Panel: Needs for Support of Computation in Physics & Astronomy

Community Building @ SECANT Workshop

Rubin H Landau, Founding Dir
Computational Physics for Undergraduates
BS Degree Program @ Oregon State University

Prior Support: NSF (CCLI, CI-Team/EPIC), OSU, MSR
Susanne’s 4 Questions

1. Students’ computational experience @ OSU
2. How effectively incorporate C & C Think?
   1. Essential CS concepts, tools & problem solving
   2. Interplay with applied math?
3. Examples where C does !⇒ understand
   1. Effective, practical way assess understanding + C
4. Faculty orientation = problem for UG?
   1. Grads + advisor = OK?
Evidence for $\Delta$(Science Ed)

- RHL Survey (Y&L)
- CSE, CP ~ balance
- Small sample
- Stereotypes
- PH Ed: imbalance?
Paradigm Physics Major (≠ CPUG)

Computational (Ph Ed) vs (Computational Ph) Ed

- Organize physics via abstract math concepts
- E.G. unique solution to math methods problems
- Geometric & visualization strategies (≠ programs)
- Many math strategies; ODE’s vs. PDE’s
- Develop problem-solving skills
- Modern pedagogical strategies
- Compute like a physicist (many tools)

Paradigms

Symmetries & Idealizations
Static Vector Fields
Oscillations
Spin & Quantum Measurements
1-D Waves
Central Forces, Energy & Entropy
Periodic Systems
Rigid Bodies / Reference Frames

Capstones

Classical Mech
Math Methods
E & M
Quantum Mech
Thermal Physics
Optics
Sci Compute I (CP)
Lab (electron/II)
vs Comp Physics Curriculum

- Problem solving (why do P, what P do)
- Learn by **doing** individual Projects
- Over-shoulder teach (lectures?)
- CS + App Math + physics in context
- More efficient, effective approach to science Ed
  - ok ↓ # “physics” courses; yet many new subjects
- Compiled language
  - see algorithm (eqtns)
  - bare bone codes given
  - “I am not a bigot!” (packages)
<table>
<thead>
<tr>
<th>Year</th>
<th>Fall</th>
<th>Winter</th>
<th>Spring</th>
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<tbody>
<tr>
<td>Soph (45)</td>
<td>Intro CS II (CS) Vector Calc II (MTH) Gen Phys II Writing II</td>
<td>Discrete Math (MTH) Infinite Series (MTH) Gen Phys III Perspective</td>
<td>Scientific Comptg II (PH) App Diff Eqs (MTH) Intro Mod Phys Linear Algebra (MTH)</td>
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<td>Jr (44)</td>
<td>CP I (PH) Symmetries (PH) Oscillations (PH) Vector Fields (PH) Writing III CP Seminar</td>
<td>CP II (PH) Data Structures (CS) 1D Waves (PH) Quantum Measures (PH) Central Forces (PH) Elective</td>
<td>Class Mech (PH) Quantm Mech (PH) Perspective Statistics (MTH) Biology</td>
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Real computation across the curriculum
Not 1 course, not just our view
Use what’s available
Computational Physics Education

Hardware
- IEEE Floating Point
- Architecture Memory Hierarchy
- Performance Tuning
- Parallel Computing

Software
- Operating Systems
- Errors & Limits
- Scientific Libraries
- Linear Algebra Matrix Computing

Numerics
- Differentiation
- Integration
- Trial & Error Searching
- Eigenvalue Problems
- Ordinary Differential Equations
- Partial Differential Equations
- Finite differences elements
- Integral Equations

Applications
- Data Analysis Interpretation
- Data Interpretation
- Statistical Fitting
- Data Structures
- Fourier Analyses
- Wavelet Analyses

Simulation
- Problem Solving
- Communication
- Molecular Dynamics (MD)
- Monte Carlo Simulations
- Stochastics
- Metropolis algorithm
- Nonlinear Systems
- Computational Fluid Dynamics

Math

Science

Content Map!
How Does this Work?

