Computational Physics at Berry College, In and Out of the Classroom

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ABSTRACT: The Berry College physics program has only 3 faculty, and of those I am the only one with significant experience in computational physics. As a result the responsibility of integrating computation into the physics curriculum has fallen largely on my shoulders. I have introduced students to computational physics in two main ways: through computational assignments in my two-semester classical mechanics sequence, and through student involvement in undergraduate research. In both of the classical mechanics courses all students are required to complete several major computational assignments using Mathematica. In the second-semester course students are additionally required to write formal papers (typeset using Mathematica or LaTeX, and incorporating figures, etc.) describing their work and the results. Student use of computation in undergraduate research has ranged from the use of Mathematica to study simple quantum systems to the creation of sophisticated FORTRAN and Java programs to conduct original research in quantum chaos.

Computational Physics at Berry College

The College:

- Four-year liberal-arts college with a few professional programs.
- Enrollment ~ 1750
- Located on a 26,400 acre campus in Northwest Georgia.

The Physics Department:

- Three full-time faculty.
- Offer major and minor in physics.
- 5 graduates in the 2006-2007 AY
- Housed in a relatively new (2001) science building.
- Computer facilities:
  - Public student computer lab with 24 Windows machines
  - Physics student projects room with 8 Windows or Mac machines
  - Computational research lab with 5 PowerMac G4s).

Computation in the Physics Major:

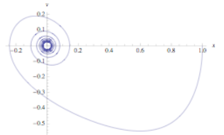
- Majors are not required to take any computer science courses, although many take a course in Java/Python programming to get a double-major in math.
- All majors will use Excel for some basic computational work in introductory labs.
- Almost all majors will use Mathematica in their Differential Equations course.
- All majors will take at least one semester of Classical Mechanics, which requires the use of Mathematica for computational projects. These projects are described in greater detail in the next part of this poster.
- Most majors will use Mathematica or other computational software to some extent in other physics or mathematics courses.
- A few majors will engage in computational physics research. Some of this research is described in greater detail later in this poster.

Computation in Classical Mechanics

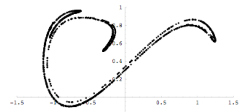
I teach a two-semester sequence in classical mechanics at Berry. It is in these courses that our physics majors receive their greatest exposure to computational physics. In each class students are asked to complete several computational projects that relate to the material covered in class.   I currently use Mathematica for these computational projects, but I am considering other alternatives. In the first semester the emphasis of the projects is on learning how to use Mathematica to solve computational problems (as well as learning physics!). Students are expected to turn in their Mathematica code and the results of their computations, along with a brief description of their results. In the second semester students are expected to turn in formal papers describing the problems they solved and their computational results (this course is part of Berry's Writing-Across-the-Curriculum Program). These papers are expected to be properly typeset (using Mathematica or LaTeX) with equations and figures included where appropriate. The table below provides details about the various projects that are assigned in each course.

Project Title	Physics Topics	Computational Tools
Classical Mechanics I (PHY 302) Projects		
Projectile motion with air resistance	Velocity-dependent forces Quadratic air resistance	Numerical solution of ODEs Plotting functions Root finding Curve fitting (polynomial) Optimization
Damped harmonic oscillator with quadratic damping	Quadratic vs. linear damping Absence of critical damping Phase space trajectories	Numerical solution of ODEs Parametric plots
Driven harmonic oscillator	Homogeneous vs. inhomogeneous solutions Transient vs. steady-state motion	Plotting multiple functions Parametric plots
Duffing oscillator	Nonlinear oscillators Limit cycles/periodic orbits Chaos	Numerical solution of ODEs Plots and parametric plots Poincare sections
Tent map	Chaos in iterated maps Lyapunov exponents Bifurcations of periodic orbits	Iteration of functions Plotting data and functions Bifurcation diagrams
Stability of circular orbits	Circular orbits for a given force law Stability of circular orbits	Root finding Numerical solutions of ODEs Parametric plots
Classical Mechanics II (PHY 402) Projects		
Projectile motion on Earth (no air resistance)	Non-inertial reference frames Coriolis and Centrifugal forces	Numerical solution of ODEs Root finding 3D parametric plots
Rigid body rotation	Principal axes and principal moments of inertia Angular momentum and rotational KE of a rigid body Parallel-axis theorem	Numerical linear algebra Eigenvalues and eigenvectors (numerical diagonalization)
Chain of oscillators	Coupled oscillators Normal modes of vibration Standing waves on a string	Eigenvalues and eigenvectors (numerical diagonalization) Plotting lists of data
Liouville's Theorem	Preservation of phase-space volume occupied by an ensemble of trajectories	Computation using ensembles of trajectories (Monte Carlo) Plotting lists of data
An area-preserving map on the unit torus	Hamiltonian chaos Fractal structures in phase space Stability of fixed points Lyapunov exponents KAM tori Homoclinic tangles	Poincare sections Iterating a 2D map Eigenvalues and eigenvectors (numerical diagonalization) Parameter searching

