How Computers are Changing Physics

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Punchlines

- Increasing importance of simulation in contrast to numerical analysis.
- Models are increasingly presented in the form of an algorithm rather than a differential equation. Introduction of digital models based on the logical manipulations of 1's and 0's rather than floating point arithmetic.
- Simple rules can yield complex behavior. Analytical methods work well only for linear systems.
- Importance of graphical display of data and visualization.
- Geometrical concepts such as clusters and fractals are becoming more important.

- Development of a computer culture is still evolving – conceptual change requires time.
- Changes in the curriculum and innovations in educational methods should be guided by developments in physics research.
- Computation has led to important conceptual advances and new ways of thinking about physical systems which should be reflected in the curriculum.
- Availability of open source software.

- Our goal should be to incorporate computational methods into the curriculum rather than computers in the classroom.
- New courses in computer simulation, computational physics, and numerical methods have been developed and many new texts are available.
- Computational physics does not yield instant gratification as found in many other computer applications. We need to provide students opportunities to learn that computers do not lessen the need for thinking deeply and that such thinking has its own rewards. Computing is not a substitute for thinking.

How are Computers Used in Physics Research?

- Computational mode
  - ⋆ evaluation of definite integrals
  - ⋆ numerical solution of simultaneous equations
  - ⋆ diagonalization of matrices
  - ⋆ solution of partial differential equations using finite element techniques

  Conceptual advance: renormalization group

- Real-time control and data analysis
- Simulation mode
  - ⋆ molecular dynamics, dynamical systems, Monte Carlo methods
- Symbolic manipulation
  - ⋆ Maple, Mathematica, Matlab, Octave
- New computer architectures

Molecular Dynamics

How can we understand dense gases, liquids and liquid-solid transitions?

Numerical solution of classical equations of motion for N interacting particles.

What is the importance of the details of the interaction to the properties of simple liquids?

What is the nature of the glass transition?

1. Choose interparticle interaction.
2. Periodic boundary conditions.
3. Choose initial conditions.

4. Determine neighbors and forces.

5. Calculate trajectory in phase space.

Verlet algorithm

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n \Delta t^2$$

$$v_{n+1} = v_n + \frac{1}{2}[a_n + a_{n+1}]\Delta t$$

6. Check conservation of energy and momentum.

7. Compute physical quantities as averages over trajectories.

What have we learned?

Qualitative features of liquids due to the repulsive part of the interparticle potential.

Present emphasis on nonequilibrium systems, glasses, and granular dynamics.

Nonlinear Dynamics

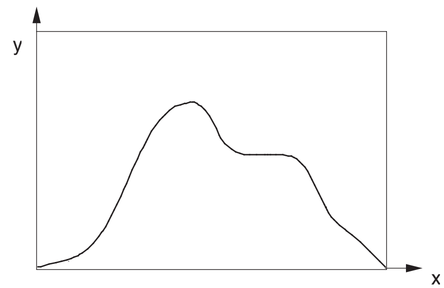
$$x_{n+1} = 4rx_n(1 - x_n)$$

A good example of a simple system for which little theory is known. Instead can do "experimental mathematics."

Monte Carlo Methods

A random walk through random walks.

Random sequences, purest expression of ignorance, give us ability to gain new knowledge.



Monte Carlo integration.

$$A \approx \frac{\text{number of splashes}}{\text{number of stones}} \times \text{area of field}$$

How can we understand the dynamics of ink in water?

Traditional continuum approach: differential equation

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}$$

$$P(x,t) = \frac{1}{2}(\pi D t)^{-1/2} e^{-x^2/4Dt}$$

Alternative approach: random walk on a lattice. applet

$$P_N(x) = \frac{N!}{(N+x/2)!(N-x/2)!}(\frac{1}{2})^N \rightarrow (\frac{2}{\pi N})^{1/2} e^{-Nx^2}$$

Can solve diffusion equation numerically **or**

Consider random walks to “simulate” diffusion on a lattice.

Quantum Monte Carlo

$$-i\hbar\frac{\partial\Psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - V(x)\Psi$$

Let $\tau = it/\hbar$, and consider random walk in imaginary time:

$$\frac{\partial\Psi}{\partial\tau} = \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - V(x)\Psi$$

Diffusion equation with source:

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} - kP$$

$$\Psi(x,t) = \sum_n a_n\psi_n(x)\exp(-E_n\tau) \rightarrow a_0\psi_0(x)\exp(-E_0\tau)$$

DLA

applet

$$N \approx R^D \qquad \text{for } N \to \infty$$

D is fractal dimension

$D = d$, space-filling (compact) cluster

$D \approx 1.7$ for DLA (fractal)

Undergraduate level textbooks

Pre 1980

1. Ehrlich, Physics and Computer (1973).
2. Potter, Computational Physics (1973).
3. Bennett, Scientific and Engineering Problem-Solving with the Computer (1976).
4. Merrill, Using Computers in Physics (1976).

1980–1989

1. Koonin, Computational Physics (1986).
2. Stauffer et al., Computer Simulation and Computer Algebra (1988).
3. MacKeown and. Newman, Computational Techniques in Physics (1987).
4. Gould and Tobochnik, Introduction to Computer Simulation Methods (1988).
5. Heermann, Computer Simulation Methods in Theoretical Physics (1988).

