ECE 695
Numerical Simulations
Lecture 36: Addressing Grand Challenges with Simulations

Prof. Peter Bermel
April 14, 2017
R&D is increasingly performed in “Pasteur’s Quadrant”

Research is inspired by:
- Consideration of use?
  - No
  - Yes
- Quest for Fundamental Understanding?
  - Yes
  - No

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<tr>
<th>Quest for Fundamental Understanding?</th>
<th>Consideration of use?</th>
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<tbody>
<tr>
<td>Yes</td>
<td>Pure Basic Research (Bohr)</td>
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<tr>
<td>No</td>
<td>Use-inspired Basic Research (Pasteur)</td>
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<td>Former University Presidents (Vest)</td>
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<td>Pure Applied Research (Edison)</td>
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Adapted from Pasteur’s Quadrant: Basic Science and Technological Innovation, Donald E. Stokes 1997
With input from people around the world an international group of leading technological thinkers were asked to identify the Grand Challenges for Engineering in the 21st Century.

From urban centers to remote corners of Earth, the depths of the oceans to space, humanity has always sought to transcend barriers, overcome challenges, and create opportunities that improve life in our part of the universe.

In the last century alone, many GREAT ENGINEERING ACHIEVEMENTS became so commonplace that we now take them mostly for granted. Technology allows an abundant supply of food and safe drinking water for much of the world. We rely on electricity for many of our daily activities. We can travel the globe with relative ease, and bring goods and services wherever they are needed. Growing computer and communications technologies are opening up vast stores of knowledge and entertainment. As remarkable as these engineering achievements are, certainly just as many more great challenges and opportunities remain to be realized. While some seem clear, many others are indistinct and many more surely lie beyond most of our imaginations.
• Proposed by a committee of amazingly accomplished and innovative people.

• Extremely challenging and important.

• Deemed to be doable in the next few decades.
NAE GRAND CHALLENGES FOR ENGINEERING

- Make solar energy economical
- Manage the nitrogen cycle
- Advance health informatics
- Prevent nuclear terror
- Advance personalized learning

- Provide energy from fusion
- Provide access to clean water
- Engineer better medicines
- Secure cyberspace
- Engineer the tools of scientific discovery

- Develop carbon sequestration methods
- Restore and improve urban infrastructure
- Reverse-engineer the brain
- Enhance virtual reality
Make Solar Energy Economical
Make Solar Energy Economical

• Key Challenges:
  – Novel earth-abundant materials
  – Reliable, low-cost packaging techniques
  – Energy storage (daily and seasonal)

• How simulations can help:
  – Provide predictions of performance of realistic, novel PV materials (e.g., using DFT)
  – Predict and optimize lifetime energy production (e.g., using ADEPT)
  – Design electrolyzers and fuel cells (e.g., using FEM multi-physics)

Engineer Better Medicines
Engineer Better Medicines

• Key Challenges:
  – Diagnose and treat people based on individual differences, known as “personalized medicine.”
  – Create inexpensive and rapid diagnostic devices such as gene chips and sensors able to detect minute amounts of chemicals in the blood

• How simulations can help:
  – Design and optimize sensitive biological sensors
  – Reverse-engineering infectious disease attacks on human DNA

Reverse-Engineer the Brain
Reverse-Engineer the Brain

- **Key Challenges:**
  - Understanding how the brain performs computation and storage
  - Applying neurological computing to repair brain injuries

- **How simulations can help:**
  - Simulate neurological electrical and chemical signal propagation (e.g., using drift-diffusion methods)
  - Predict impact of neural prostheses, artificial retinas, electo-ceuticals, etc.

Secure Cyberspace

• Key Challenges:
  – Prevent hackers from shutting down communication, transportation, and other critical systems
  – Taking more pro-active approaches than frequent patches

• How simulations can help:
  – Authenticate hardware, software, and data in computer systems
  – Verifying user identities using biometric technologies
  – Programming languages that have security protection built in
  – Better security for data flowing over the internet

Provide Access to Clean Water
Provide Access to Clean Water

• Key Challenges:
  – Removing natural and manmade toxins from freshwater
  – Desalinating water at a reasonable cost

• How simulations can help:
  – Designing nanofiltration membranes (e.g., using DFT)
  – Designing low-cost, renewable desalination plants
    • Nano-osmosis (e.g., using molecular dynamics)
    • Multi-stage flash powered by solar heat (e.g., using MEEP)

Provide Energy from Fusion

The ITER Fusion Project

Comments on “Provide Energy from Fusion”

SHAPE THE FUTURE

NAE Grand Challenges Scholars Program

Vest Scholars Program

Global Summit
Provide Energy From Fusion

• Barriers to Success:
  – materials that can withstand the assaults from products of the fusion reaction
  – confining/removing radioactivity induced by neutrons
  – preventing releases of radioactive tritium fuel
  – Better superconductors and vacuum systems

• How simulations can help:
  – ab initio materials modeling (e.g., tight-binding, DFT)
  – Drift-diffusion modeling of radioactive ion transport

Enhance Virtual Reality

• Key Challenges:
  – Generating optically realistic environments at high frame rates
  – Reproduce realistic feelings of touch and motion

• How simulations can help:
  – The purest simulation challenge!
  – Ray-tracing and transfer matrices can help with efficiently modeling optics in real-time
  – Providing touch feedback via electrorheological fluids, which alter their thickness when exposed to electric fields of different strengths

Engineer the Tools of Scientific Discovery
Engineer the Tools of Scientific Discovery

• Key Challenges:
  – biochemical methods of probing the body’s cellular and molecular machinations
  – sustainable sources of food, water, and oxygen for space exploration
  – detecting infrared and gravitational waves from distant galaxies

• How simulations can help:
  – New mathematical and computing methods, incorporated into the emerging discipline of “systems biology,” may show the way to better treatments of disease and better understanding of healthy life
  – Synthetic biology may enable the design of entirely novel biological chemicals and systems for food, water, and oxygen
  – Systematically reducing noise in detectors susceptible to the environment
Next Class

• Next time, we will discuss our presentation program and evaluation criteria for the last week of classes

• Note that there’s no class next Wednesday & Friday (Apr. 19 & 21)