Integrated Computational Materials Science & Engineering

3/3/2012

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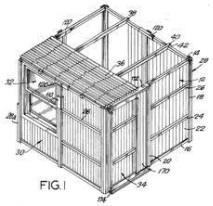
Thesis Statement

Future innovation in defense-related products is critically dependent upon *simultaneous co-selection* of material properties, product design, and manufacturing process.

Material Choices:
- Brick
- Straw
- Wood
- Composite
- Gingerbread

Interdependent!

Manufacturing Process:
- Whittle down sticks
- Bundle 10 to a tow
- Precision placement
- Glue?



Product:
- Roof, walls, door
- Hurricane Safe
- Well-ventilated (airflow/hour)
- Max Cost < $1000
- Max Weight
- Min Volume

Thesis Statement

This type of co-design is *only possible* with the maturation of advanced computational methods:

1. **Multiscale modeling**
2. **Material informatics**
3. **Computational manufacturing**

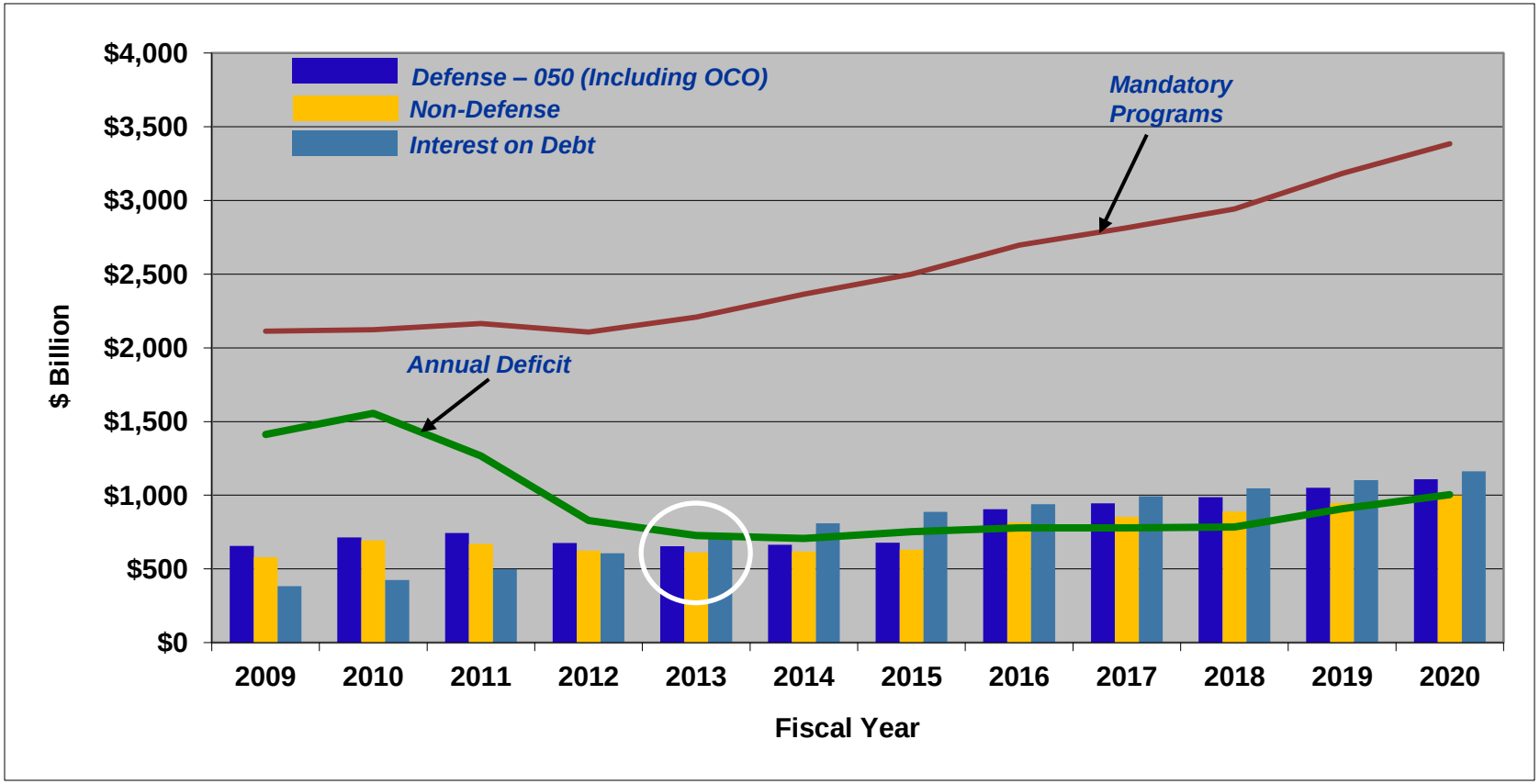
The ultimate goal of ICMSE (Integrated Computational Materials Science & Engineering) is to demonstrate we can do simultaneous co-design!

