NE 155
Introduction to Numerical Simulations in Radiation Transport

Lecture 1: Introduction

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PREVIEW

$$[\hat{\Omega}\cdot\nabla + \Sigma(\vec{r},E)]\psi(\vec{r},\hat{\Omega},E) = \chi(E)\int_0^\infty dE'\,\nu\Sigma_f(\vec{r},E')\int_{4\pi} d\hat{\Omega}'\,\psi(\vec{r},\hat{\Omega}',E') + \int_0^\infty dE'\int_{4\pi} d\hat{\Omega}'\,\Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega}',E')$$

Learn methods to translate equations like the *Boltzmann Transport equation* into computer-generated solutions

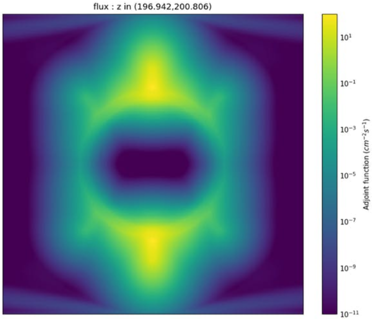


Figure 1: Watts Bar Flux

Categories

Experiment: Experimental scientists work by observing how nature behaves

Theory: Theoretical scientists use the language of mathematics to explain and predict the behavior of nature

Computation: Computational scientists use theoretical and experimental knowledge to create computer-based models of aspects of nature

Computational Science/Engineering

Computational Science seeks to gain understanding principally through the analysis of mathematical models on high performance computers.

The term computational scientists has been coined to describe scientists, engineers, and mathematicians who apply high performance computer technology in innovative and essential ways to advance the state of knowledge in their respective disciplines.

Thus, we distinguish it from computer science, which is the study of *computer and computation* and *theory and experiment*, the traditional form of science.

SOLVING PROBLEMS

1. Identify the problem
2. Pose the problem in terms of a mathematical model
3. Identify a computational method for solving the model
4. Implement the computational method on a computer
5. Assess the answer in the context of the
    - Implementation (computer language and architecture)
    - Method (discrete or continuous)
    - Model (symbolic or numerical)

    Using
    - Visualization and interpretation
    - Experimental comparisons
    - Analytical comparisons
    - Engineering judgement

Big Challenges

- Science
  - Global climate modeling
  - Astrophysical modeling
  - Biology: genomics; protein folding; drug design
  - Computational Material Sciences and Nano-sciences
- Engineering
  - Earthquake and structural modeling
  - Computational fluid dynamics
  - Analysis and design of nuclear reactors
- Business
  - Financial and economic modeling
  - Transaction processing, web services, and search engines
- Defense
  - Nuclear weapons – test by simulations
  - Cryptography and cybersecurity

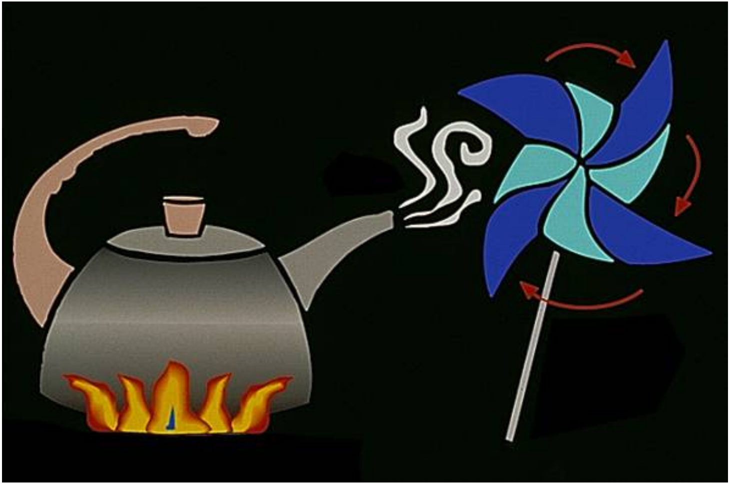
What are we trying to accomplish?

