Why the '*Rocket Science*' for Such Everyday Products?

- Products must *perform* ...2nd moment of truth.

- *Performance* ... is often about Fundamental Science & Engineering Contradictions.

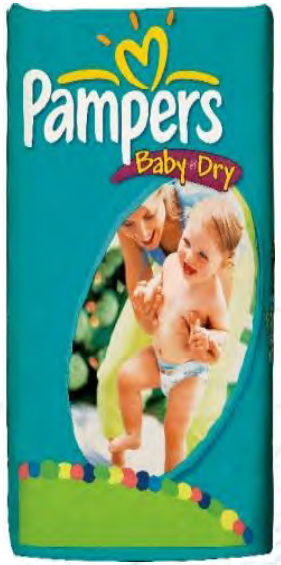
Modeling & Simulation

The power to transform

Engineering 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.

The Cleaning Contradiction…

- Remove or make unnoticeable: ‘Soil’ , ‘Stains’ & ‘Odors’

- Leave the rest unaltered: Fibers, Dyes, Surfaces, Hair, Skin, pets

Except…

‘what it smells like…’

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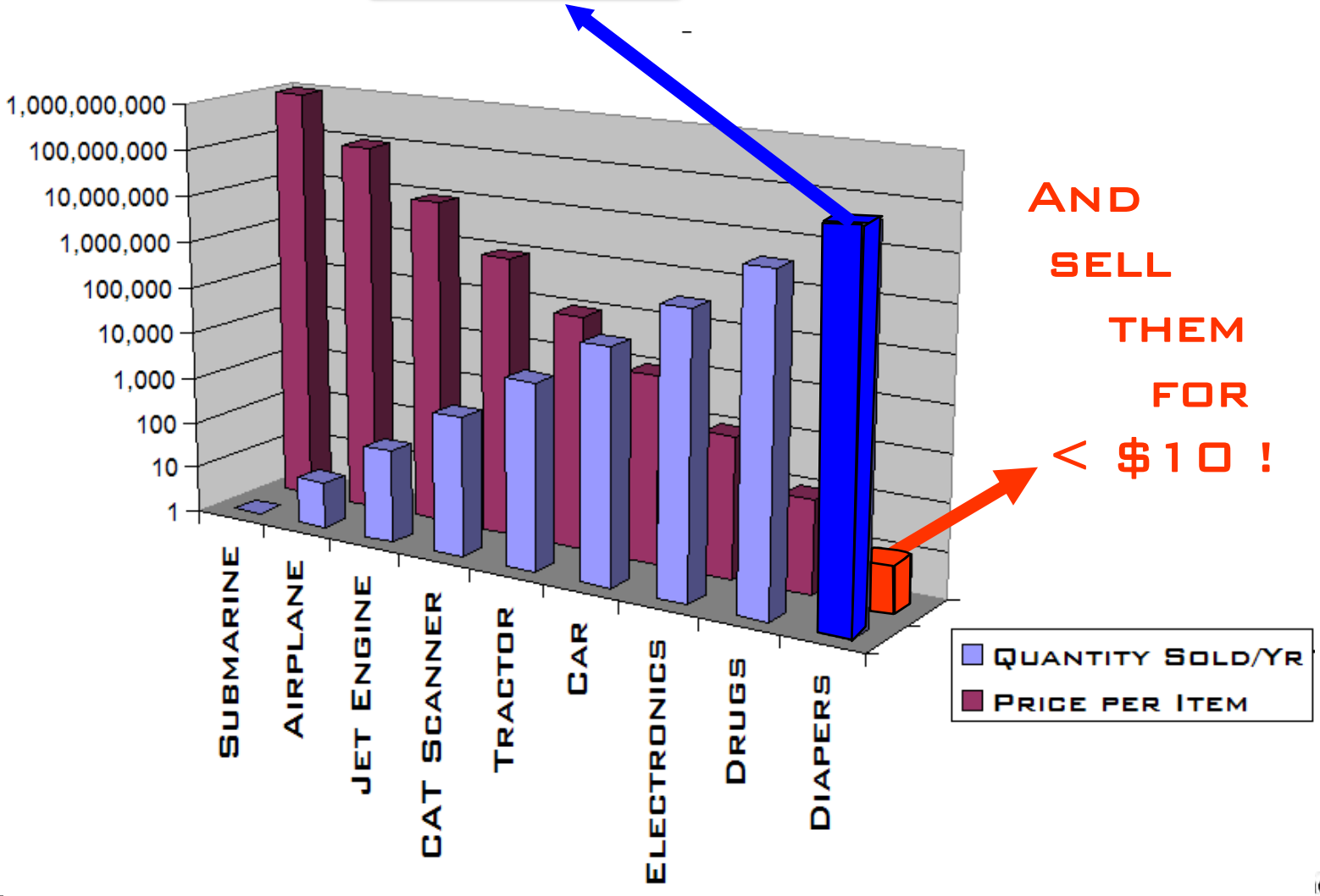
Scale: Sell a Billion $