Outline

- **Introduction: Why do we need ICMSE?**
- Case Studies
- Conclusion and Future Work: *What problems need to be solved?*

Federal Budget Outlook

(Outlays $ Billions)

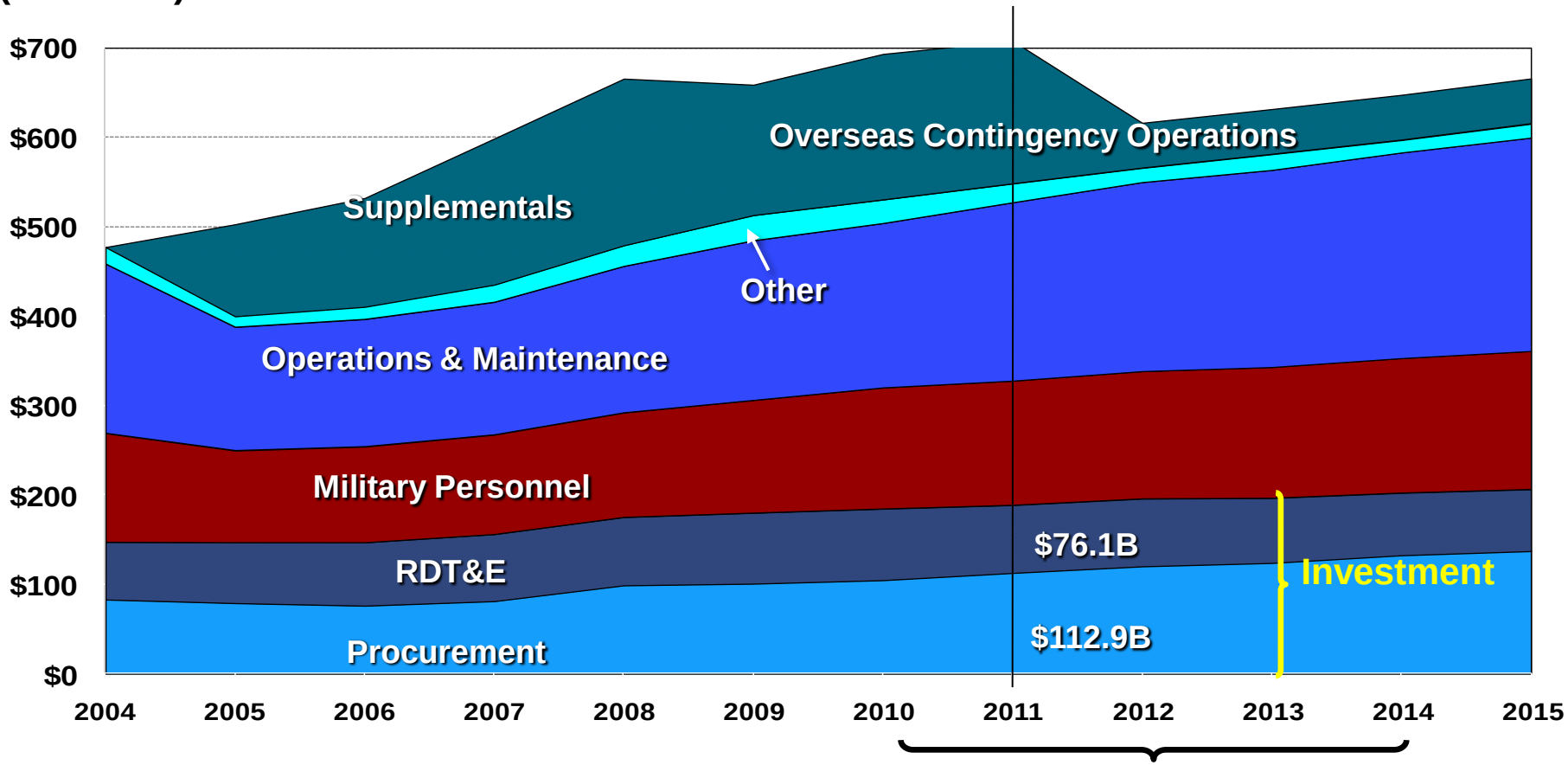


Source: OMB

Interest on Debt Exceeds Defense Spending Starting in FY2013

DOD Budget by Title

($ Billions)



