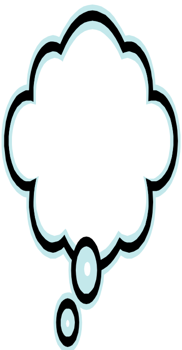
Computational Physics:

- A Model for Physics Education

-A Model for Future eTextBook



Rubin Landau
Physics Professor Emeritus
Oregon State University
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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
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- Sally Haerer, Saturo S. Kano (consultants, producers)
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- Hans Kowallik (Computational Physics text, sounds, codes, LAPACK, PVM)
- Matthew Ervin Des Voigne (tutorials)
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- 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)
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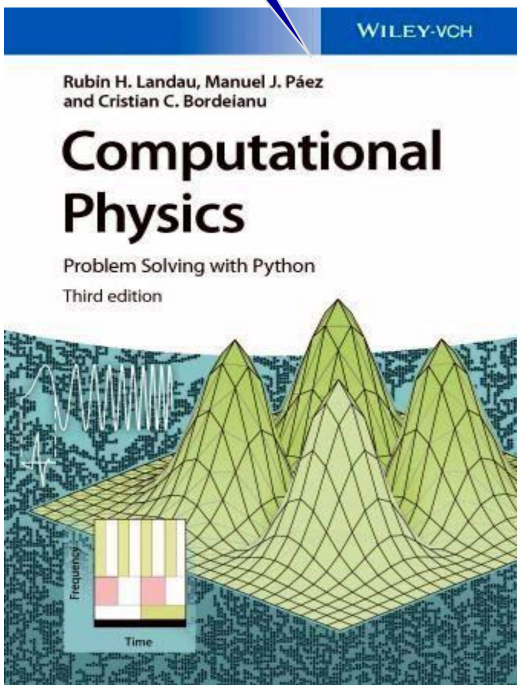
- Paul D. Hillard, III (REU, Summer 96; Southern Univ, LA)
- Kevin Wolver, (REU, Summer 96; St Ambrose, IA)

And all the suffering students!

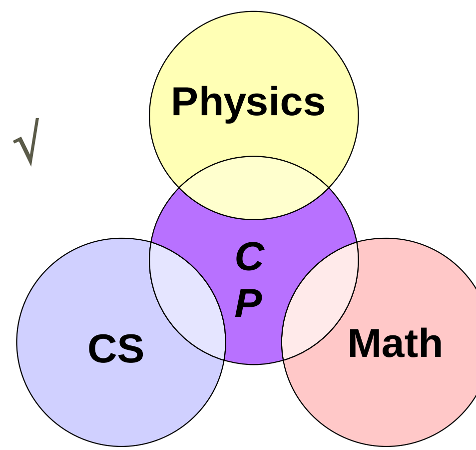
Preview (CP-2 Resource Letter, AJP)

D of SC



Python Version
Wiley 2015

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**
9. **Digital Libraries, eTexts √**
   - a. **Subroutine libes**
   - b. **General DLs**



Changing the Status Quo?