We make **BILLIONS** of products a year...



And sell them for < $10 !

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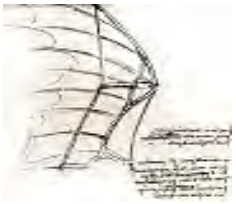
Innovation Learning Cycle



- 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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Modeling & Simulation has 'Transformed' Industries?

1940's-1970's

Defense

1970's-1980's

Aviation

1980's-1990's

Automotive

1990's-2010+

Consumer Goods

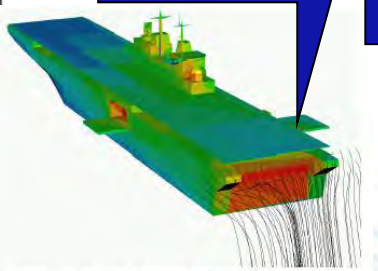
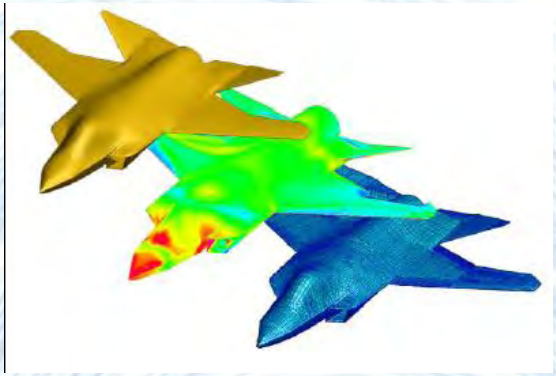
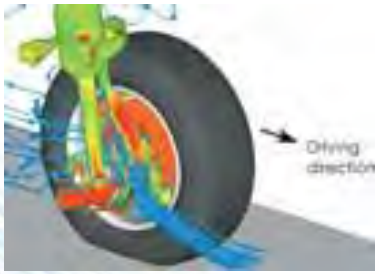
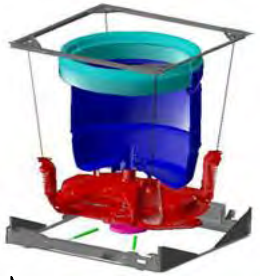
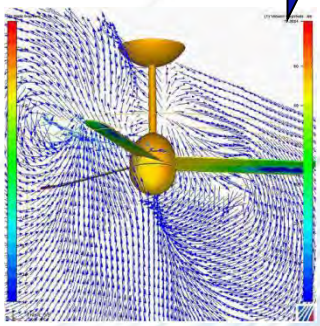


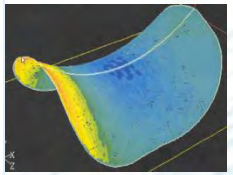
Figure 11: Simulation of full LHA and V/STOL aircraft with the FPV model.











Now CPG ...