1990 –

1. Baker and Gollub, Chaotic Dynamics: An Introduction (1990) and (1996).
2. Heermann, Computer Simulation Methods in Theoretical Physics (1990).
3. Haile, Molecular Dynamics Simulation: Elementary Methods (1992).
4. Thompson, Computing for Scientists and Engineers: (1992).
5. Stauffer et al., Computer Simulation and Computer Algebra (1993).
6. Crandall, Projects in Scientific Computing (1994).
7. DeVries, A First Course in Computational Physics (1994).
8. Garcia, Numerical Methods for Physics (1994).
9. Vesely, Computational Physics (1994).
10. Zimmerman and Olness, Mathematica for Physics (1995).
11. Baumann, Mathematica in Theoretical Physics (1996).
12. Crandall, Topics in Advanced Scientific Computation (1996).
13. Gaylord, Kamin, and Wellin, Programming with Mathematica (1996).

14. Gould and Tobochnik, Introduction to Computer Simulation Methods (1996).
15. Giordano, Computational Physics (1997).
16. Landau and Paez, Computational Physics (1997).
17. MacKeown, Stochastic Simulation in Physics (1997).
18. Pang, Computational Physics (1997).
19. Danby, Computer Modeling (1998).
20. De Jong, Mathematica for Calculus-Based Physics (1999).

Complete listing at sip.clarku.edu/books.

Texts can be grouped into three classes:

- numerical methods
- simulation
- symbolic manipulation

What choice should we make?

Computer Simulation Laboratory

- Computer simulations provide opportunity for doing physics closer to the way research is done.

laboratory experiment	computer simulation
sample	model
physical apparatus	computer program
calibration	testing of program
measurement	measurement
data analysis	data analysis

- Approach close to laboratory experiments.
- Numerical methods more meaningful when part of a simulation, than when taught only as a tool.

- Computer simulations encourage a broader vision of physics than is usually taught.
- Simulations provide a way of reaching a deeper understanding of fundamental physical concepts, particularly by writing programs with graphics and user interaction.
- Project oriented, minimum background required.
- Students learn programming skills in context of physics.
- Simulations encourage open-ended questions and creative thinking in contrast to routine problem solving.
- Students might reform the curriculum.

Disadvantages

- Difficult to add course to curriculum.
- Laboratory course open-ended and time consuming.

Understanding physics comes from reading, studying, solving problems, doing experiments, and doing simulations.

Examples of recent student projects

Application of genetic algorithm to find minima of spin glass (computer science major).

Percolation-based model of stock trading (economics major).

Relaxation method solution and MC solutions of Laplace's equation.

Ising model using finite size scaling and flat histogram method.

Application of the invaded cluster algorithm to Widom-Rowlinson model.

Evolution of river networks. How do river channels form?

1. At each site, specify height of land and height of water (integers).

2. Choose site at random. If surface height (water plus land) is lower on a neighboring site, move water units to bring surfaces as close to even as possible.

3. For each water unit moved, a unit of land is dissolved away only if the land is lower at the destination site.

4. Additional water falls on a site as precipitation at random intervals.

Choice of Programming Language

Desirable features

- Portable.
- Inexpensive.
- Easy to learn.
- Built in graphics.
- Allow event-based programming.
- Capable of performing numerical functions.
- Structured, preferably object-oriented.
- Useful outside of physics so that language will be maintained and improved and provide a marketable skill for students.
- Allow bit manipulation.
- Parallel programming capability.
- Fast.

True BASIC $\longrightarrow$ Java

Focus on parts of the language that are useful for doing computer simulations and provide templates and utilities. `<www.opensourcephysics.org>`.

Integrating computational physics into the curriculum

Most texts and courses treat the computer as an add-on. Such use is ineffective.

Need to teach a separate course and make fundamental changes in existing courses.

Two notable exceptions:

- Ruth Chabay and Bruce Sherwood, Matter & Interactions, John Wiley & Sons. Two-volume introductory calculus-based physics curriculum that engages students in the process of modeling physical systems using a small number of fundamental principles and integrates computer modeling into the curriculum. Book uses VPython.
- Physlets, Wolfgang Christian. Java applets built into Web pages using Javascript. Common user interface and good sets of questions.

Desired change: make courses less theoretical. Teach courses from a computational point of view and reduce problem solving.

Statistical and Thermal Physics

Most natural area in which to incorporate computation.

- Nature of probability.
- Approach to equilibrium. Increase of entropy.
- Microcanonical simulations (MD or demon) and compute subsystem probability to motivate Boltzmann probability.
- Compare different ensembles by doing MC simulations. Compare time averages to ensemble averages by doing MD.
- QMC with noninteracting particles to understand better the significance of indistinquishability.
- Flat broad histogram method to improve understanding of density of states.
- Random walks and diffusion.
- Maximum entropy and image enhancement.
- Traffic flow.

applets and in particular An ideal thermometer.

Most important goal: Develop a community of teachers and students to generate course materials and exchange ideas in an “open source” environment.

Making Teaching Count

The use of the Internet as a vehicle for delivering curricular materials allows us to share course materials and our approach with instructors at other institutions.

One reason that teaching is not taken as seriously as research is that our teaching reputations are local and the quality is not easily evaluated. The advent of the Web has already started to change this situation.

We can use the Web to develop curricular materials in a way that takes advantage of the collective work of many people. Can there be “open source” curriculum development projects in physics and other areas?