Lecture 29:
Verification & Validation -- and Some Examples
May 6, 2008

Jeffrey C. Grossman
Elif Ertekin
Accuracy and Validation

• Verification and validation (V&V) are processes that help to ensure that models and simulations are correct and reliable.

• Verification: “Did I build the thing right?”
  – Have the model and simulation been built so that they fully satisfy the developer’s intent?

• Validation: “Did I build the right thing?”
  – Will the model or simulation be able to adequately support its intended use? Is its fidelity appropriate for that?

*After Dale Pace

Accuracy and Validation

- V&V must be easy, right? Sure, see below:
Accuracy and Validation

• How important is V&V?

• Well, at least one of them is in our case (we often assume the other one is ok).

• Validation, that is.

• That would be, validation is the one we need to worry about. Let’s discuss.

• And both are becoming part of grant solicitations.
Amorphous vs. Crystalline Silicon Solar Cells

- Gap: 1.12 eV
- Lower absorption coefficient, device ~100 μm
- Mobilities:
  - electron: 250 μm in 1 ns
  - hole: 250 μm in 3 ns

- Gap: 1.6-1.8 eV
- High absorption coefficient, device ~1 μm
- Mobilities:
  - electron: 0.25 μm in 1 ns
  - hole: 0.25 μm in 200 ns

Staebler and Wronski found that under illumination, a-Si:H films suffer from strongly reduced photoconductivity and dark conductivity.

These properties return to their as-deposited values after annealing at temperatures above 160 C.

Despite sustained and intense efforts to eliminate SWE it has remained a problem for thirty years.

Severely limits the opto-electronic properties and device performance.

D. Osborn, Spectrum Energy, Inc.
Bond Switches

Rotation of a single Si-Si bond
All atoms remain 4-fold coordinated

Energetic cost in crystalline Si
~ 4.5 eV

Energetic cost in amorphous Si
much lower, as little as 0 eV
New Microscopic Picture of SWE

Incident light

Delocalized mobile hole

Bond switch

Localized bound hole
Confined Water


Still many open issues:
New Ice-phase stabilized in confined media at room T?
Will viscosity remain close to bulk value?
Confined Water in Hydrophobic Channels

Distinguish between surface and confinement effects

- **32 water mol.**
  - \(d = 10.09\ \text{Å}\)
  - 156 atoms – 384 el.
  - Simulation time 25 ps

- **54 water mol.**
  - \(d = 14.41\ \text{Å}\)
  - 222 atoms – 672 el.
  - Simulation time 25 ps

- **34 water mol.** in (14x0) NT
  - 438 atoms – 1616 el.
  - \(d = 11.1\ \text{Å}\)
  - Simulation time 20 ps

- **54 water mol.** in (19x0) NT
  - \(d = 15\ \text{Å}\)
  - 466 atoms – 1648 el.
  - Simulation time 20 ps

Rayleigh-Taylor Instability

This awesome example comes from Leo P. Kadanoff’s presentation entitled “The Good, the Bad, and the Awful -- Scientific Simulation and Prediction.”

You can listen to and watch (yes, audio and video) his half hour presentation on the nanoHUB. Highly recommended!

Rayleigh Taylor Instability

Source of Instability:
- Hotter fluid tends to rise
- Cooler, more dense, fluid
- Hotter, less dense, fluid
Rayleigh-Taylor Instability

- Idea: occurs anytime a dense, heavy fluid is accelerated into a light fluid or lesser density
- Slight perturbations to plane parallel interfaces are unstable …fingers grow into sets of inter-penetrating fingers
- Observed in weather inversions, salt domes, star nebulae
- How to model this process? Requires solving hydrodynamics equations.
Rayleigh-Taylor Instability

This awesome example comes from Leo P. Kadanoff’s presentation entitled “The Good, the Bad, and the Awful -- Scientific Simulation and Prediction”

The Raleigh Taylor Instability.

Small deviations from perfect surface flatness triggers an instability. The two fluids penetrate into one another. Analysis (dimensional and RG arguments) suggest a penetration distance

\[ h = \alpha Agt^2 \]

with \( A \) being the Atwoods number (density contrast) and \( \alpha \) being dimensionless---and also Universal (!?).

About 15 groups have measured or calculated \( \alpha \). Their results are important for us (a DOE supported astrophysics group) because the instability occurs on the surface of an exploding star.

This awesome example comes from Leo P. Kadanoff’s presentation entitled “The Good, the Bad, and the Awful -- Scientific Simulation and Prediction”

**Summary of Different Studies**


The ‘b’ refers to the bubble, which the denser fluid penetrates as spikes.