1. Challenging for some students (intro*, multidisciplinary)
2. Unhappy with grade if just ran code, no thought, no time
3. Students often thankful when/that over (career)
4. Tears, emotion; human-C interaction = complex
5. Excitement; human-C interaction = complex, emotional
6. “This combo is what I interested in, but had to pick 1”
7. “Why have we studied fluids only in our freshman year?”
8. “Now I know what
9. “Gave me an entirely new view of integration, series, ”
10. “Now Laplace’s equation makes sense”
11. “I was up all night.”
12. Chaotic scattering: several MS, 1 Ph D
13. “MD: way I thought simulations should
15. Women: didn’t know liked C, problem solving
# Two Lower-Division Courses

<table>
<thead>
<tr>
<th>Course</th>
<th>Topics</th>
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<tbody>
<tr>
<td><strong>Physics/Math/CS 265, Scientific Computing I</strong> (A First Course, Princeton)</td>
<td>OS, Basic Maple, Number Types</td>
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<td>Logical control, plotting</td>
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<tr>
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<td>Maple Functions, Number types, Symbolics</td>
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<td>Visualization, Loops, Integration</td>
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<td>Calculus, Equation Solving</td>
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<td>Objects, Complex Arithmetic</td>
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<td>Introductory Java</td>
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<td>Web Computing: Applets</td>
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<td>Limits, Methods (functions)</td>
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<td>Arrays, File I/O</td>
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<tr>
<td><strong>Physics 464/564, Intro Computational Science</strong> (Computational Physics, Wiley)</td>
<td>Unix Editing and Running*</td>
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<td>Monte Carlo Techniques</td>
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<td>Floating Point Errors &amp; Uncertainties</td>
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<td>Random Walk, Decay Simulation*</td>
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<td>Limits: precision, under/overo ws</td>
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<td>Interpolation, cubic spline</td>
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<td>Matrix Computing with JAMA libe</td>
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<td>Least-squares t, Quadrature</td>
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<td>Differentiation, ODEs, ODE Eigenvalues</td>
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<td>Hardware: Memory, CPU, Tuning</td>
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## Contents of Upper-Division Courses

### Physics 465–6/565–6 Computational Physics *(Computational Physics, Wiley)*

<table>
<thead>
<tr>
<th>Course</th>
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<tbody>
<tr>
<td>Realistic, Double Pendula*</td>
<td>Quantum Path Integration*</td>
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<tr>
<td>Fourier &amp; Wavelet Analyses</td>
<td>Fluid Dynamics</td>
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<tr>
<td>Predators &amp; Prey: Nonlinear Mappings*</td>
<td>Electrostatic Potentials</td>
</tr>
<tr>
<td>Chaotic Pendulum/Scattering*</td>
<td>Parallel Computing (MPI), Heat Flow</td>
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<tr>
<td>Fractals, Aggregation, Trees, Coastlines*</td>
<td>Waves on a String</td>
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<tr>
<td>Bound States via Integral Eqtns</td>
<td>Shock Waves &amp; Solitons</td>
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<tr>
<td>Quantum Scattering, Integral Equations</td>
<td>Molecular Dynamics Simulations</td>
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<tr>
<td>Thermodynamics: The Ising Model</td>
<td>Electronic Wave Packets</td>
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### Physics 467/567 Advanced Computational Laboratory

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<tr>
<th>Course</th>
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<tbody>
<tr>
<td>Radar Maps of Archaeological Tells</td>
<td>Density Functional Theory</td>
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<tr>
<td>Molecular Dynamics Simulations</td>
<td>Gamow States of Exotic Atoms</td>
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<tr>
<td>Meson-Nuclei p-Space Scattering</td>
<td>Pion Form Factor Data Analysis</td>
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<tr>
<td>Wavepacket-Wavepacket Interactions</td>
<td>Particle Hydrodynamics</td>
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<tr>
<td>Serious Scientific Visualization</td>
<td>Brain Waves Principal Components</td>
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<td>Earthquake Analysis</td>
<td>Quantum Chromodynamics</td>
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