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:

Quest for Fundamental Understanding?	**Consideration of use? No**	**Consideration of use? Yes**
Yes	Pure Basic Research (Bohr)	**Use-inspired Basic Research (Pasteur)**
No	**Former University Presidents (Vest)**	Pure Applied Research (Edison)

Adapted from *Pasteur's Quadrant: Basic Science and Technological Innovation*, Donald E. Stokes 1997

14 Grand Challenges for Engineering in the 21st Century

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.

Engineers Can Make A World of Difference

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- Proposed by a committee of amazingly accomplished and innovative people.
- Extremely challenging and important.
- Deemed to be doable in the next few decades.

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www.engineeringchallenges.org

Energy
Environment
Global Warming
Sustainability

Reducing Vulnerability to
Human and Natural Threats

Improve Medicine and
Healthcare Delivery

Expand and Enhance
Human Capability
And Joy

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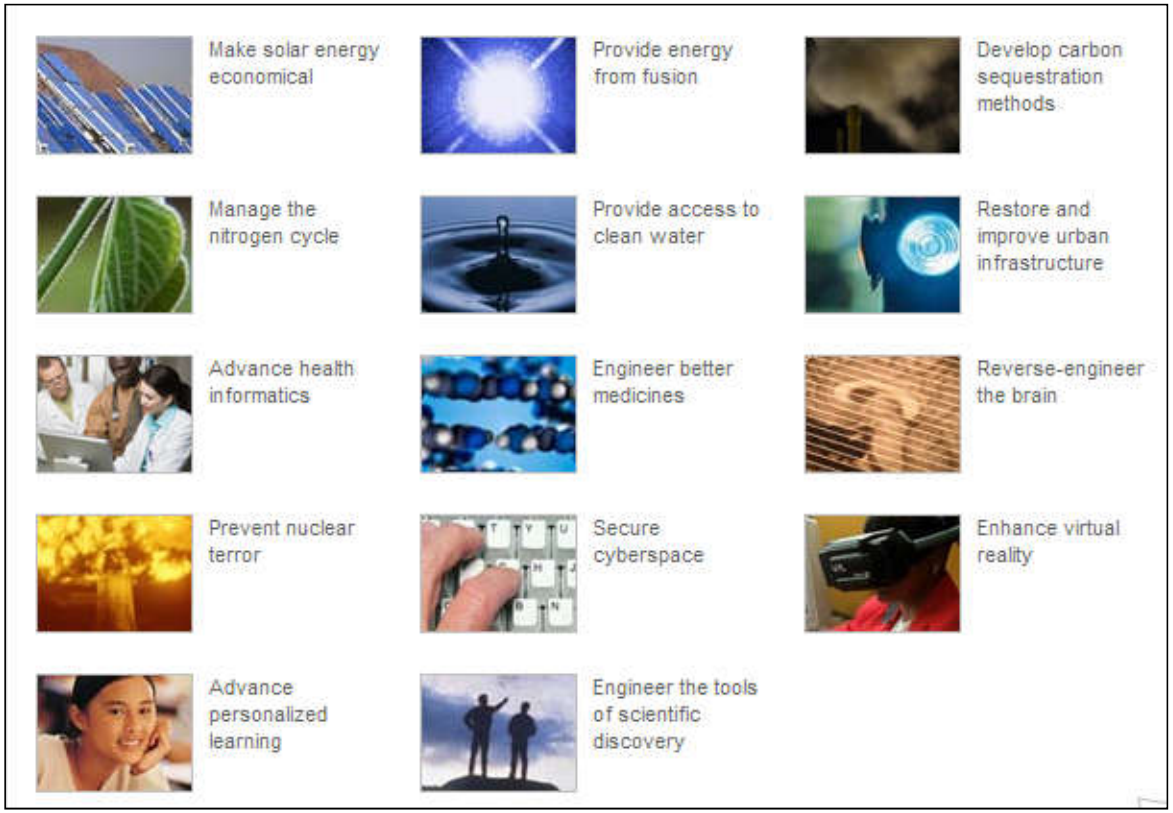

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14 Grand Challenges for Engineering in the 21st Century

Home > Challenges > Make Solar Energy Economical

MAKE SOLAR ENERGY ECONOMICAL

- U.S. Department of Energy Solar Energy Technologies Program
- Comments on "Make Solar Energy Economical"

SHAPE THE FUTURE

- NAE Grand Challenges Scholars Program
- Vest Scholars Program

Make Solar Energy Economical

Overview

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)

Lewis, N.S. 2007. Toward Cost-Effective Solar Energy Use. Science 315(5813): 798-801. DOI: 10.1126/science.1137014

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14 Grand Challenges for Engineering in the 21st Century

Home > Challenges > Engineer Better Medicines

ENGINEER BETTER MEDICINES

Comments on "Engineer Better Medicines"

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- NAE Grand Challenges Scholars Program
- Vest Scholars Program
- Global Summit Student Day

Engineer Better Medicines

Overview

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

L.J. Lesko, "Personalized Medicine: Elusive Dream or Imminent Reality?" *Clinical Pharmacology & Therapeutics* 81 (June 2007), pp. 807-816.