Source: OMB and DOD FY11 Budget Request Documents

Eng. and Mfg. Affordability are King in next Decade(s)

Funding covers much wider threat spectrum; flexibility needed

Solution: Advanced Materials

- e.g., carbon nanostructures
- Need <u>multiscale modeling</u> with <u>robust model linkages</u>
  - ***<u>Fast, simultaneous co-design</u> in simulation to reduce redesign***
  - ***Virtual Microscope***
- Simultaneously, maximize performance and efficiency (cost, weight, manufacturability)

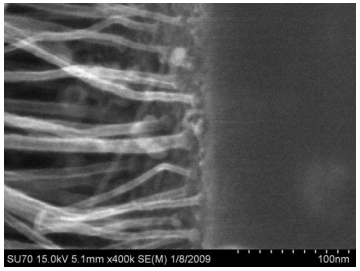
device / structure

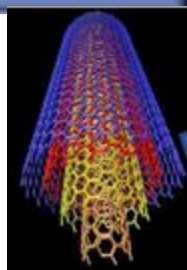
micro scale

meso scale

Atomic scale

Quantum Scale





Improved products at for lower cost

Outline

- Introduction: What is ICMSE, why do we need it?
- **Case Studies**
- Conclusion and Future Work: *What problems need to be solved?*

Scalable Nanocomposites

CW COMPOSITESWORLD

CW WEEKLY E-NEWSLETTER

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HIGH-PERFORMANCE Composites

May 2011

Nanotechnology: Into the realm of real

Fast, scalable process grows nanostructures directly on composite reinforcements for a "drop-in" use in volume production processes.

Author: Sara Black
| Posted on: 5/2/2011
High-Performance Composites

52

A new partnership between Applied Nanostructured Solutions (ANS) and Owens Corning seeks t...

Step 1: The enclosed

Nanocomposites research and the massive benefits it promises have attracted considerable press coverage over the past decade. Actual commercial development of nano-based products for composites, however, has been slow. But a new partnership between Applied NanoStructured Solutions LLC (ANS, Baltimore, Md.), a Lockheed Martin subsidiary, and Owens Corning (Toledo, Ohio) is about to accelerate growth. ANS has worked for more than three years to develop a rapid, scalable manufacturing process that can produce reinforcements infused with carbon nanostructures (CNS) for composites fabrication. With Owens Corning now on board as a joint development partner, ANS seeks to commercialize the process for high-volume applications.

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From specialty fillers to space elevators
Nanomaterials research and early commercialization set stage for promising future of nanocomposites....