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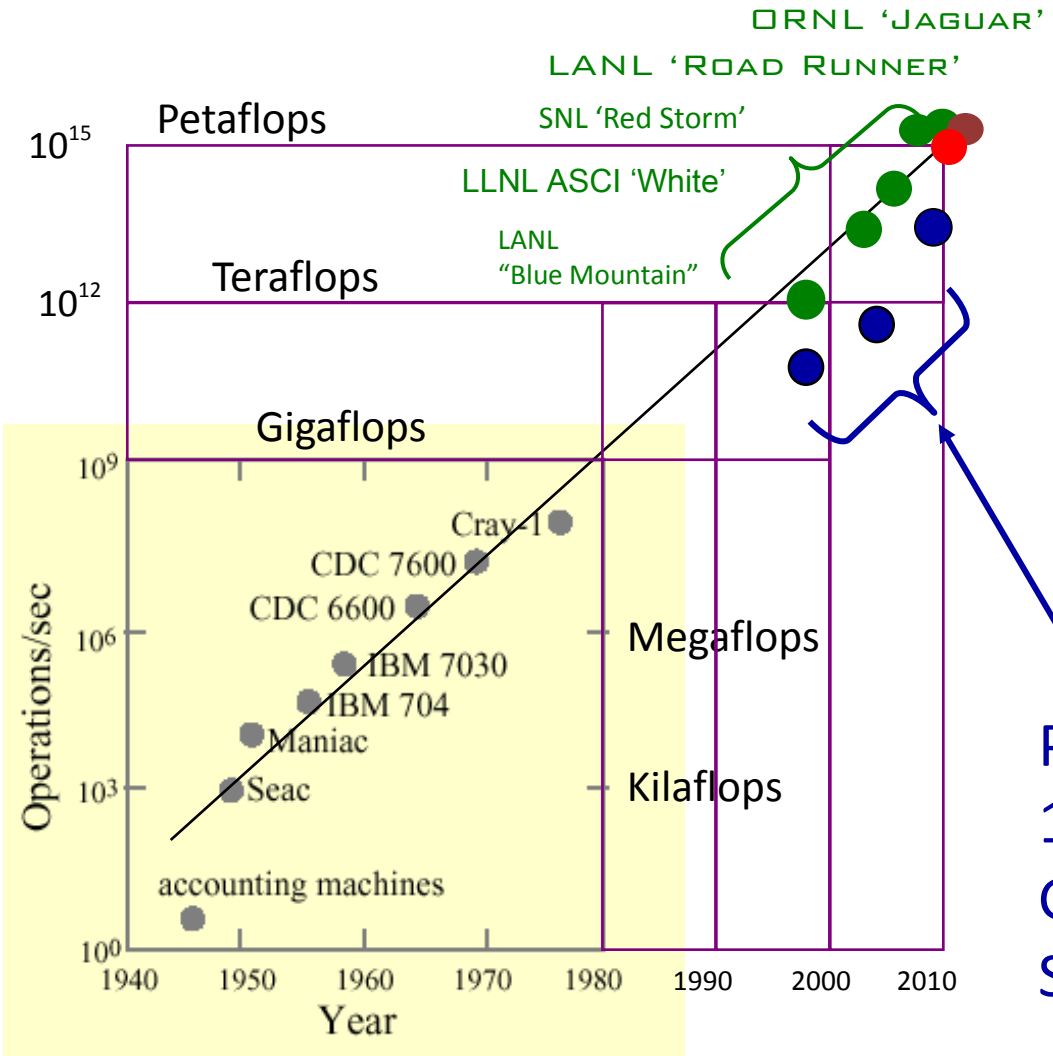
A Trend I Bet on…'Moore's Law'

Computing Hardware Performance



U.S. Dept. of Energy 'Leadership' Class Machines

U.S. NSF 'Tier 1' Blue Waters

Chinese Gov't

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

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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What are we going to do with All that Power?

Modeling & Simulation
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‘Cash in’ Moore’s law

Replace:

Slow and Expensive Learning Cycles

With:

Faster, Smaller Experiments; Virtual Models & Simulations

Modeling & Simulation
The power to transform

Replace 'Physical' with 'Virtual'?

THE PURSUIT OF

...

REALISM

Modeling & Simulation
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Realism Requires...

- Tackling 'Full Complexity' Problems
- solving Larger equation sets...
  - (Billion Elements, Billion Atoms/Molecules...etc.)
- parametric studies vs. point estimates
  - (Stochastic parameter inputs)
- Non-Experts do Analysis...
  - Automate for Practitioners, what requires an expert today

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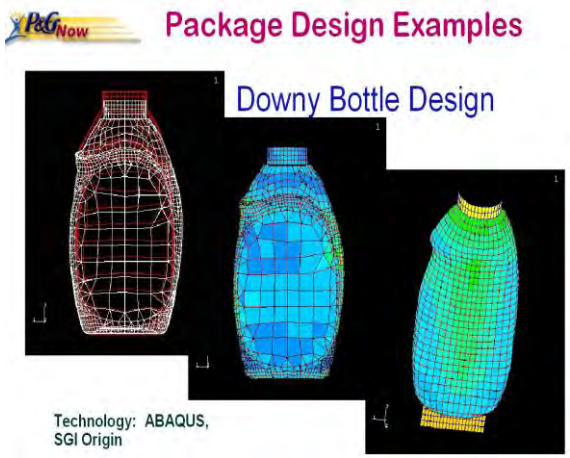
Our M&S Approach...