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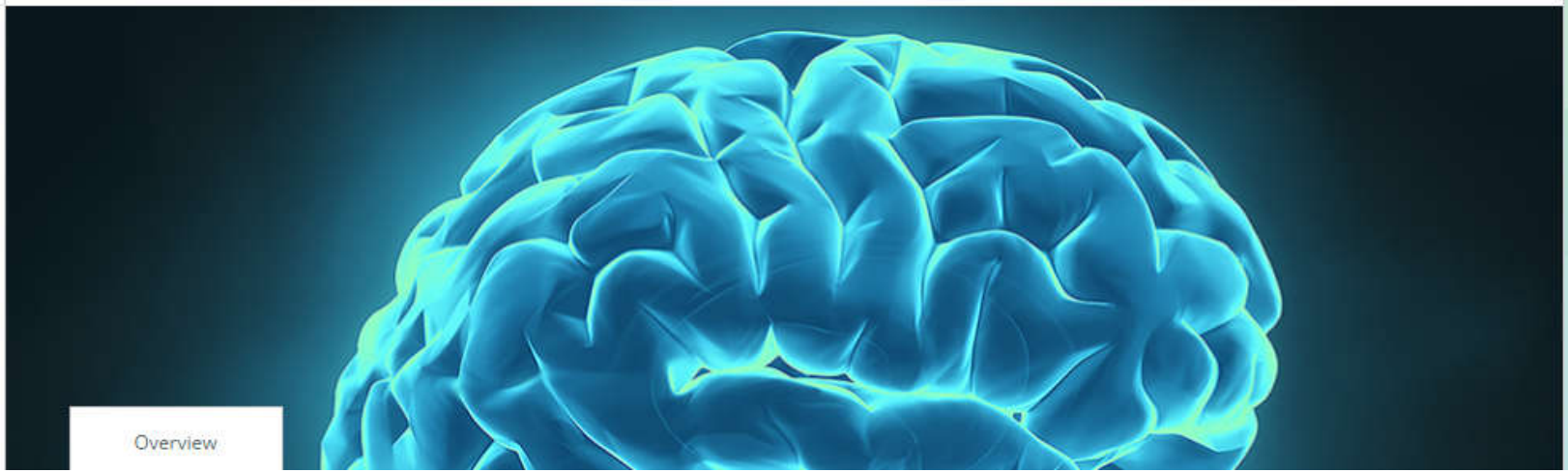
14 Grand Challenges for Engineering in the 21st Century

Home > Challenges > Reverse-Engineer the Brain

REVERSE-ENGINEER THE BRAIN

Comments on "Reverse-Engineer the Brain"

Reverse-Engineer the Brain



Overview

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- Global Summit Student Day

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, electro-ceuticals, etc.

Hapgood, F., "Reverse-Engineering the Brain," *MIT News Magazine* (July 1, 2006).

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Home > Challenges > Secure Cyberspace

SECURE CYBERSPACE

Comments on "Secure Cyberspace"

Secure Cyberspace

Overview

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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

Harrison, K. et al., "Security Through Uncertainty," *Network Security* (February 2007), pp. 4-7.

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Home > Challenges > Provide Access to Clean Water

PROVIDE ACCESS TO CLEAN WATER

- Comments on "Provide Access to Clean Water"
- Safe Drinking Water Is Essential
- Dean Kamen Appears on The Colbert Report

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- NAE Grand Challenges Scholars Program

Provide Access to Clean Water

Overview

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)

Gleick, Peter H. *The world's water volume 8: The biennial report on freshwater resources*. Vol. 8. Island Press, 2014.

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Home > Challenges > Provide Energy from Fusion

PROVIDE ENERGY FROM FUSION

- The ITER Fusion Project
- Comments on "Provide Energy from Fusion"