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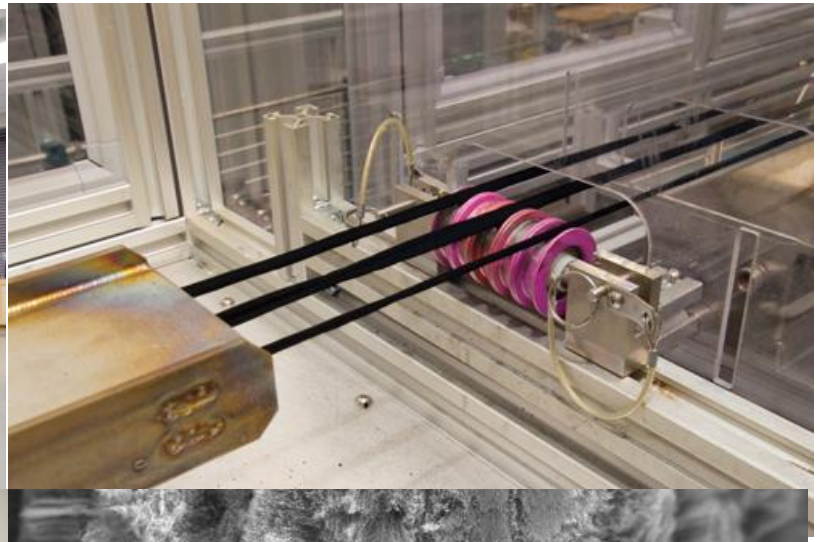
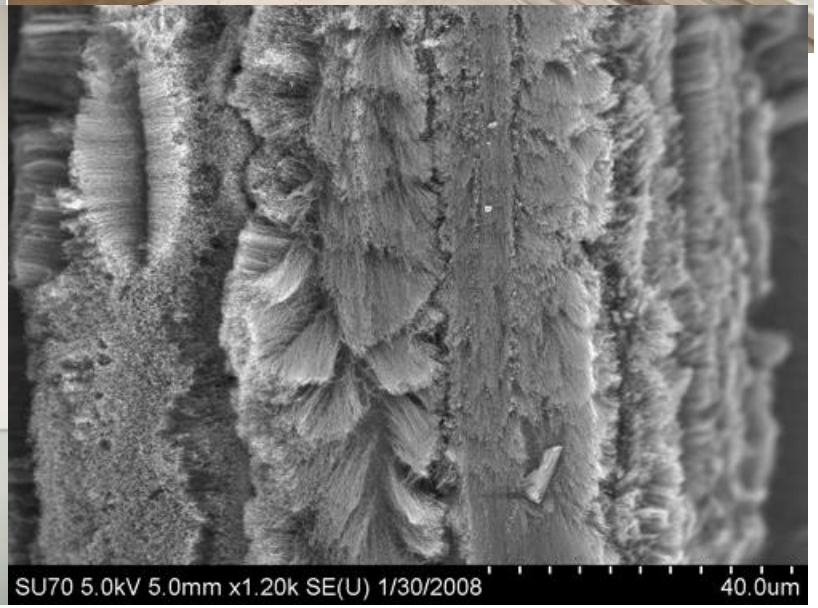
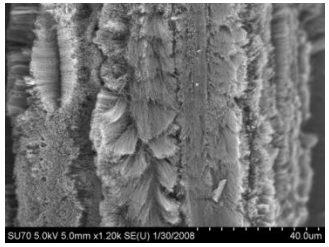
Scalable Nanocomposites