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

'VIRTUAL' ones that...



- Fit
- Work
- Make Financial Sense

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

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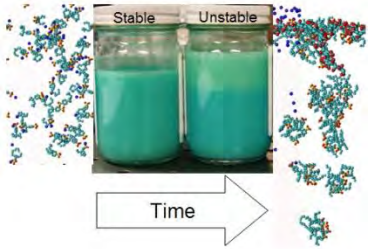
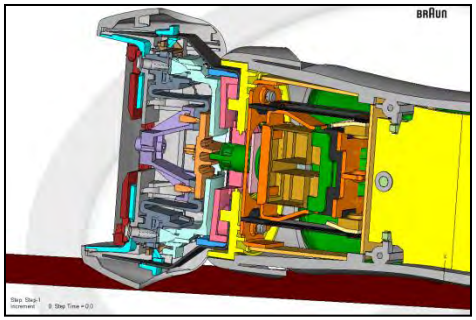
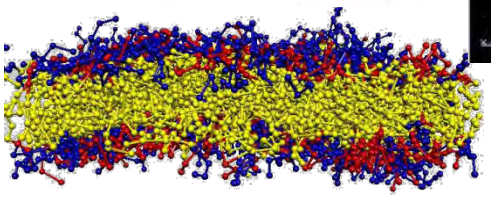
...Atoms to the Enterprise

