Paradigms and Paradoxes of Computational Physics

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ISU Physics Colloquium
5 March 2012
Computers are Everywhere!

[photos of computers in various settings]
...Including Physics Careers

Field of employment for physics bachelor's in the private sector, classes of 2006 & 2007.

- Engineering: 32%
- Computer Science or Information Technology: 16%
- Non-STEM: 29%
- Other Technology: 9%
- Other Natural Sciences: 7%
- Physics or Astronomy: 5%
- Math: 1%
- Science Education: 1%

STEM: Natural Science, Technology, Engineering and Math

Physics bachelor's who regularly perform the following activities or use the following skills, class of 2007.

- Employment in Engineering
- Employment in Computer Science or Information Tech.

- Solve Technical Problems: 95%
- Work on a Team: 87%
- Technical Writing: 80%
- Knowledge of Phys. or Ast.: 80%
- Perform Quality Control: 78%
- Manage Projects: 75%
- Work with Customers: 75%
- Use Specialized Equip.: 73%
- Design & Development: 72%
- Programming: 70%
- Advanced Math: 69%
- Simulation or Modeling: 67%
- Manage People: 65%
- Computer Admin.: 62%
- Manage Budgets: 60%

Percentages represent the proportion of physics bachelor's who chose “daily”, “weekly”, or “monthly” on a four-point scale that also included “never or rarely”.

http://www.aip.org/statistics
...Including Physics Careers

Scientific and Technical Knowledge Regularly Used by New Physics PhDs, Classes of 2007 and 2008 Combined.

- Basic Research
- Basic Physics Principles
- Programming
- Advanced Physics Principles
- Advanced Math
- Technical Problem Solving
- Simulation and Modeling
- Specialized Equipment
- Applied Research
- Design and Development
- Perform Technical Support
- Perform Quality Control

Percent who use regularly

Note: Percentages represent the proportion of physics PhDs who chose “daily”, “weekly” or “monthly” on a four-point scale that also included “never or rarely”.

Data are limited to PhDs who earned their degrees from a US institution and remained in the US.

http://www.aip.org/statistics
Hence the Paradox:

Computational physics is not part of the standard physics curriculum for undergraduate or graduate students.
To clarify:

• Physics students DO use computers, like all other students.
• Physics students DO use computers in physics-specific ways, e.g., data acquisition, symbolic integration.
• Many physics programs DO offer courses in computational physics.
• Most physics students DO learn computing in the course of research.
But:

- There is no standard content for a computational physics course.
- Computational courses are often optional for a physics degree.
- Employers cannot assume that physics graduates know how to program.
- Computational physics is virtually absent from the physics GRE.
1. CLASSICAL MECHANICS — 20%
(such as kinematics, Newton’s laws, work and energy, oscillatory motion, systems of particles, central forces and celestial mechanics, Hamiltonian formalism, noninertial reference frames, elements of mechanics of continuous systems, and fluid mechanics)

2. ELECTROMAGNETISM — 18%
(such as electrostatics, currents and DC circuits, magnetic fields and forces, electromagnetic fields, Maxwell’s equations and their applications, electromagnetic waves, AC circuits, and electromagnetic radiation)

3. OPTICS AND WAVE PHENOMENA — 9%
(such as wave properties, superposition, interference, diffraction, polarization, dispersion, and coherence)

4. THERMODYNAMICS AND STATISTICAL MECHANICS — 10%
(such as the laws of thermodynamics, thermodynamic processes, equations of state, ideal gases, kinetic theory, ensembles, statistical concepts and calculation of thermodynamic quantities, thermal expansion and heat transfer)

5. QUANTUM MECHANICS — 12%
(such as fundamental concepts, solutions of the Schrödinger equation (including square wells, harmonic oscillators, and hydrogenic atoms), spin, angular momentum, wave function symmetry, elementary perturbation theory)

6. ATOMIC PHYSICS — 10%
(such as properties of electrons, Bohr model, energy quantization, atomic structure, atomic spectra, selection rules, black-body radiation, x-rays, atoms in electric and magnetic fields)

7. SPECIAL RELATIVITY — 6%
(such as introductory concepts, time dilation, length contraction, simultaneity, energy and momentum, four-vectors and Lorentz transformation, velocity addition)

8. LABORATORY METHODS — 6%
(such as data and error analysis, electronics, instrumentation, radiation detection, counting statistics, interaction of charged particles with matter, lasers and optical interferometers, dimensional analysis, fundamental applications of probability and statistics)

9. SPECIALIZED TOPICS — 9%
Nuclear and Particle physics (e.g., nuclear properties, radioactive decay, fission and fusion, reactions, fundamental properties of elementary particles). Condensed Matter (e.g., crystal structure, x-ray diffraction, thermal properties, electron theory of metals, semiconductors, superconductors). Miscellaneous (e.g., astrophysics, mathematical methods, computer applications)
Plenty of good reasons:

• Physics teachers are the most conservative people on the planet.
• We only know how to teach what we were taught as students.
• We don’t teach anything else more recent than 1925.
• Computer programming is hard.
• We can’t rely on CS departments.
Too much diversity!

- Languages
- Operating systems
- Development environments
- Libraries
No standard textbook
Other frustrations

• Computers are unforgiving—no partial credit.
• Students come in with vastly different backgrounds.
• Hard to find good homework assignments and test questions.
A crucial insight: Teach computational physics in a lab setting.
Computational Physics at WSU

- Two spreadsheet “lab” exercises in introductory physics
- Mathematica prerequisite for most upper-division courses
- Required course in computational physics
- New computational physics degree option that includes CS, numerical analysis, and a second computational physics course
Essential skills to teach

• Algorithmic thinking
• Writing legible code
• Debugging
• Understanding numerical errors
• Testing results
• Using natural units
Paradigms in standard courses

- Projectile motion
- Atwood’s machine
- Planetary orbits
- Simple harmonic oscillator
- Standing waves on a string
- Ideal gas
- Two-state paramagnet
- Einstein solid
- Hydrogen atom
Paradigms in computational physics

• Projectile motion with air resistance
• Chaotic pendulum
• 3-body orbits
• Lennard-Jones molecular dynamics
• Random walks
• 2-D Ising model via Metropolis algorithm
• Laplace’s equation via relaxation method
• Quantum bound states via shooting method
• Lattice-Boltzmann fluid dynamics?