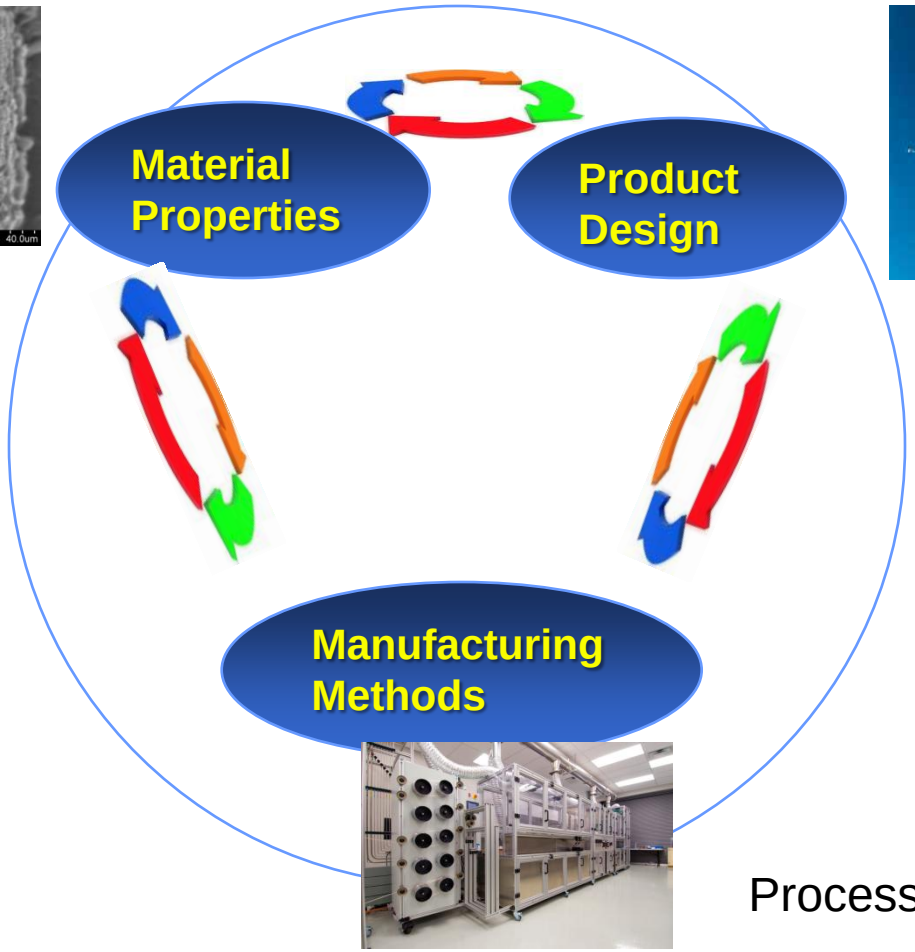


Multiscale Modeling in the Loop

Material models from nano to micro

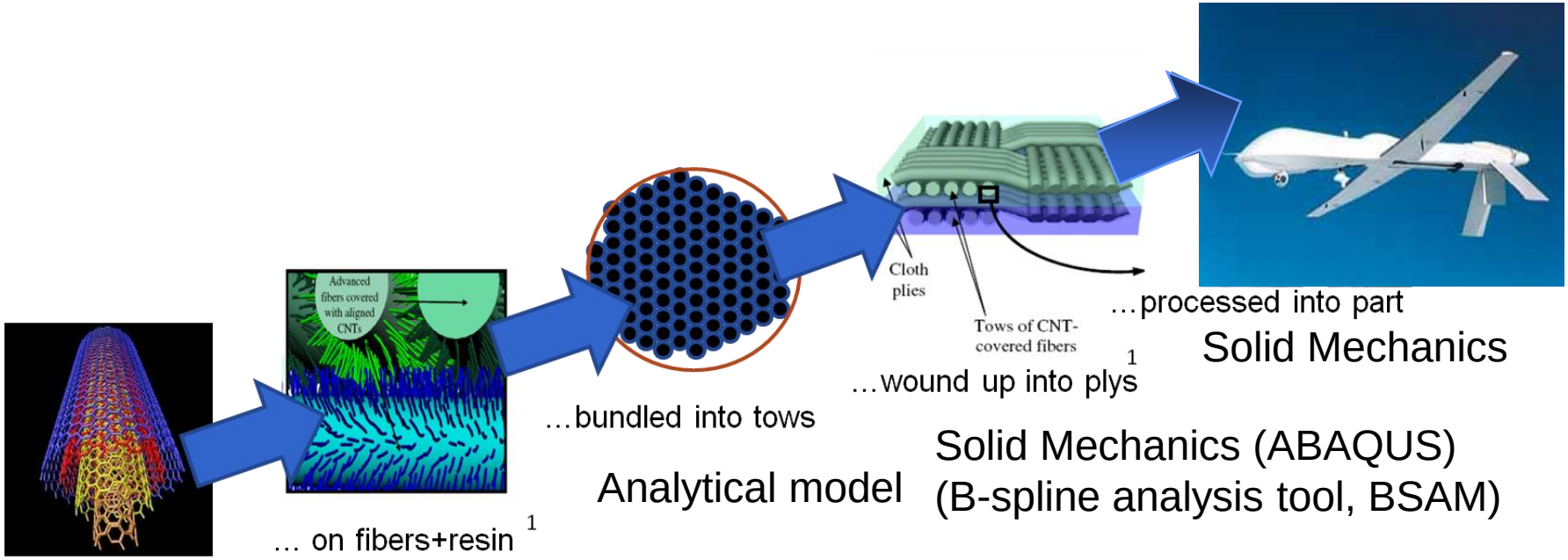


Macroscale models of Product Topological optimzation



Process Models

Multiscale Modeling Hierarchy



CNTs

… on fibers+resin [1]

…bundled into tows

…wound up into plys [1]

…processed into part

Molecular Dynamics (LAMMPS),
Concurrent Finite Element (ABAQUS, MDS)

Analytical model

Solid Mechanics (ABAQUS)
(B-spline analysis tool, BSAM)