- The challenge of designing a nuclear reactor is to make it as **economical** as possible while ensuring its **safety**.

- This is not an easy task!

- The principle of a nuclear reactor is relatively simple:
  - Fission creates heat within the nuclear fuel,
  - The heat is conducted to the fuel cladding surface and to the coolant,
  - The heat is subsequently transported by a coolant through heat exchangers and ultimately to a steam conversion plant.

EASY?



What are we trying to accomplish?

- In order to design economical and safe reactors, one must choose among a vast range of competing designs:
  - What are the best fuels, structure, and coolant materials; what are their appropriate ratios?
  - How does the reactor respond to component failures?
  - How does one balance those choices given competing goals of performance, lifetime, safety, and capital cost?
- Ideally, one would like to base these choices on theory rather than experimental trial and error
- This is where computational science fits in...

Early Days

Before much computer use (e.g., 1943), things took a long time

Project	Est. Time
Density distribution in difficult system	2 weeks
Integral equation for absorption in Al slab	2 weeks
Slowing-down length in H_2O & related calcs	3 weeks
Albedo problems	1 week

Adolescence – Early 1980s

- NE was at the forefront of computer applications (!)
- Major early success story in the computational sciences:
  - Reduced the burden of experiment
  - Contributed greatly to reactor design
- However, modeling was severely constrained
  - Unable to explicitly model the key physical phenomena within a reactor
  - Low-dimensional representation
  - Lumped parameter models
  - Empirical correlations with tunable parameters established largely by experiments

Adolescence → Today's Challenges

- Computing limitations caused
  - Heavy reliance on expensive and often complicated experiments
  - Inaccuracy resulted in *significant design margins* → negative impact on plant economics
  - Exploration of novel reactor design concepts was greatly constrained

- Many codes developed then are still used

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- What methods will take us into the future?

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- What will the architectures look like?

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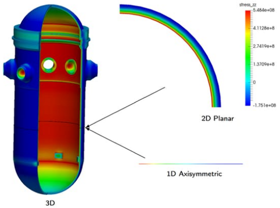
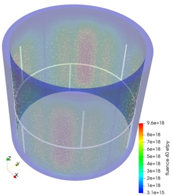
- Do we need to design new tools?
- What methods will take us into the future?
- What will the architectures look like?
- How do we successfully navigate that interplay?

Current State

Major modeling and simulation efforts in nuclear energy

- Nuclear Energy Advanced Modeling and Simulation Program (NEAMS) is geared for advanced reactors
  https://inl.gov/neams/
- Consortium for Advanced Simulation of Light Water Reactors (CASL) is for light water reactors
  https://www.olcf.ornl.gov/tag/casl/





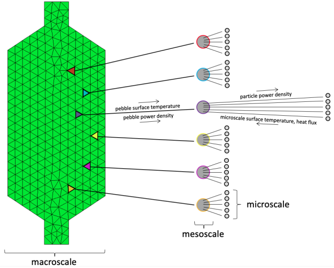
SUPERCOMPUTING IN RESEARCH

These kinds of simulations require time on the fastest computers in the world

- Summit #2 (ORNL): 2.41M cores are a mix of CPUs, GPUs, AI chips; 148.6 petaflops
- Sierra #3 (LLNL): 1.57M cores are a mix of CPUs, GPUs, AI chips; 94.64 petaflops

What Can We Accomplish?

- Predictive simulation
- Model entire facilities at a new level of fidelity
- Coupled multi-physics



What Can We Accomplish?

Integrate

- existing nuclear energy and nuclear national security modeling and simulation capabilities
- and associated expertise
- with high-performance computing

to solve problems that were *previously unthinkable or impractical* in terms of the computing power required to address them.

However, these computer simulations will not completely eliminate the need for *experimental or measurement data* to confirm or "validate" the software.

John Wagner, INL

Are You Up To the Challenge?