**Result**

Don’t trust the value of $\alpha$.
It is not universal and depends on the details of the calculation being done.
Don’t trust any Rayleigh Taylor calculation with zero surface tension or zero viscosity.
Mathematically, these can give ill posed problems in which answers depend upon details of what happens at the earliest time.
Ion Beam Synthesis of Nanocrystals

Amorphous $\text{SiO}_2$

$^{74}\text{Ge}^+$

Ge atom

atoms “diffuse”

clusters coarsen

ion damage

Energetic ion

Thermal Annealing at 900°C


Courtesy: C. W. Yuan, D. C. Chrzan
Goals & Outline

• Goal: Quantitative model for ion beam synthesis of nanocrystals
  – predict: cluster size distributions
  – identify: experimental parameters that control distribution

• How would you do it??

Courtesy: C. W. Yuan, D. C. Chrzan
Kinetic Processes - Fragmentation

- **statistical approach**
  - ion collision displaces atoms randomly/simultaneously
    - displacement probability $f(\rho)$
    - $\lambda$ determined through TRIM.
  - rapid “reclustering”

- **power law fragment size distribution**
  - MD simulation of ion-induced fragmentation of Au cluster reported by Kissel & Urbassek.
  - incorporate into rate equations

\[
f(\rho) \propto \exp\left(-\frac{\rho}{\lambda}\right)
\]

Results - kinetic Monte Carlo

Courtesy: C. W. Yuan, D. C. Chrzan
KMC vs RE

- \( F = 1.5 \times 10^{12} \text{ cm}^{-2} \text{ s}^{-1} \)
- \( D = D_0 = 6.5 \times 10^{10} \text{ cm}^2 \text{ s}^{-1} \)
- \( \gamma = 0.2 \text{ J m}^{-2} \)
- \( N = 4 \times 10^{16} \text{ cm}^{-2} \)
- KMC and RE display good agreement
  - log-normal-like size distribution!
- Simulations approach a steady-state
- Use RE to explore key parameters that govern size distribution
  - Implantation rate vs. relaxation rate
  - Interface energy

Courtesy: C. W. Yuan, D. C. Chrzan
Theory vs. Experiment

- $D \sim 10^2 D_0$ agrees well with several experimentally-observed as-implanted size distribution
- Indicates that the value of $F/D$ may be intrinsic to the implantation process

Courtesy: C. W. Yuan, D. C. Chrzan

Theorem: given any plane separated into connected regions, the regions may be colored using no more than four colors in such a way that no two adjacent regions receive the same color.

First proposed in 1852 when a student realized while coloring the counties of England that only four colors were needed.

Not proven until 1976 by mathemagicians at U. of Illinois.

How might one go about proving this?

http://www.emu.edu.tr/%7Ecahit/
Several failed attempts at analytically proving the theorem …

In fact, this is considered to be the first major theorem proven with a computer

Thus, it is not accepted by all mathematicians because it is unfeasible for a human to verify by hand - must trust the compiler and the hardware

Basic approach: the set of all possible maps can be reduced to 1476 “reducible configurations”. A computer was used to verify these configurations.

By the way, there is no extension of the theorem to three-dimensional space.

http://www.emu.edu.tr/~cahit/
One last example … read about it on your own time (nice write up in Wikipedia)


Data from thermometers (red) and from tree rings, corals, ice cores and historical records (blue).
Hockey Stick Controversy

• Issues raised relate to:
  – Validity of various temperature proxies
  – Reasonableness of the Global Climate Model used
  – Implementation of “principal component method” used to reduce dimensionality of large data sets for simpler analysis

• Ensuing debate involving National Research Council, National Academy of Sciences, American Geophysical Union, Congress
Hockey Stick Controversy

One last example … read about it on your own time (nice write up in Wikipedia)

Reconstructions of Northern Hemisphere temperatures according to older (blue), newer (red), and recorded data (black)
Hockey Stick Controversy

Paleoclimate findings by the IPCC before and after the Hockey Stick Controversy:

Before: 2001 (page 2)[53]

"proxy data for the Northern Hemisphere indicate that the increase in temperature in the 20th century is likely to have been the largest of any century during the past 1,000 years. It is also likely that, in the Northern Hemisphere, the 1990s was the warmest decade and 1998 the warmest year."

After: Current SPM statement from 2007 (page 10)[54]

"Average Northern Hemisphere temperatures during the second half of the 20th century were very likely higher than during any other 50-year period in the last 500 years and likely the highest in at least the past 1300 years. Some recent studies indicate greater variability in Northern Hemisphere temperatures than suggested in the TAR, particularly finding that cooler periods existed in the 12 to 14th, 17th, and 19th centuries. Warmer periods prior to the 20th century are within the uncertainty range given in the TAR."