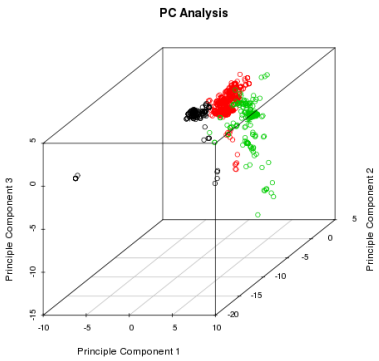
Solid Mechanics

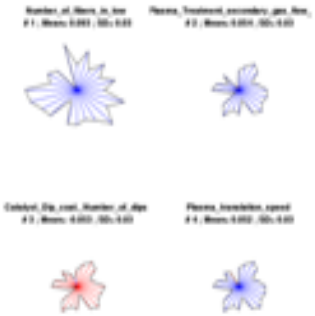
First Principles (VASP)
Molecular Dynamics (LAMMPS)

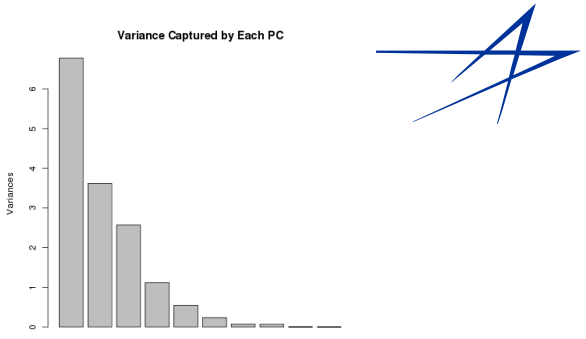
Multiscale Modeling can be an Art, Few Standard Tools.
Sometimes problems can be too complex to model!

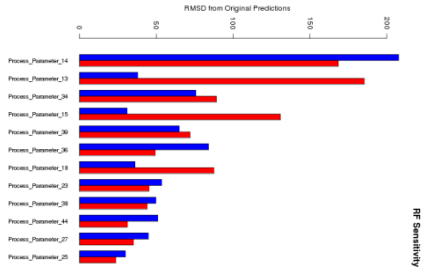
[1]Picture credits: Brian Wardle, *et al*.

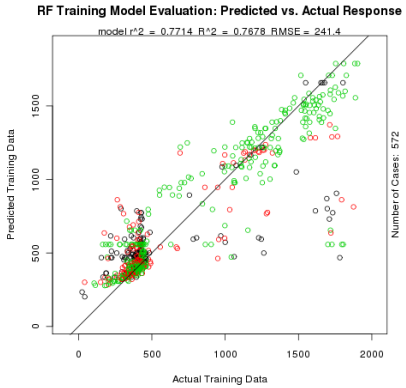
Informatics Analysis Tools



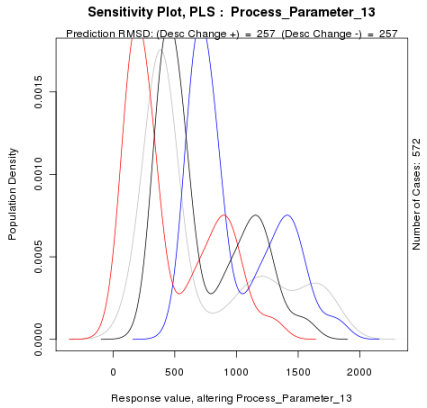








- Multiple Linear Regression (MLR)
- K – Means Clustering (PCA)
- Partial Least Squares (PLS)
- Support Vector Machines (SVM)
- Random Forest (RF)
- Star Plots
- Y-Scramble Validation
- Predictive Analysis
- Sensitivity Analysis
- Multivariable Comparative Analysis
- Multivariable Predictive Analysis
- Inverse-QSAR



A combination of linear and nonlinear modeling with data visualization addresses model interpretability and predictivity

The Importance of Informatics

The hot tech gig of 2022: Data scientist

FORTUNE

By Jessi Hempel, writer January 6, 2012: 5:00 AM ET

By the end of the decade 50 billion devices will be emitting information nonstop. Data scientists will help manage it all.

FORTUNE -- A decade from now the smart techies who decided to become app developers may wish they had taken an applied-mathematics class or two. The coming deluge of data (more on that in a moment) will create demand for a new kind of computer scientist -- a gig that's one part mathematician, one part product-development guru, and one part detective.