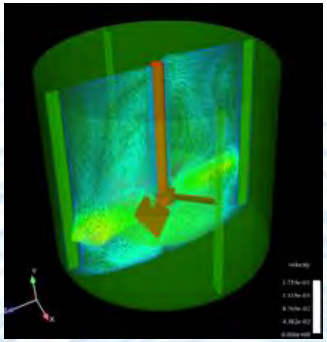
Product/ Device/ Package

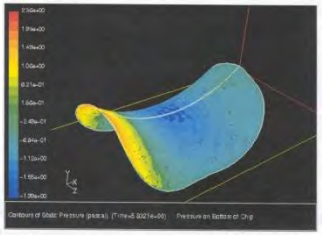




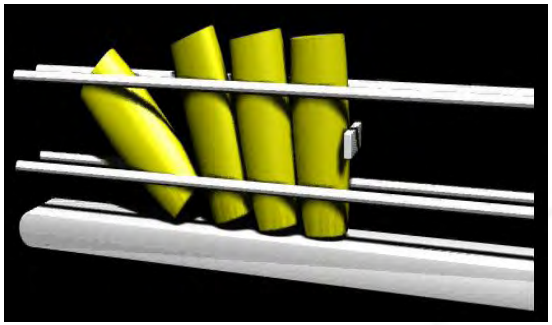


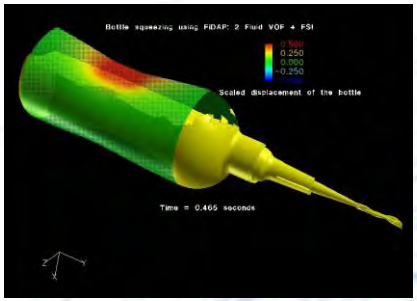
Process



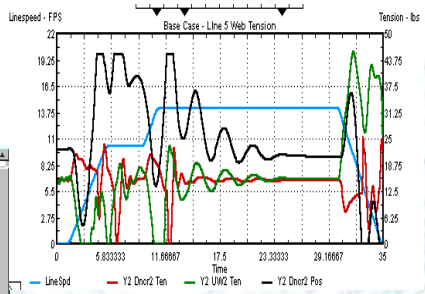


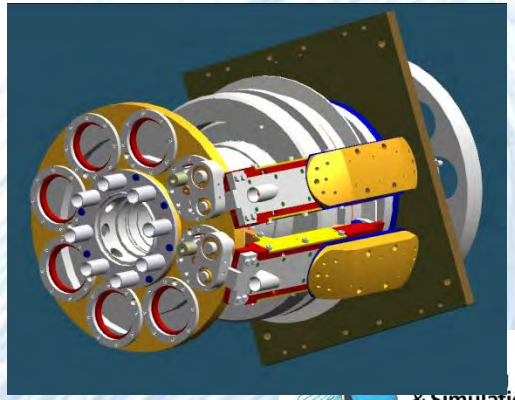
Pressure on the Bottom of the Chip



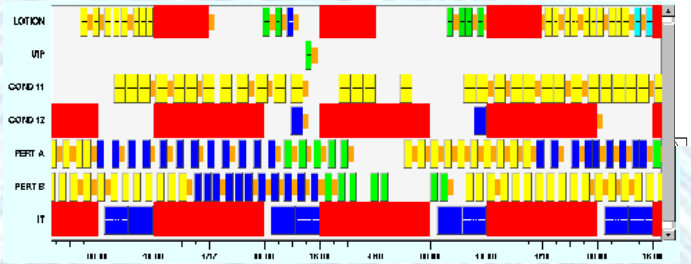


Mechanical & Converting





Supply Chain, Through-put, & Reliability



& Simulation

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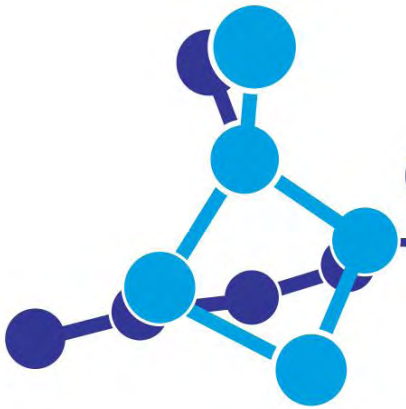
Examples

M&S 'Brands'



Computational Chemistry

CAE

computer aided engineering

Modeling & Simulation

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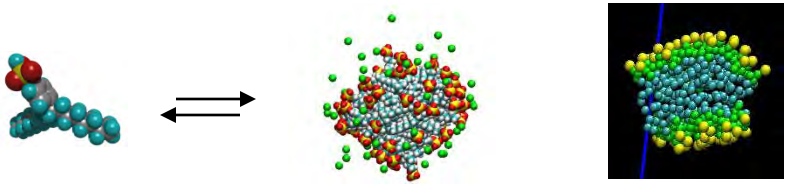
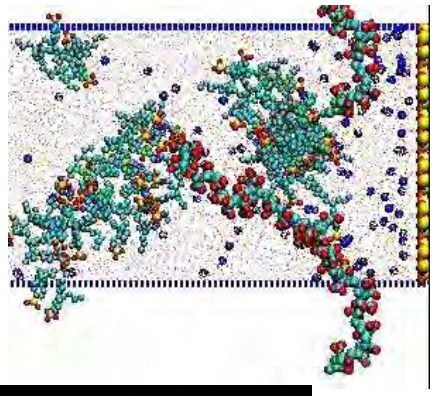
Formulations & Cleaning

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



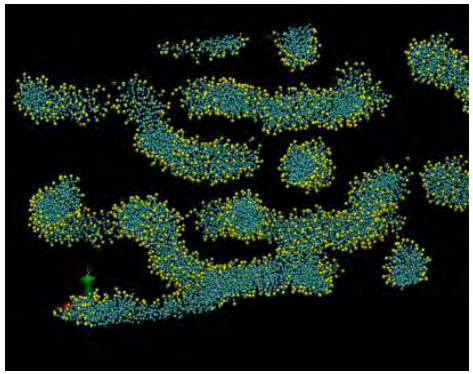
Spherical or lamellar (bilayer)

