3rd LBRN-LONI Scientific Computing Bootcamp

Introduction to Scientific Computing

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June 1, 2020

Outline

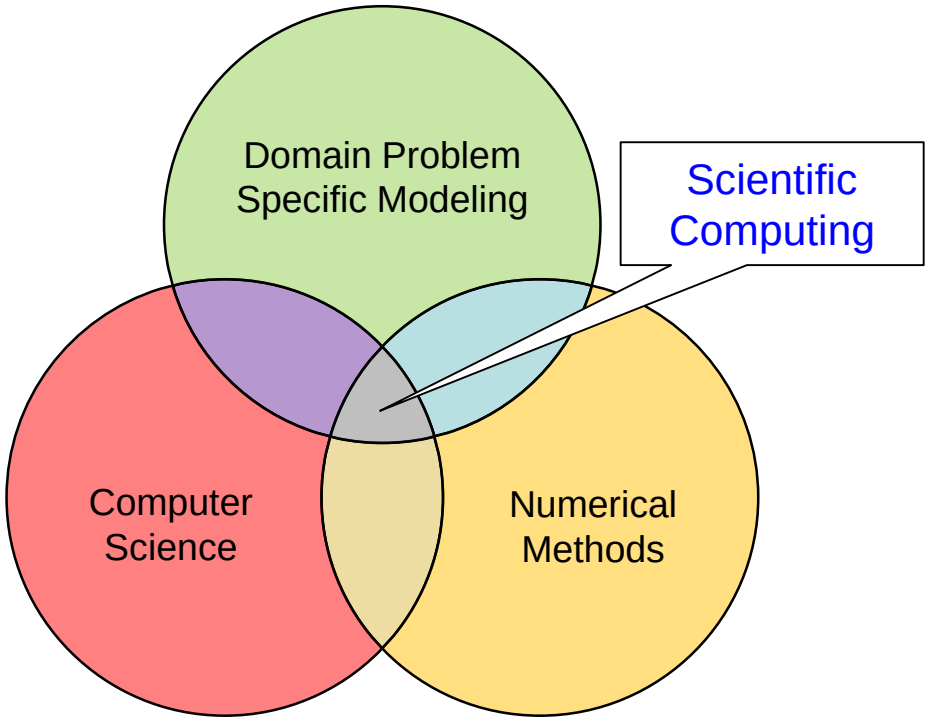
A very brief overview of scientific computing

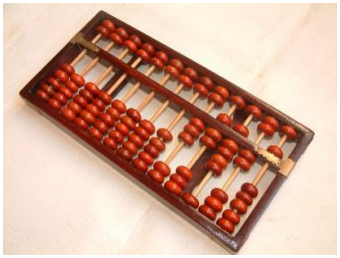
Agenda for the bootcamp

Computing Platform

What is Scientific Computing?

- ***"Scientific Computing is the collection of tools, techniques, and theories required to solve on a computer mathematical models of problems in Science and Engineering." –*** *(Golub & Ortega 1992)*
- **It is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems.**



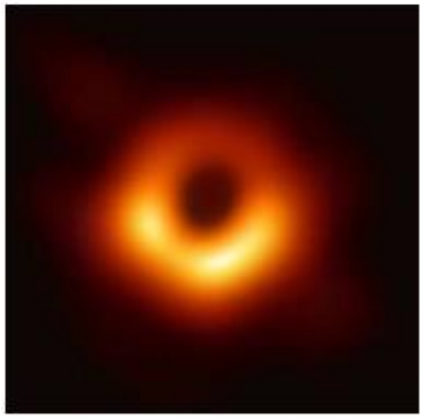


Abacus

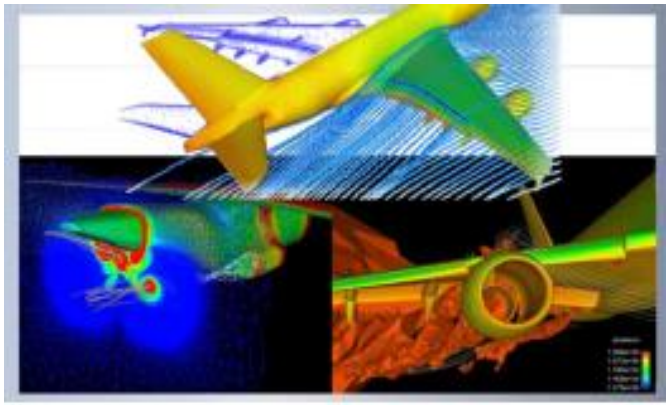
Calculating-Table by Gregor Reisch: Margarita Philosophica, 1503.