D.J. Patil is a pioneer in the field of data science, a new discipline that aims to organize and make sense of all the data generated by machines. It's a challenge that will grow exponentially over the next decade.

Tech in 2012: Face-offs, failures and fairly big changes at the office

Today there are some 400 million devices connected to the Internet, mostly phones and computers. By 2020 some 50 billion devices, from cars to appliances, will be

PHOTO: CODY PICKENS

D.J. Patil: "If you can't measure it, you can't fix it."

http://tech.fortune.cnn.com/tag/data-scientists/

3D Printing Revolution

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Video: First flight of 3D printed plane

The future of flight? (Image: University of Southampton)

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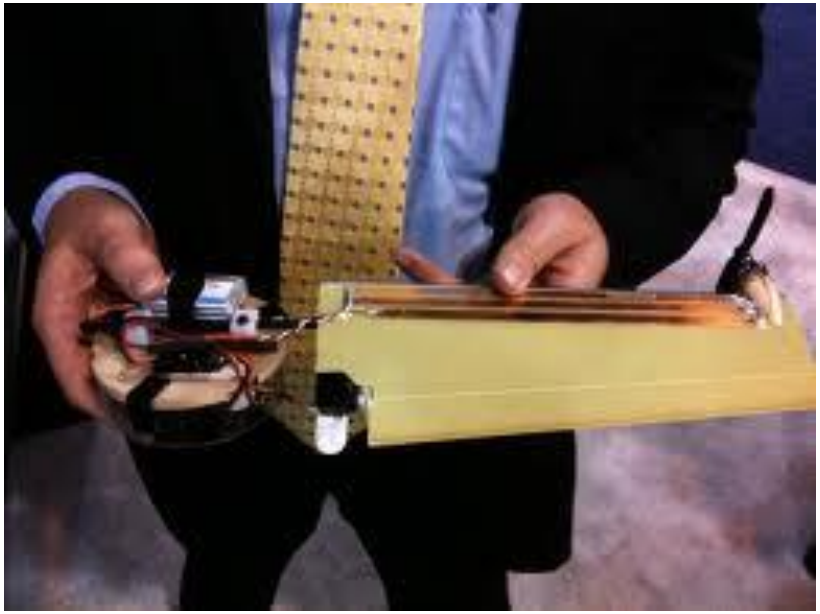
Computational Manufacturing



PRINTED SAMARAI:
(3D printed; <15 mins assembly)

Need to understand:

- **What are the properties of the material you create?**
- **What beneficial design changes does this allow you to make?**

Pouring an Airplane?

Flightglobal serious about aviation

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Lockheed Martin reveals F-35 to feature nanocomposite structures

By: STEPHEN TRIMBLE WASHINGTON DC 02:00

Source: FLIGHT INTERNATIONAL

Lockheed Martin has revealed the F-35 Lightning II will be the first mass-produced aircraft to integrate structural nanocomposites in non-load bearing airframe components.

A thermoset epoxy reinforced by carbon nanotubes will replace carbon fibre as the material used to produce F-35 wingtip fairings beginning with low rate initial production (LRIP)-4 aircraft, said Travis Earles, a manager for corporate nanotechnology initiatives.

Meanwhile, the same carbon nanotube reinforced polymer (CNRP) material is being considered to replace about 100 components made with other composites or metals throughout the F-35's airframe, he said.

The shift to CNRP as an airframe material has been anticipated ever since carbon nanotubes were discovered in 1991. It is widely considered one of the strongest materials ever invented - several times stronger than carbon fibre reinforced plastic (CFRP), yet lighter by about 25-30%.

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Conclusion

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This type of co-design is only possible with the maturation of advanced computational methods:

- **Multiscale modeling**
- **Material informatics**
- **Computational manufacturing**

Future Critical Needs for ICMSE

- **Automated, dynamically reconfigurable factories for the production of any product using any material with tailored properties in small quantities**
- **Foundational failure physics method development**
  - **Bonded joints / Large fastened structures**
  - **Moisture intrusion / impact in sandwich structures**
- **Rigorous quantification of model error**
- **Scale linkages in multiscale modeling: Mapping from first principles to semi-empirical**
- **Standardization of model interoperability (process models and material models)**
- **Multiscale *meta-workflows* and data shared across the community of interest**

Android Analog for Interoperable Structural Models and Design Tools