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

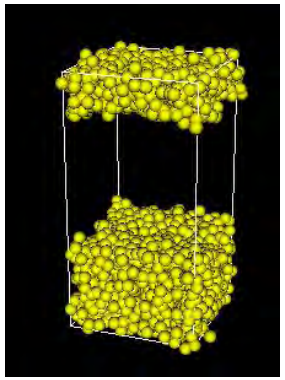


Surfactant at a clay surface

- **'Soil' Removal**
  - Emulsification
  - Solubilization



cylindrical micelles



oil-water interfaces

Computational Chemistry CADMol

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

Modeling & Simulation
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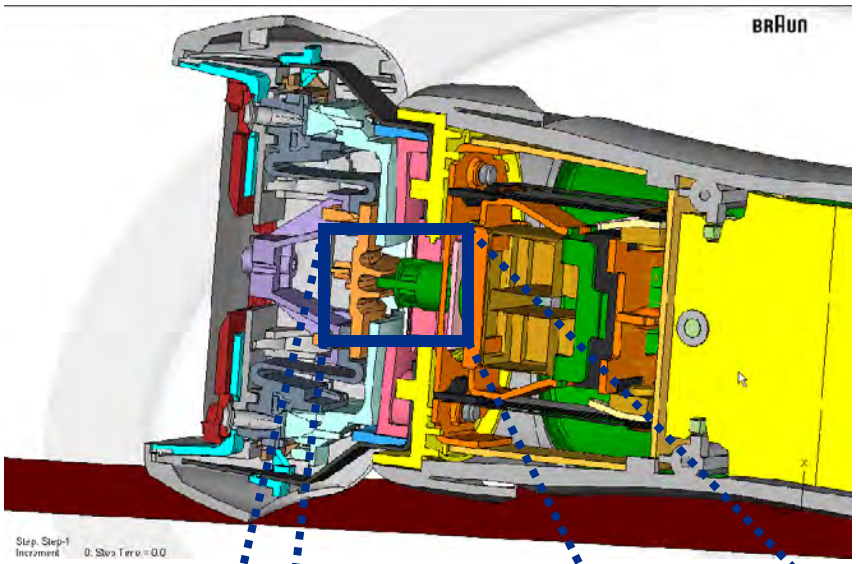
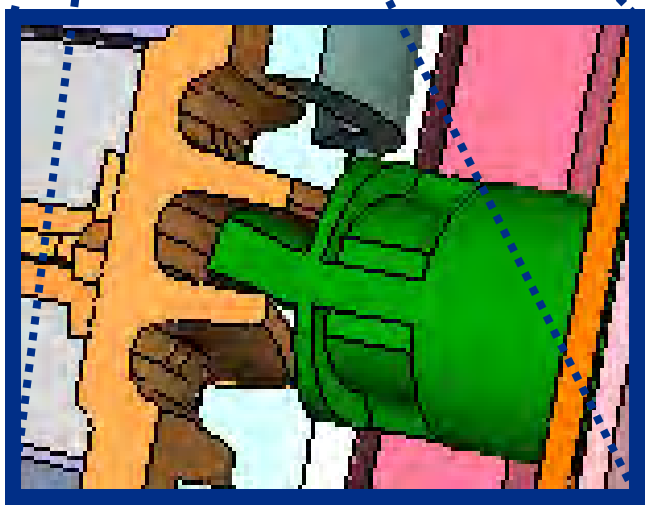
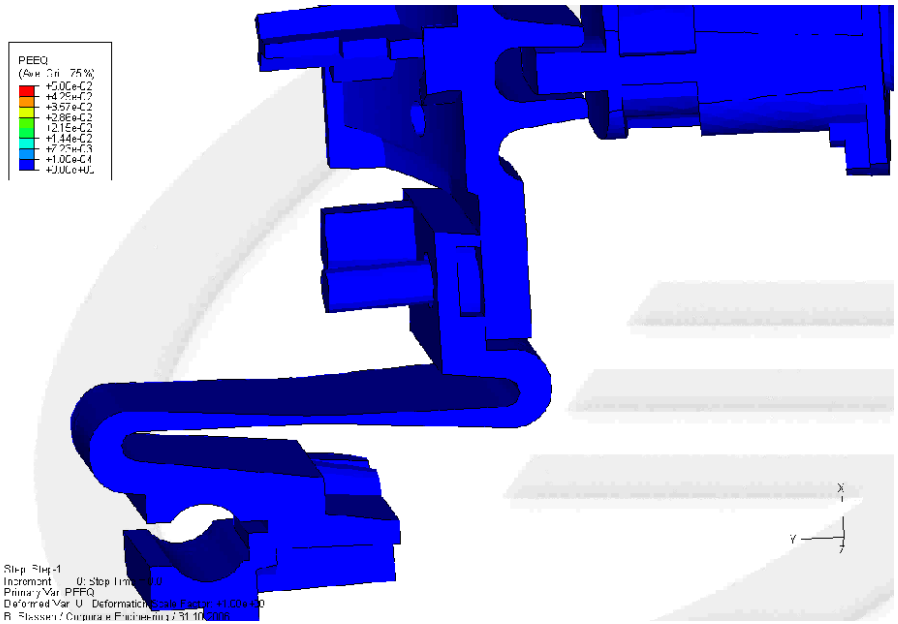
Bathroom Floor Drop







