Proposal for a

COMPUTATIONAL PHYSICS CONCENTRATION

at the University of Virginia

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At present our Department offers only one course in computational physics: Phys 551 "Methods of Computational Physics". This course is meant to address the needs of advanced undergraduate physics majors and of certain, primarily beginning, graduate students. Given the overwhelming relevance of computational methods in modern physics, we have felt that this course alone does not address the needs of our students adequately, nor in a timely manner. By itself, Phys 551 cannot expose the interested students to a wider array of techniques and knowledge in this discipline. Consequently, we may be losing potential students (majors) to other disciplines which may not address adequately their interest in physics and the sciences.

We have furthermore felt that our undergraduate majors do not have an adequate opportunity to acquire basic computational skills as would be relevant to our discipline. Consequently, we find that most of our students lack these skills even as they graduate.

In order to provide a systematic course of study of the elements and techniques of computational physics, we propose the following curriculum for a "Concentration in Computational Physics", to be offered to our undergraduate majors.

The Concentration will rely on a sequence of three courses, one of which is to be required of all BSc and distinguished BA physics majors, and two electives open simultaneously to our graduate students. Short descriptions of the courses follow.

> **Phys 254**: Fundamentals of Scientific Computing (3 credit hours)
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> PREREQUISITES: one semester of calculus, and one semester of introductory physics, e.g., Phys 151, 231, 142E, or 201, or instructor permission.
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> The class will teach the applications of computers to basic problems in the physical sciences. Computing topics will include an introduction to programming, usage of external libraries, and implementation of basic algorithms such as Monte Carlo methods. Mathematics covered will focus on the numerical methods of solving common problems in physics and other sciences, as well as error analysis and data fitting. The course will make extensive use of problems such as radioactive decay, satellite trajectories, random walks, population dynamics, etc. No previous computer experience is required.

The class will meet weekly for one one-hour lecture session, and for two two-hour laboratory sessions in the computer lab with a TA and/or professor.

Phys 254 will be required of all BSc and distinguished BA physics majors, and will normally be taken during the student's first year at the University.

Note: Phys 254 is a new course which represents a net addition to our undergraduate majors' curriculum, with a two-fold purpose. Its first goal is to ensure that our majors attain a basic level of scientific computing literacy. In this sense the course will also be suitable for other science majors in the College, including pre-medical majors, as well as undergraduate engineering students. Secondly, Phys 254 will be the first course in the new Computational Physics concentration course sequence.

Phys 553: Computational Physics I (3 credit hours)

PREREQUISITES: knowledge of vector calculus, ordinary differential equations, and introductory physics, including modern physics.

The class will review elementary computational methods for differentiation, integration, interpolation, zeros, extrema, etc., and concentrate on numerical solutions of differential equations, basic spectral analysis, numerical methods for matrices, Monte Carlo simulation.

Note: Phys 553 will be offered in the fall semester, and will be normally taken by undergraduate students in their third year, but will also be open to graduate students. This course replaces Phys 551, which will revert back to being a "special topics" course.

Phys 554: Computational Physics II (3 credit hours)

PREREQUISITES: Phys 553 (or instructor permission)

The class will address more advanced topics in computational physics, such as: numerical methods for partial differential equations, Green's function method, advanced Monte Carlo modeling, advanced iteration methods for linear systems.

Note: Phys 554 will be offered in the spring semester. Undergraduate students will normally take it in their third or fourth year. The course is also open to graduate students.

Tentative syllabi for the four courses are outlined below.

Proposed Topics for a Phys 254 Syllabus

Outline:

1. Introduction to computers and programming (e.g., operating systems, editors, input/output, simple programs)
2. Numerical differentiation and integration
3. More advanced programming (e.g., subroutines, functions)
4. Error analysis and limits to precision
5. External Libraries
6. Data Fitting
7. Root Finding/ Maxima and Minima Finding
8. Matrices
9. Monte Carlo simulation methods

Note: Phys 254 syllabus will rely heavily on the subject matter covered in Phys 151, but will also include basic topics of interest to science in general.

