Computational Physics:
- A Model for Physics Education
  - A Model for Future eTextBook

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1st = Computational subatomic few-body systems (1966-2003)
2nd = Research developments (1988-) → broaden, ed dream

Computational Physics for Undergraduates
Supported by NSF (CCLI, CI-Team/EPIC), OSU, MSR
Contributing Group

- Manuel J Paez, University of Medellin, Colombia, SA, CoAuthor
- Cristian Bordeianu, University of Bucharest, Romania, CoAuthor [deceased]
- Paul Fink, Robyn Wangberg, CoAuthors
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- Melanie Johnson (Unix Tutorials)
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- Matthew Ervin Des Voigne (tutorials)
- Bertrand Laubsch (Java sound, decay simulation)
- Jon J Maestri (vizualizations, animations, quantum packets) [deceased]
- Al Stetz, David McIntyre (First Course)
- Juan Vanegas (OpenDX)
- Connelly Barnes (OOP, PtPlot)
- Phil Carter, Donna Hertel (MPI)
- Zlatko Dimcovic (Wavelets, Java I/O)
- Joel Wetzel (figures)
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- Brandon Smith, (REU, Summer 97; Chico State/SDSC, CA)
- Paul D. Hillard, III (REU, Summer 96; Southern Univ, LA)
- Kevin Wolver, (REU, Summer 96; St Ambrose, IA)

And all the suffering students!
Preview (CP-2 Resource Letter, AJP)

1. Need Comp Science & Engr (data) √
2. Computational Courses √
3. Comp Physics Approach & Contents √
4. Journals
5. Conferences & Organizations
   b. SC Center & Grids
   c. CSE Ed Focus Groups √
6. Books √
7. Tools, Languages, Environments √
8. Parallel Computing
   a. Subroutine libes
   b. General DLs
Changing the Status Quo?

- If work paradigm changes, education paradigm changes.

- ... the greatest thing a human soul ever does in this world is to see something, and tell what it saw in a plain way. Hundreds of people can talk for one who can think, but thousands can think for one who can see.

- You never change something by fighting the existing reality. To change something, build a new model that makes the existing model obsolete.

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Premise: Need $\Delta$ (Phys Ed)

- Historical rapid $\Delta$ in how/what do science
  - $\uparrow$ computer power & pervasiveness
- $\Rightarrow$ $\Delta$ undergrad Ph Ed $>$ delivery (C tool)
  - Proper for P Ed $\Delta$ content: more C, Understand C
  - CSE view; Toolset freedom, Compt Science Think
- Physics Choice: like Classic Greek, or living?
  - “we are teaching the same things we taught 50 years ago”
    (APS/AAPT Taskforce on Grad Ed., R Diehl)
- PH(t) narrows, CSE do Fluids, MD, NLinear, data mining
- Simulation: Solitons, QCD, Stars, Black holes, Particle-Astro
Premise (cont): Need △ (Phys Ed)

- Physics = problem solving describing physical world
- From Basic principles + math tools
- Now + Computation = tool
- National Labs Research → CSE
- CSE Educational view
  - ⇔ research (creative) = Hi Quality education
  - = Physics Education + Research Attitude
  - ≠ Physics Education Research (inward)
Evidence for ∆ (Physics Ed) 1

Software

What's Important in 5-7 Years? (AIP)

- Software development
- Comp. programming
- Product design
- Modeling or simulation
- Knowledge of physics
- Scientific software
- Lab or instrumentation skills
- Physics principles
- Mathematical skills
- Synthesizing info
- Scientific problem solving

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Evidence for $\Delta$ (Physics Ed) 2

- National Science Board: remain in field
  - 35% of CS, math BS (74% PhD)
  - 22% of physical, biological (52%)
  - $\neq$ bad thing!

$\Rightarrow$ Undergrad Physics overemphasize Physics!
  - = weaker preparation for career
  - "In the new economy, computer science isn't an optional skill"  
    B. Obama, 2016
Evidence for $\Delta$ (Physics Ed) 3

- Number US STEM grads decreasing
- Yet Numb ≠ issue!, $t_{HW} = 24\text{hr} \rightarrow 15\text{ hr}$
- Bristol Comp Ph Exam: 75% (1990) $\rightarrow 50\%$ (2000)
- Though entrance grades increased (B $\rightarrow$ A)
Where Do Physics BS's Go?