Lots of Small Parts...

...Everyone must work!

Modeling & Simulation

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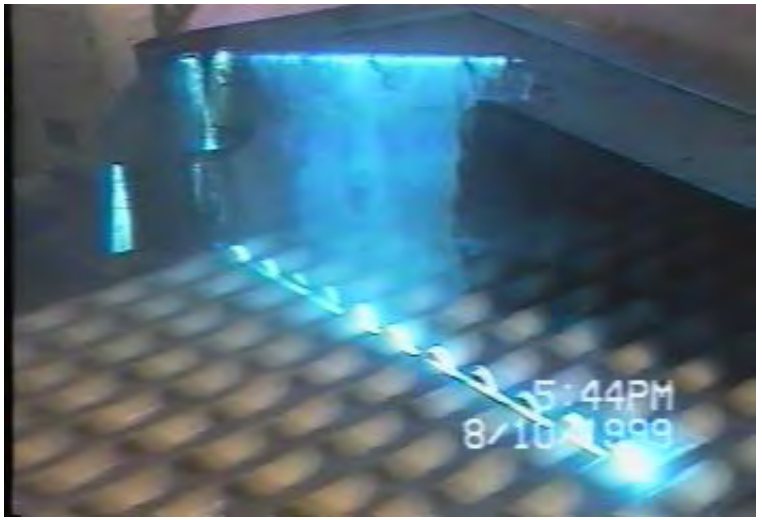
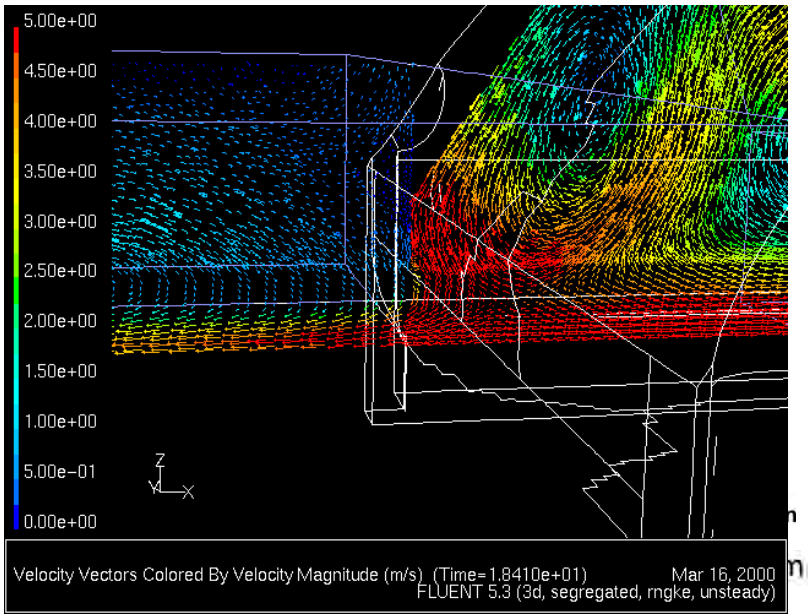
Fluids / Thermal

- **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

Modeling & Simulation
The power to transform

Making a 10^9 Pringles?