Possible Syllabus Units in More Detail:

(a subset of these topics would actually be taught)

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1. Introduction to computers
   Handouts: Using Galileo, Using Emacs, Using Gnuplot
   Computing concepts:
        What are memory, disk space, cache, CPUs, etc?
        How does an OS work?
        How does a program run?
        What is a programming language?
        How are programs created?
   Examples:
        'Hello World'

2. Introduction to programming I
   Physics concepts:
        Position, velocity and acceleration in 1 dimension
   Computing concepts:
        Variables
        Statements
        Editing a program
        Compiling a program
        Running a program
   Examples:
        Compute speed and time at the end of a body's fall

3. Introduction to programming II
   Physics concepts:
        Position, velocity and acceleration in 2 dimensions
   Computing concepts:
        Control structures
        Built-in functions
        Arrays
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        Memory overruns
   Examples:
        Compute position and velocity vs. time for a projectile
        (1) writing output directly to a file and (2) storing
        values in an array.  Compute average velocity.

4. Functions and subroutines
   Physics concepts:
        Circular motion
   Computing concepts:
        Calling subroutines
        Calling functions
        Return values
        Memory overruns
   Examples:
        Compute x,y coordinates of a particle in uniform circular
        motion, given r and theta.  Create a subroutine to perform
        this calculation, producing a table of r,theta,x,y for
        0 <= theta <= 2*pi.  Create a function that returns r,
        the distance from the origin, for any point x,y.

5. Input and output
   Physics concepts:
        Force diagrams
   Computing concepts:
        Reading and writing data
   Examples:
        From a file, read x,y components of forces acting on a body
        in a plane.  Compute the total force acting on the body.

6. Errors and Uncertainties in Computations
   Physics concepts:
        Work, Potential energy, conservation of energy
   Computing concepts:
        Roundoff error
        Truncation error
        Small size of random errors
   Examples:
        Compute the change in potential energy of a bucket of water after
        the addition of another drop, given M (the original mass of the
        water), m (the mass of the drop) and h (the height of the
        bucket).  Use a loop to produce a table of potential energy
        difference vs. drop mass for a wide range of drop masses.  Do
        the computation two ways:  (1) by adding the masses, then computing
        the potential energy, (2) by computing the potential energy, then
        adding.  Modify your program to calculate the total amount of
        work done in adding all of these drops.

7. Numerical differentiation and integration
   Physics concepts:
        Center of mass
   Computing concepts:
        Finite difference
        Simple sum
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Trapezoid rule
Simpson's rule
Examples:
1. Compute z vs. t for a falling body. Use finite difference methods to find the body's velocity at each point.
2. Find the area under the curve y = 9 - x**2, for -3 < x < 3.
3. Find the center of mass of an object with the above shape, and a uniform density and thickness.

8. Using external libraries
Physics concepts:
Center of mass
Computing concepts:
Linking programs with external libraries
Numerical integration using library routines
Examples:
Rewrite previous example, calling library functions to do the work.

9. Limits to precision
Physics concepts:
Kepler's laws, Gravitation
Computing concepts:
float vs. double
Examples:
1. Determine the magnitude and direction of the gravitational field at the center of a circle of identical, evenly-distributed point-masses by summing the contributions of each mass. What is the force acting on one of the masses, due to the other masses?
2. Modify the program to read in a list of point-masses in the x,y plane and calculate the magnitude and direction of the gravitational field at a given x,y position.

10. Root finding
Physics concepts:
Kepler's laws, Gravitation
Computing concepts:
Bracketing and bisection
Secant method
Newton-Raphson
Examples:
A spacecraft ``orbits'' back and forth through a hole drilled completely through the earth, passing through earth's center. At apogee, the satellite is above the surface of the earth. Determine, using each of the three methods above, when the spacecraft will cross the earth's surface.

