PY502, Computational Physics

Instructor: Prof. Anders Sandvik

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Lectures: Tuesday/Thursday 5:00 - 6:15 PM in SCI B58

- Discussions, Friday 2:30 – 3:20 PM in PRB 148

Homework: ≈7 assignments

- Gabe Schumm (gschumm@bu.edu) is the grader

Grade: 100% homeworks

- active participation can increase grade by 1 step if points close

Course web site

http://physics.bu.edu/py502

- Lecture presentations and notes
- Example programs
- Homework assignments and solutions
- Messages (“Course News”)

Submitting homework

Email (Gabe will give further instructions later)

Some discussion/collaboration on homework problems is allowed, but each student has to turn in her/his independently written programs and reports.

Computers and programming language

- Bring your own laptop to class if possible
  - operating system: Linux/Unix (similar under OSX)
  - install emulator software if you use Windows
  - computer help from Guoan Hu (office PRB 453)
- The Julia language will be used in lectures
- You can possibly use other languages for homework
  - but I strongly discourage this!
- Introduction to Julia will be given (~4 lectures)
- Extensive background in programming not needed
- Some Unix/Linux knowledge assumed (e.g., text editing)
- Come to office hours if you need help!

- Access to SCC computing cluster will be arranged (will be discussed on Friday)

Course material

- Materials will be posted on the web site ahead of the lectures
- Online resources pointed out
- No additional required text

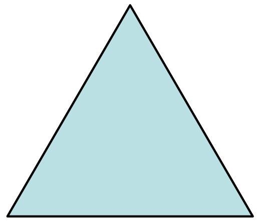
Recommended reading

- Computational Physics, by J. M. Thijssen
- Computational Physics, by N. J. Giordano and H. Nakanishi
- Numerical Recipes, by W. H. Press et al.
  (free on-line with codes in many languages: http://numerical.recipes)

What is computational physics?

• "Scientific computing" in physics

- Studies of models of physical systems using computers
  - Numerical solutions of equations that cannot be done analytically
  - Direct studies of models to "simulate" a system
- Most subfields of physics use some computations, e.g.,
  - Dynamics of solar systems, galaxies, etc
  - Studies of mechanical models of earthquakes
  - Fluid dynamics; turbulence
  - Molecular dynamics of gases, fluids
  - Electrostatics and dynamics (Maxwell's equations)
  - Electronic structure of materials
  - Statistical mechanics of polymers, magnetic systems, etc.
  - Lattice gauge theory (numerical QCD)
- Some times considered third "branch" of physics
  - Experimental, theoretical, computational



- Most physicists need to do some computational work

Topics covered in PY502

- The Julia programming language
- Numerical integration (principles and Julia practice)
- Numerical solution of differential equations
  - classical and quantum mechanics problems
- Monte Carlo simulations (statistical mechanics)
- Basic methods for quantum many-body (lattice) systems

Goals

- Learn the basics of the above techniques
- **Gain proficiency in “computing thinking”**

Teaser: **The last topic of the course will combine several of the previous methods we have learned to study:**

Quantum Annealing (a paradigm for quantum computing)

You will learn what is going on in annealing devices made by D-wave, Google,….