Computational Methods for Nonlinear Systems

- Graduate computational science laboratory course developed by Myers & Sethna
  - lectures are minimal
  - class work focused on self-paced implementation of computer programs from hints and skeletal code
- Developed originally to support Cornell IGERT program in nonlinear systems
  - graduate fellowship program supporting interdisciplinary group of students
  - a Core Course in graduate Computational Science & Engineering (CSE) minor
- Hands-on introduction to scientific computing, algorithms, programming, and simulation techniques
  - in the context of IGERT focal themes: complex networks, biolocomotion & manipulation, pattern formation, and gene regulation
  - also includes: statistical mechanics, chaos in nonlinear systems, molecular dynamics, random matrix theory, constraint satisfaction, etc.
- Most exercises incorporated into Sethna’s textbook, “Statistical Mechanics: Entropy, Order Parameters, and Complexity”
Programming

- all programming done in Python (www.python.org)
  - 3rd party Python libraries for numerics, graphics, visualization, etc.
  - e.g., NumPy, SciPy, pylab, Python Imaging Library
- course hints files provide documented code fragments to be fleshed out by students
- graphical tools provided to give immediate feedback, help debug, etc.
- why Python?
  - interpreted: rapid program development and interactive access
  - built-in data structures & high-level syntax
  - rich standard library and 3rd party libraries (for science, visualization, databases, internet programming, etc.)
  - supports procedural programming, object-oriented programming, functional programming, scripting, large systems
  - free software (monetarily and intellectually)
Course modules

- Small-world networks
- Invariant measure
- Cardiac dynamics
- NP-completeness
- Percolation
- Chaos & Lyapunov
- Random matrix theory
- Ising model
- Pendulum
- Fractal dimensions
- Stochastic cells
- Molecular dynamics
- Walker
- Period doubling
- Repressilator
- plus a few others
Small-world networks

- **Science**
  - small world networks (Watts & Strogatz)
  - “six degrees of separation”
  - shortest path lengths in randomly wired graphs
- **Computing**
  - data structure for undirected graphs
    - good introduction to built-in Python containers (lists and dictionaries)
  - object-oriented encapsulation of complex data structures
  - graph traversal algorithms (breadth-first search) for shortest path and betweenness
  - simple graph visualization software supports debugging and provides quick feedback
Percolation

• Science
  - statistical mechanics of percolation
    ▸ connected clusters in randomly wired graphs (e.g., bond percolation on a lattice)
    ▸ universality of phase transitions

• Computing
  - reuse of objects with generic interface
    (reuse of UndirectedGraph class from small-world network module)
  - graph traversal algorithms (breadth-first search) for cluster finding
  - scaling collapses
Walker

- **Science**
  - Simple model of bipedal walker (Ruina and coworkers)
    - double pendulum with impulse for heelstrike
    - single pendulum as warmup
  - period-doubling bifurcations in physical system

- **Computing**
  - integration of ODEs
    - finite differences, time-step dependence, integration schemes (stability, fidelity, accuracy)
    - calling 3rd party numerical libraries
  - change of integration variables for event detection (heelstrike)
  - tracking unstable periodic orbit
  - visualization tools for animation
Maps & dynamical systems

- **Science**
  - bifurcations and chaos in iterated maps
  - period doubling in logistic map
  - density (invariant measure) in chaotic regime
  - Lyapunov exponents: divergence of nearby trajectories
  - fractal dimensions of attractors
  - renormalization group of logistic map & universality of period doubling route to chaos

- **Computing**
  - iterating maps
  - root-finding
  - fitting
Cardiac dynamics

- **Science**
  - pattern formation in excitable medium
  - FitzHugh-Nagumo model (type of reaction-diffusion equation)
  - spiral defects forming in electrical pulsing can lead to cardiac arrhythmias
  - model extensions to simulate dead tissue, cardiac chambers, etc.