Why Scientific Computing?

- **Scientific Computing is nowadays:**
  - The “third pillar of science”, in addition to theoretical analysis and experiments for scientific discovery.
- **Sometimes other means are:**
  - Impossible
  - Costly (time and money)
  - Dangerous or undesirable



Astrophysics



Aircraft design

In lieu of testing nuclear weapons, second-generation designers judge the condition of the aging stockpile based on tests of weapon subsystems, computer simulations of both physics phenomena (shown here) and weapon behavior, and knowledge gained from past nuclear tests.

Nuclear weapon tests

How to Conduct Scientific Computing?

- **Scientific theory and algorithm**
  - From your own study/research background
- **Software**
  - General purpose
    - Excel
    - Matlab
    - Python/R/Perl/C/Fortran, etc.
  - Dedicated software, such as:
    - Ansys (CFD, Structural/Solid Mechanics/Electronics)
    - Lammps/Gromacs/Amber (Molecular Dynamics)
  - Most cases, we need both
- **Hardware**
  - Your laptop/desktop/lab server
  - Cloud Computing ✓
    - Will be used in this bootcamp
  - Supercomputers

LONI QB2 cluster

Purpose of This Bootcamp

- **Understand the basic usage of popular scientific computing programming tools**
  - **Python**
  - **R**
- **One application of the programming tools**
  - **Deep Learning**

Google Colaboratory

- **Colaboratory, or "Colab" for short, allows you to write and execute Python and R in your browser, with**
  - Zero configuration required
  - Free access to GPUs
  - Easy sharing

- **Allows you to focus on learning the Python or R language itself instead of working on installing and configuring a programming environment.**

  - From https://colab.research.google.com/notebooks/intro.ipynb

Agenda

- **Day 1**
  - Introduction and Python Basics
- **Day 2**
  - Scientific Computing with Python
- **Day 3**
  - Introduction to R
- **Day 4**
  - Intermediate R
- **Day 5**
  - Introduction to Deep Learning
- **Our source code repository:**
  - https://github.com/lsuhpchelp/lbrnloniworkshop2020
- **Computing Environment:**
  - **Google Colab**
    - **See** https://github.com/lsuhpchelp/lbrnloniworkshop2020/blob/master/day1/python_test.ipynb

Lectures and Hands-on sessions

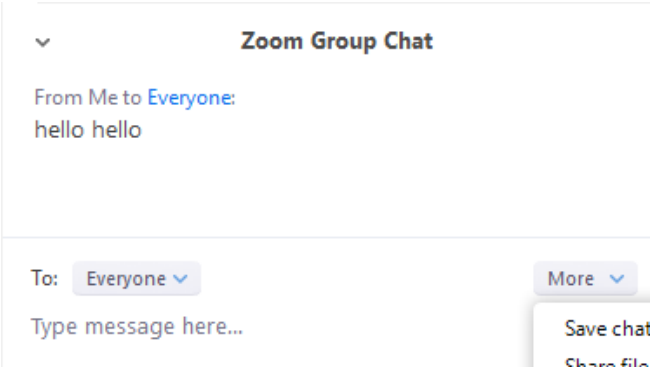
- **Morning sessions 9am-12noon**
  - **Lecture**

- **Afternoon sessions 1pm-4pm**
  - **Zoom session using breakroom**

- **Although recordings will be available, we strongly recommend you try to follow the live session.**

Questions?

- ✓ **Type your question in the Zoom chat window. (Preferred)**



- ✓ **Raise your hand if you do want to ask a question with your microphone, we can unmute you.**