11. Finding maxima and minima
Physics concepts:
Kepler's laws, Gravitation
Computing concepts:
Golden section search
Brent's method
Using first derivatives

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    Examples:
        Given two spherical masses, M and m, find the position
        on the line joining their centers at which the gravitational
        field has its minimum magnitude.

12. Curve fitting
    Physics concepts:
        Rotational dynamics
        Error analysis
    Computing concepts:
        Computing Chi**2
        Least-squares fit to a simple function (straight line, Gaussian)
    Examples:
        A small mass is connected to a string wound around a wheel.
        The mass is dropped, and its velocity is measured at various
        heights as it falls.  Given a data file containing the measurements
        of velocity, determine the moment of inertia of the wheel.
        Given a data file containing several measured values of the
        falling mass's acceleration, determine the best-fit value of
        the acceleration.

13. Pseudo-random numbers and Monte Carlo methods I
    Physics concepts:
        Radioactive decay
        Population dynamics
    Computing concepts:
        Pseudo-random number generation
        Monte Carlo methods
    Examples:
        Use Monte Carlo methods to simulate simple problems in sequential
        radioactive decay and/or population dynamics in biology.

14. Matrix methods
    Physics concepts
        Normal modes
    Computing concepts:
        Algorithms for eignenvalues and eigenvectors
    Examples
        Find the resonant frequencies for coupled harmonic oscillators.
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Proposed Sample Syllabus for Phys 553

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1. Review of Elementary Numerical Methods
    - Differentiation and integration
    - Interpolation and extrapolation methods
    - Zeros and extrema of single variable functions
      Newton-Raphson method
    - Random number generation
    - Sorting algorithms

2. Numerical Solution of Ordinary Differential Equations
    - Runge-Kutta method
    - Adaptive stepsize methods
    - Predictor-corrector methods
    - Shooting method--eigenvalue problems for the Schroedinger equation

3. Numerical Methods for Matrices
    - Solving systems of linear equations
    - Matrix eigenvalue problems
    - Gaussian elimination
    - Tridiagonalization and the Lanczos algorithm

4. Spectral Analysis
    - Fourier transform methods
    - Fast Fourier transforms
    - Orthogonal functions
    - Gaussian quadrature
    - Spectra of random matrices - theoretical and computational issues
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Note: The line of demarcation between the syllabi of Phys 553 and 554 will be somewhat fluid, and topics listed here under one course may be taught in the other, as seen fit by the instructor.

Proposed Sample Syllabus for Phys 554

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5. Partial Differential Equations
     - Discretization of PDE's on a lattice
     - Heat flow problems and relaxation methods
       Jacobi and Gauss-Seidel iteration
     - Minimization methods and the conjugate gradient algorithm
     - Green's function methods
       Propagators and correlators
     - Real-time solution of PDE's
       Importance of unitarity and conservation laws
       The Crank-Nicholson algorithm

6. Monte Carlo Methods
     - Monte Carlo integration - Vegas?
     - Partition functions in statistical physics
     - Markov chains and the Metropolis algorithm
     - Heat bath techniques
     - Hybrid methods and detailed balance
     - Monte Carlo simulation of Ising model in 2-D and 3-D
       Seeing phase transition on the computer
     - Path integrals in QM and QFT
       The stat-mech - QFT connection
       Monte Carlo simulation of quantum field theories

7. Advanced Iteration Methods for Linear Systems
     - Theory of the conjugate gradient method
       Orthogonal directions and conjugate directions
       Bi-orthogonalization
     - Preconditioning in the CG method
     - LU decomposition
     - Orthogonality and Singular Value Decomposition
     - Krylov subspaces
     - Lanczos and Arnoldi methods for eigenvalue problems
       Tridiagonalization of matrices
       Roundoff issues and Cullum-Willoughby filtering for large
       eigenvalue problems

8. Topics in Computational Physics
     - Exploring statistical mechanics, condensed matter physics,
       and particle physics with computer intensive methods
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