- **Computing**
  - numerical solution of PDEs
    - finite-differences, operator stencils
  - nullcline analysis for single cell (root-finding)
  - simple animation tool allows interactive steering of simulation (needed to provide targeted electrical pulses and “defibrillator” shock)
Cell dynamics: stochastic cells and Repressilator

• Science
  - Repressilator (Elowitz & Leibler): genetic oscillator from realm of synthetic biology
    ‣ oscillatory mRNA/protein dynamics from mutually repressing proteins
  - telegraph noise and shotgun noise in stochastic systems
• Computing
  - chemical kinetics and reaction networks
    ‣ Petri nets
    ‣ synthesis of aggregate kinetic equations from network
  - Monte Carlo algorithms (Gillespie)
  - stochastic vs. deterministic descriptions
• Additional projects exploring other gene regulatory networks (switches, feed-forward loops, etc.)
NP-completeness & constraint satisfaction

- Science
  - NP-complete problems
  - phase transitions in 3SAT and parametric complexity
  - integer partitioning problem

- Computing
  - algorithms for NP-complete problems
  - backtracking, recursion
Random matrix theory

• Science
  - eigenvalue spacings in random matrices
  - developed originally to describe energy level spacings in quantum systems

• Computing
  - random matrix generation
  - eigenvalue computation (numpy)
Molecular dynamics

- Science
  - thermodynamics: emergence of effective properties from molecular chaos

- Computing
  - design of large software systems
  - geometric data structures
  - integration of ODEs
  - thermodynamics
    - pressure
    - pair distribution functions
Ising model

- Science
  - phase transitions in simple model of magnetic system
    - nucleation
    - self-similarity
    - fluctuation-dissipation

- Computing
  - Monte Carlo algorithms
    - heat bath
    - Metropolis
    - cluster flipping
Randomness: random walks & Gumbel distributions

• Science
  - ensembles and distributions
    ▸ averages
    ▸ extremal behavior
    ▸ emergent symmetries

• Computing
  - random number generation
  - statistical analysis of ensembles
Motion capture and data-driven dynamical systems

A new group project to be fleshed out in collaboration with John Guckenheimer and Madhu Venkadesan

- **Science**
  - data-driven dynamical systems
    - attractor reconstruction
    - model inference
    - control
    - connections to biolocomotion

- **Computing**
  - interfacing to hardware
  - analyzing noisy experimental data
  - integrating ODEs
Working with course modules

- Course web page
  - www.physics.cornell.edu/~myers/teaching/ComputationalMethods
- Module web pages
  - www.physics.cornell.edu/~myers/teaching/ComputationalMethods/ComputerExercises
  - linked from “Computer Exercises and Hints” on course web page
- For a given module:
  - download (and print out, if desired) “Exercise” pdf file (e.g., Small World Exercise)
  - download “Hints” file and save to disk (e.g., SmallWorldNetworksHints.py)
  - copy “Hints” file to working file
    - e.g., cp SmallWorldNetworksHints.py SmallWorldNetworks.py
  - edit working file
    - e.g., emacs SmallWorldNetworks.py
  - read exercise file and comments in working/hints file
  - remove Python instruction “pass” and fill in body of code to implement exercise
  - start up ipython interpreter
  - run the module (e.g., %run SmallWorldNetworks.py)
Important third-party Python modules

- NumPy (Numerical Python) [www.scipy.org/NumPy]
  - grew from a merger of Numeric and numarray; converging toward version 1.0
  - provides (in a compiled library) high-level array syntax, linear algebra, random number generation, Fourier transforms

- SciPy [www.scipy.org]
  - Python interfaces to well-tested compiled numerical routines, interfaced to work with NumPy arrays
  - provides routines for integration of functions and differential equations, root-finding, minimization, etc.

- pylab (a.k.a. matplotlib) [matplotlib.sourceforge.net]
  - provides 2D (x-y) plotting, histograms, etc.

- Python Imaging Library (PIL) [www.pythonware.com]
  - image creation and manipulation
  - forms the basis of several course visualization modules

- ipython [ipython.scipy.org]
  - enhanced alternative to the standard python interpreter
  - command completion & history, “magic” functions, etc.