Evidence for $\Delta$ (Physics Ed) 4
Evidence for \( \Delta \) (Science Ed)

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

<table>
<thead>
<tr>
<th></th>
<th>CS</th>
<th>CSE</th>
<th>CP</th>
<th>PH</th>
</tr>
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<tbody>
<tr>
<td>Other</td>
<td>31</td>
<td>29</td>
<td>32</td>
<td>36</td>
</tr>
<tr>
<td>Application</td>
<td>17</td>
<td>28</td>
<td>28</td>
<td>45</td>
</tr>
<tr>
<td>Math</td>
<td>12</td>
<td>23</td>
<td>19</td>
<td>17</td>
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<tr>
<td>Comp</td>
<td>40</td>
<td>20</td>
<td>20</td>
<td>2</td>
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</tbody>
</table>
What = CP, How CP

- Problem solving (why do P, what P do)
- Learn by doing individual Projects
- Over-shoulder teach (lectures?)
- Practical ≠ “Theory of CP” (grad, math); doer
- CS + Math + physics in context
- More efficient, effective approach to science Ed
- ok ↓ # “physics” time
- Compiled language
  - see algorithm (eqtns)
  - bare bone codes given
- “I am not a bigot!” (Python, packages)
President’s Info Tech Advisory Committee:
CS departments alone can’t meet need, not diverse, “computational science indispensable in every sector,… need be recognized by governments & universities”

Changing Physics Courses May help
# BS in CP @ OSU

<table>
<thead>
<tr>
<th>Year</th>
<th>Fall</th>
<th>Winter</th>
<th>Spring</th>
</tr>
</thead>
<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>
</tr>
<tr>
<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 (CS) Quantum Measures (PH) Central Forces (PH) Elective</td>
<td>Class Mech (PH) Quantm Mech (PH) Perspective Statistics (MTH) Biology</td>
</tr>
</tbody>
</table>

Real computation across the curriculum
Not 1 course, not just our view
Use Available & New Courses < 7 years
## Computational Degree Programs

*Abbassi, Swanson, Epic, Mariasingam, L*

*≈ 5x(2001)*

<table>
<thead>
<tr>
<th>Computational Physics</th>
<th>Computational Mathematics</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Houghton C</td>
<td>1. Arizona State</td>
</tr>
<tr>
<td>2. Illinois State</td>
<td>2. CUNY Brooklyn</td>
</tr>
<tr>
<td>4. SUNY Buffalo</td>
<td>4. Missouri So State</td>
</tr>
<tr>
<td>5. Chris Newport (BS/MS+CS)</td>
<td>5. Rice</td>
</tr>
<tr>
<td><strong>Computational Science</strong></td>
<td><strong>Computational Biology</strong></td>
</tr>
<tr>
<td>2. SUNY Brockport</td>
<td>2. U Pennsylvania</td>
</tr>
<tr>
<td>3. Stevens Inst Tech</td>
<td>4. UC Berkeley</td>
</tr>
<tr>
<td>4. UC Berkeley</td>
<td>5. Rice</td>
</tr>
<tr>
<td><strong>Computational Biology</strong></td>
<td><strong>Foreign Programs</strong></td>
</tr>
<tr>
<td>3. National U Singapore (CSE)</td>
<td>8. U Waterloo (CSE)</td>
</tr>
<tr>
<td>4. Trinity C, Dublin (CP)</td>
<td>9. Utrecht U (CSE)</td>
</tr>
<tr>
<td>5x(2001)</td>
<td></td>
</tr>
</tbody>
</table>
### Other UG Computational Programs

What's in a name? That which we call a rose by any other name would smell as sweet.

**Minor, Concentration, Track, Emphasis, Option, Focus (23) (all politics are local)**

<table>
<thead>
<tr>
<th>Computational Physics</th>
<th>Computational Science</th>
</tr>
</thead>
<tbody>
<tr>
<td>4. Penn State Erie</td>
<td>3. Old Dominion</td>
</tr>
<tr>
<td>5. U Arkansas</td>
<td>4. RPI</td>
</tr>
<tr>
<td><strong>Computational Mathematics</strong></td>
<td>5. Salve Regina</td>
</tr>
<tr>
<td>2. San Diego State (App &amp; CM)</td>
<td>7. U Wisconsin Eau Claire</td>
</tr>
<tr>
<td>3. U Central Florida</td>
<td>8. U Wisconsin LaCrosse</td>
</tr>
<tr>
<td><strong>Computational Biology</strong></td>
<td>10. Wittenberg</td>
</tr>
<tr>
<td>1. UC Merced</td>
<td>11. Wofford C</td>
</tr>
<tr>
<td>2. Center CB (Colo)</td>
<td></td>
</tr>
</tbody>
</table>

(NY Botanical) © Rubin Landau, OSU
DOE Awards, Fellowship

**XSEDE (NSF)**
(Extreme Sci & Engr Discovery Environ)

= \sum \text{SuperComputer Centers}

**Education People**

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**It Takes a Village**

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**Engaging People In Cyberinfrastructure**