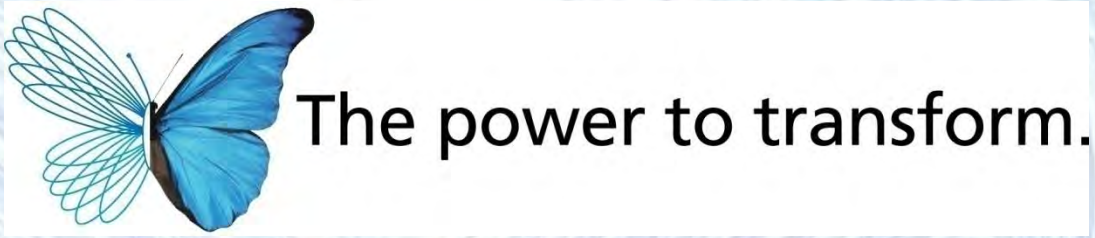




How long does it Take to make a **Billion** Pringles?

What are the areas of Challenge & Research?

Multi_Physics…



Multi-Scale challenges

High Performance Computing using 10^3 - 10^4 processors Enables:

- Spatial Domain De-composition of large complex problems

Multi-Scale Problems Also Require:

- Temporal Domain compression or De-composition to enable large numbers of processors to solve.

Modeling & Simulation
The power to transform

Multi-Physics Challenges

Chemical Systems Multi-Physics :

- Crystallization, Agglomeration, Chemical RX
- Reactor Designs

Structure / Fluid Coupling:

- Free Surface Flow on and through Compressible
- Partially Saturated Porous Media

Fluids / structure Interaction FSI:

- Flexible Films in Fluids e.g. 'flag waving'
- Squeezing to Dispense from Bottles
- Container Sloshing, Bottle Drop

Modeling & Simulation

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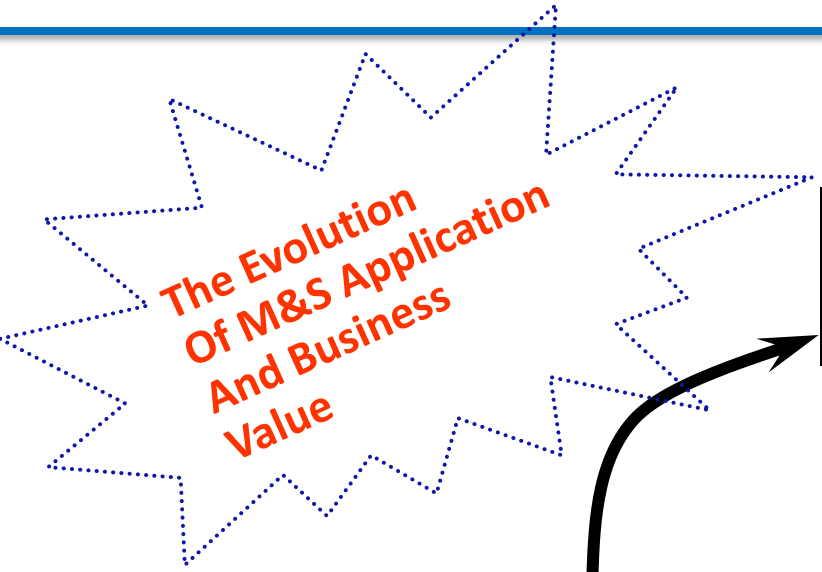
...How do we USE the Power!



"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

Modeling & Simulation
The power to transform

M&S Work Process

What if ? ,
Why not ?,
How much?

Define Problem

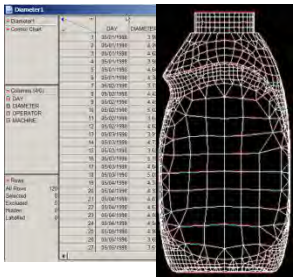
1. Translate Business Challenge into Science question

2. Express Science in Equations

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

Gather Input Data

Consumer, Reliability Material Properties, Geometry etc.

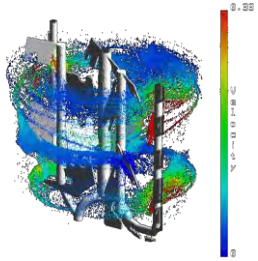


Solve Equations

1. Solve Equations
2. Build Simulation

Display & Validate

Display results
For non-expert understanding



Shape Decisions

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

Modeling & Simulation
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Themes for the Future

- Moore's law...but Parallel
- Application Software...the current 'issue'
- 'Democratization' of Analysis
- Business value...replacing slow & expensive learning with virtual
- Computing Skills & computational Awareness the MOST important trend for practicing Engineers

Modeling & Simulation
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