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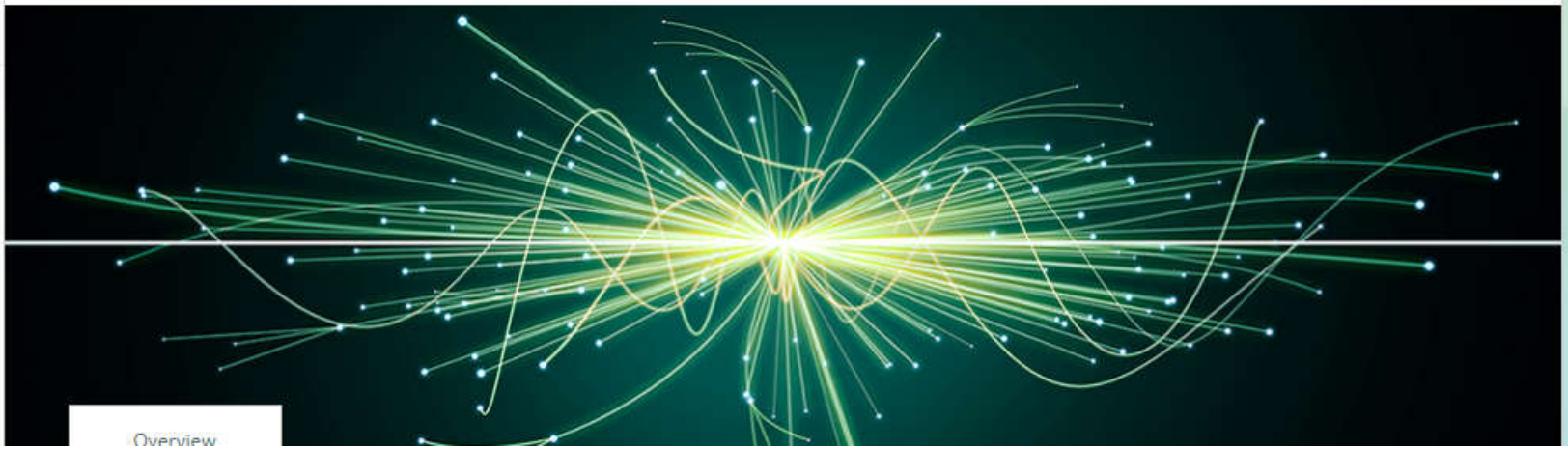
- Vest Scholars Program
- Global Summit

Provide Energy from Fusion



Overview

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

Magaud, P., G. Marbach, and I. Cook. 2004. Nuclear Fusion Reactors. Pp. 365-381 in Encyclopedia of Energy, Volume 4, ed. C.J. Cleveland. Elsevier Science: Oxford, U.K. DOI: 10.1016/B0-12-176480-X/00305-3.

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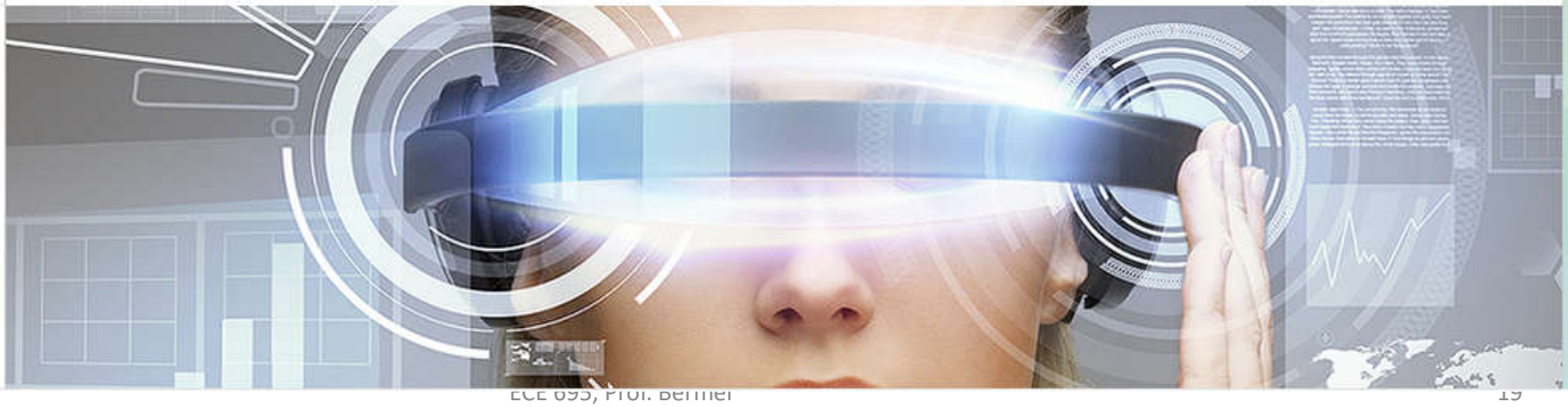
14 Grand Challenges for Engineering in the 21st Century

Home > Challenges > Enhance Virtual Reality

ENHANCE VIRTUAL REALITY

Comments on "Enhance Virtual Reality"

Enhance Virtual Reality



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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

Doug A. Bowman and Ryan P. McMahan, "Virtual Reality: How Much Immersion Is Enough?" *Computer* 40 (July 2007).

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14 Grand Challenges for Engineering in the 21st Century

Home > Challenges > Engineer the Tools of Scientific Discovery

ENGINEER THE TOOLS OF SCIENTIFIC DISCOVERY

Comments on "Engineer the Tools of Scientific Discovery"

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- Vest Scholars Program
- Global Summit Student Day

Engineer the Tools of Scientific Discovery

Overview

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)