- **Human Development**
- **Curriculum Development**
- **Tool and Resource Development**
- **Engaging Diverse Communities**
- **Minority Serving Institutions**
- **Informal Science Communities**
- **K-12 Community**
- **Science and Technology Centers**
- **EPIC Partners**
- **2&4 Year College and University Community**
- **Focused Development Areas**

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**National Science Digital Library**

**Math Science Partnerships**

**Advanced Technology in Education Centers**

**TeraGrid and Supercomputing Centers**

**Information Technology Research Centers**

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**Computational Science Education and Training**

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**Access to Advanced Technologies and Tools**

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**Foundational Strategies**

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**Mission**
CP Research, eg 7 Supernova on Demand

- Particle physicists data-intensive computing meets astronomy
- Measure: expansion rate of universe via Type Ia supernovae
  - standard candle, 2-pt correlation function

Epoch 1

- Nat Roe: Physics student coding
  - Poor documentation
  - Poor structure

Movie ↓
Intellectual Content
Computational Physics Ed

- *Elements of Computational Science & Engineering Ed*, Yasar & L (SIAM)
- Prerequisite establish Computational Physics course
- Include CP Examples in classes
- Easy (too) expect 1 course teach entire subject (programming?)
- Historically guided by research needs; grad study = easy
- See *Student Learning Outcomes (AIP)* for specific subjects
- ≠, don’t need CP BS, 7 years
## Examples for Physics Courses

<table>
<thead>
<tr>
<th>Physics Courses</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spontaneous Decay Simulation</td>
<td>Realistic Waves</td>
</tr>
<tr>
<td>Classical Chaotic Scattering</td>
<td>Shock Waves</td>
</tr>
<tr>
<td>Proper ODE Solution</td>
<td>Solitons</td>
</tr>
<tr>
<td>Double &amp; Chaotic Pendula</td>
<td>Sonifications</td>
</tr>
<tr>
<td>Nonlinear Dynamics, Bifurcation</td>
<td>Fluid Dynamics</td>
</tr>
<tr>
<td>Fractals &amp; Statistical Growth</td>
<td>DFT, Wavelet Analysis</td>
</tr>
<tr>
<td>Laplace &amp; Possion Equations</td>
<td>Feynman Path Integrals</td>
</tr>
<tr>
<td>Realistic PDE Solutions</td>
<td>Wavelet Analysis</td>
</tr>
<tr>
<td>Molecular Dynamics</td>
<td>Prin Component Analysis</td>
</tr>
<tr>
<td>Quantum Wave Packets</td>
<td>Data Intensive</td>
</tr>
</tbody>
</table>
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, excitement; human-C interaction = complex
5. “This combo is what I’m interested in, but had to pick 1”
6. “Why have we studied fluids only in our freshman year?”
7. “Now I know what...”
8. “Now Laplace’s eq...”
9. “I was up all night.”
10. Chaotic scattering: several MS, 1 Ph D
11. “MD: way I thought simulations should
13. Women: didn’t know liked C, problem solving
Online Courses

- Web N is here to stay & grow
- Challenge use it well for Education
- Not: general ed, weak discipline, motivation

N Feynman Path Integrals I

G

Computational Physics II, 465/565
Oregon State University
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CCLI-0836971

Hamilton’s Principle of Least Action (Classical)

Newton’s Law \( \delta S[\mathbf{x}(t)] = 0 \)

“The most general motion of a physical particle moving along the classical trajectory \( \mathbf{x}(t) \) from time \( t_a \)

to \( t_b \) is along a path such that the action \( S[\mathbf{x}(t)] \) is an extremum.”

Dynamic slide

\[
\delta S = \delta S[x(t)] + \frac{\delta x(t)}{2} - \frac{\delta S[x(t)]}{2} = 0 \quad (1)
\]

(Constraint) \( \delta (x_0) - \delta (x_0) = 0 \quad (2) \)

\[
[x(x')] = \text{functional}
\]

\[
S[\mathbf{x}(t)] = \int_{t_a}^{t_b} dt L[x(t), x'(t)] \quad (3)
\]

\[
L = \text{Lagrangian} = \mathcal{T}[x, x'] - \mathcal{V}[x] \quad (4)
\]

Free Online Lecture and Slides (N-D Search)

RHL: Hybrid Course Online Lectures
Lecture time \( \rightarrow \) Lab time
"Kindle, Nook, Sony Reader... I say, Hardwick, this sure is an impressive library."
Digital Book

