacks, Coffee & Pet Care

Blades & Razors

Duracell & Braun
Why Brands?
The Two Moments of Truth
OK…
Enough of the B School take on things…
Second moment of Truth

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

**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.
We make billions of products a year…

And sell them for < $10 !
Make a Billion Diapers…

How long does it take to make a billion Pampers?
Splicing Webs…

What Happens…
When you miss!
'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
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

Now CPG… FMCG
...Atoms to the Enterprise

Product/Device/Package

Process & Making

Mechanical & Converting

Supply Chain Throughput & Reliability
Scales of Modeling

- Quantum Chemistry - subatomic
- Molecular Mechanics - atoms, molecules
- Coarse Grain or Mesoscale Modeling – Polymers
- Continuum or Finite Difference Finite Element
- MechEng/ChE (Closed Form Equations)
- Computer Aided Engineering (CAE)

- Industrial Eng/Operations Resrch (Statistical, Discrete Event, Agent Based)

Time: ns, ms, sec, hrs, days
Distance: angstroms, nm, microns, mm, m, km
Empirical & Optimization

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

Winner of Several Joint Awards with Los Alamos National Laboratories

***Collaboration began in 1994

2002 T&B Award

2003 Research Collaboration Award

2003 Council for Chemical Research (CCR)

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Solid Mechanics:

- Rigid Body Kinematics
- Finite Element Analysis (FEA):
  - Implicit
  - Explicit
  - Linear
  - Non-linear
  - Massive Contact
The new premium shaver …
Braun Drop

Lots of Small Parts...

…Everyone must work!
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
Optimizing the bottle weight: profiling the parison.
Load Cases

Top Load Empty

Pressure

Vacuum

Squeeze

Top Load Filled

Hydrostatic
Can We Pack it?

Bottle Race Track
‘Circa 2000’
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
Mixing liquids:

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Mixing Dense Viscous Fluids
Make a $10^9$ Pringles?

How long does it Take to make a Billion Pringles?
Make a Billion Pringles…

…Aerodynamics are Relevant
Virtual Filling

Air Entrainment During Process Of Bottle Filling

No air entrainment    150 oz - time = 0.05    With air entrainment
What are the areas of Challenge & Research?

Multi_Physics...
Liquid Bottle Drop

What You Don’t In WalMart
Or Your Laundry Room!
Material Properties Are The Key To Predicting Reality!
FSI: Fluid Structure Interaction

Sheet Flutter
Sheet Flutter w/flow Field
Computational Chemistry Disciplines

Atomistic & Quantum Methods

Molecular Dynamics

Meso-scale Methods

QSAR/QSPR

Virtual Library Synthesis

Nearest Neighbor Searches
Quantum Chemistry

- Electronic properties
  - Reactivity
  - Structural details
  - Spectral properties

- Femto-seconds, tens of atoms

- Challenges: simulating dynamic reactivity
  - Hardware capacity
  - Theory (shortcuts) and software development
**Perfume Residuality QSAR**

5 Variable Model, $R^2 = 0.95$

$N = 30$

Log Observed Headspace Conc.

**Good**

Damacenone

**Poor**

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

Modeling identified new technology which was not apparent from empirical testing

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Stability of Complex Fluids

Increasing Age

Increasing ‘Phase Separation’
Multi-Scale Problem: Predict Viscosity Stability

Molecular Dynamic Simulations → Microscopic Flow Models → Probability Functions

- rigid blob model of active ingredients
- 2 interacting bilayers
- interactions of vesicles
- implications for liquid flow and stability
- Shelf Life Prediction

Nano-Meters → Nano-Seconds → Centimeters → Months
Coarse-Grained Molecular Dynamics of Suds / Cleaning

Kelly Anderson, Xibing He, Russell Devane, Michael Klein (Upenn)

Phospholipid membrane... interacting with a vesicle.
**Multi-scale modeling of surfactant lather for shampoos**

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

New surfactants designed for consumer preference
Predicting equilibrium surface structure

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.
Initial: Surface Area / Molecule = 45 Å^2

Final: Surface Tension = 43 mN/m

Initial: Surface Area / Molecule = 22 Å^2

Final: SA/M = 46 Å^2
ST = 45 mN/m

Predicting equilibrium surface properties
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
The Grand Cleaning Model

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

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

- ‘Soil’ Removal
  - Emulsification
  - Solubilization
Modeling of formulations shows the spontaneous formation of vesicles. Is this realistic or a finite size effect? Attempted fusion of two vesicles (cross section). Fusion is not spontaneous!
The High Performance Computing ‘opportunity’
‘Moore’s Law’
Computing Hardware Performance

U.S. DOE ‘Leadership’ Class Machines

P&G’s 1st, 2nd, & 3rd Generations

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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.
Future of HPTC…

What are we going to Do with All that Power?
How do we cash-in ‘moore’s Law?
How do we cash-in ‘moore’s Law?

Pursue Realism...

Replace Full scale/speed Tests!!
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
The Challenge?...
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)