All Mathematica notebooks for these projects are available at:
http://fsweb.berry.edu/academic/mans/ttimberlake/comp_phys/

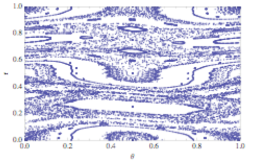


Phase space trajectory for a quadratically damped harmonic oscillator.



Poincare section for the driven Duffing oscillator.

Comparison of trajectories of projectiles on Earth with and without inertial forces.

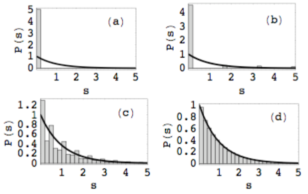


Poincare Section of an area-preserving map on the unit 2-torus

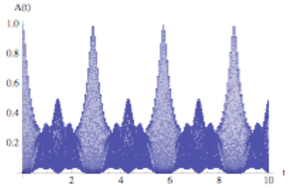
Undergraduate Research in Computational Physics

Over the past six years I have supervised a variety of undergraduate research projects, all of which have had a significant computational component. The table below provides information about some of these projects.

Project Description	Platform	Computational Tools
Correlation of the photodetachment rate of a scarred resonance state with the classical Lyapunov exponent	FORTRAN MPI Mac cluster Windows cluster	Complex-coordinate scaling Solving large systems of ODEs Numerical diagonalization Numerical husimi distributions Numerical Lypunov exponents
Parabolic fixed points of an area-preserving map on the unit 2-torus	Mathematica	Poincare sections Iterating a 2D map Numerical diagonalization Trajectory ensembles
Localization of a driven particle in the infinite square well	FORTRAN Mathematica	Solving large systems of ODEs Numerical diagonalization Computing statistical measures of localization Numerical husimi distributions Monte Carlo estimate of the area of a chaotic region in the phase space
Eigenvalue statistics of weakly driven systems	Mathematica FORTRAN	Modular arithmetic Computational statistics
Wavepacket revivals in the asymmetric infinite square well	Mathematica	Root finding Solving the time-dependent Schrödinger equation Computing autocorrelation function
Statistical measures of the randomness of prime numbers	Java Mathematica	Generation of primes and random primes Computational statistics on large datasets
Statistics of mixed eigenvalue sequences	Mathematica Java	Constructing and diagonalizing random matrices Computational statistics Nonlinear curve fits



Eigenvalue spacing distributions for the weakly driven infinite square well.



Autocorrelation function for a special wavepacket in the asymmetric infinite square well.

Computational Physics Publications

Technical

T. Timberlake and J. V. Foreman, "Correlation of the Photodetachment Rate of a Scarred Resonance State with the Classical Lyapunov Exponent," *Physical Review Letters* **90,** 103001 (2003).

T. Timberlake, F. Petruzielo, and L. E. Reichl, "Localization of Floquet states along a continuous line of periodic orbits," *Physical Review E* **72,** 016208 (2005).

Pedagogical

Todd Timberlake, "A computational approach to teaching conservative chaos," *American Journal of Physics* **72**, 1002-1007 (2004).

Todd Timberlake, "Random numbers and random matrices: Quantum chaos meets number theory," *American Journal of Physics* **74**, 547-553 (2006).