Technology Catching Up

- Exploring since 1996 WWW
- Multiple senses
- High accessibility potential
- Δ learning approaches
- Students: integrated package
- Vision: Interactive eqns, figs
- Python notebook (TOC -8 euler, abm)
~rubin/Books/CPbook/eBook/Notebooks

Not There Yet

- Exec files, OS’s incompatible
- Very large files (→ cloud)
- Validate data & codes?
- Security concerns
- No standard readers, writers
- ≠ deep subject mastery
- Mastery >> scanning
- No page numbers

A good book has no ending. –R.D. Cumming
Take Home Lessons

- Physics now done with computation
- Physics now done with other sciences
- Physics Ed now done with 50-100 year old stuff
- Students are people; more product than customer
- Agree: bad math means unreliable science?
- So bad computation means unreliable science
- Computation too important to leave to CS
- www.science.oregonstate.edu/~rubin
Conclusions & Summary

- Suggest: rejuvenate Phys Ed with modern Res (+CP)
- Need $\Delta$ curriculum: learn P + CS + math in context
- CP courses, materials: More efficient, effective *Model*
  - learning within problem solving, emotional connect
  - learn all 3 better, frees t for C, M
  - Freedom: common toolset & mindset CSE
- Thank you!
- www.science.oregonstate.edu/~rubin
Skills Expected of Physics UnderGraduates (AAPT)

Plot functions and data
Visualization complex data
Numerical integration, diff
Limits of algorithms
Programming*, compiled language
Several operating system

ODEs, PDEs
Matrix operations
Fourier transforms, FFT
Statistics, data fitting
Computational thinking
Symbolic programming
LATEX
Evidence for $\Delta (Physics\ Ed)$


- **Engineering**: 45%
- **Computer and Information Tech.**: 24%
- **Other Natural Science, Technology and Math**: 14%
- **Physics or Astronomy**: 10%
- **Non-STEM**: 7%

Knowledge and Skills Regularly Used by Physics Bachelor's Employed in the Private Sector, Classes of 2011 & 2012 Combined.

- **Employment in Engineering**
- **Employment in Computer Science or Information Technology**

- Solve Technical Problems
- Work on a Team
- Technical Writing
- Design & Development
- Use Specialized Equip.
- Perform Quality Control
- Manage Projects
- Knowledge of Phys. or Ast.
- Programming
- Work with Customers
- Advanced Math
- Simulation or Modeling
- Manage People
- Manage Budgets

Percentages represent the physics bachelor's who chose "daily," "weekly," or "monthly" on a four-point scale that also included "never or rarely."

http://www.aip.org/statistics

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# Two Lower-Division Courses

<table>
<thead>
<tr>
<th><strong>Physics/Math/CS 265, Scientific Computing I</strong> <em>(A First Course, Princeton)</em></th>
</tr>
</thead>
<tbody>
<tr>
<td>OS, Basic Maple, Number Types</td>
</tr>
<tr>
<td>Maple Functions, Number types, Symbolics</td>
</tr>
<tr>
<td>Calculus, Equation Solving</td>
</tr>
<tr>
<td>Introductory Java</td>
</tr>
<tr>
<td>Limits, Methods (functions)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Physics 464/564, Intro Computational Science</strong> <em>(Computational Physics, Wiley)</em></th>
</tr>
</thead>
<tbody>
<tr>
<td>Unix Editing and Running*</td>
</tr>
<tr>
<td>Floating Point Errors &amp; Uncertainties</td>
</tr>
<tr>
<td>Limits: precision, under/overo ws</td>
</tr>
<tr>
<td>Matrix Computing with JAMA libe</td>
</tr>
<tr>
<td>Differentiation, ODEs, ODE Eigenvalues</td>
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</tbody>
</table>
# Contents of Upper-Division Courses

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

<table>
<thead>
<tr>
<th>Course Title</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Realistic, Double Pendula*</td>
<td>Quantum Path Integration*</td>
</tr>
<tr>
<td>Fourier &amp; Wavelet Analyses</td>
<td>Fluid Dynamics</td>
</tr>
<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>
</tr>
<tr>
<td>Fractals, Aggregation, Trees, Coastlines*</td>
<td>Waves on a String</td>
</tr>
<tr>
<td>Bound States via Integral Eqtns</td>
<td>Shock Waves &amp; Solitons</td>
</tr>
<tr>
<td>Quantum Scattering, Integral Equations</td>
<td>Molecular Dynamics Simulations</td>
</tr>
<tr>
<td>Thermodynamics: The Ising Model</td>
<td>Electronic Wave Packets</td>
</tr>
</tbody>
</table>

**Physics 467/567 Advanced Computational Laboratory**

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