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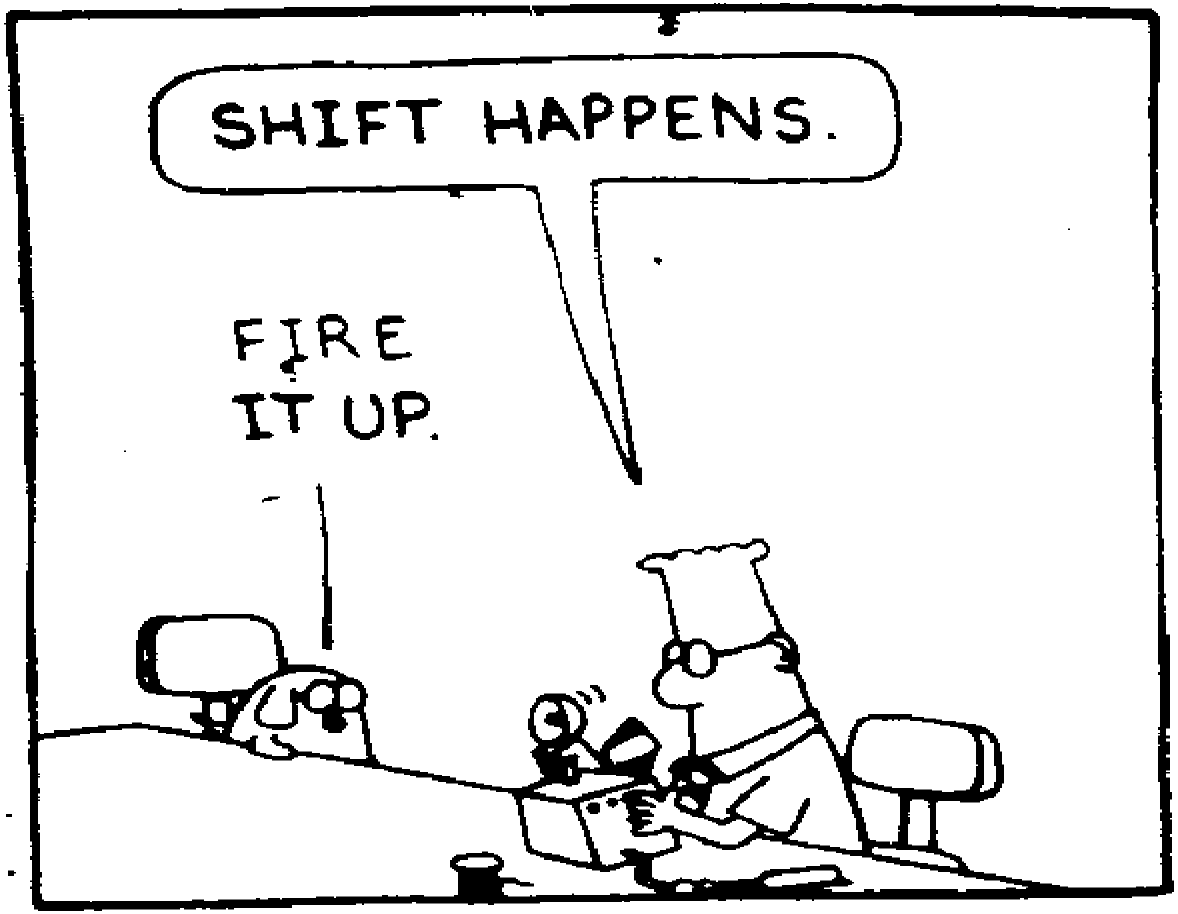

- You r g the
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ernie?)

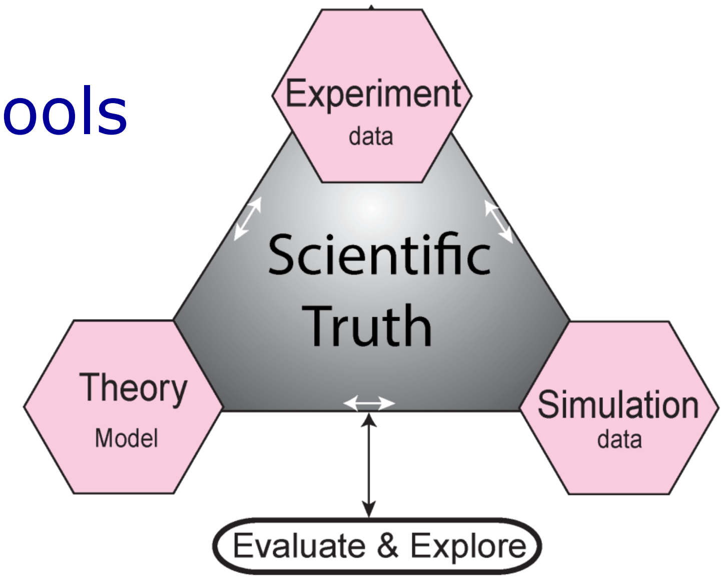
Premise: Need Δ (Phys Ed)

- Historical rapid Δ in how/what do science
  - ⇑ computer power & pervasiveness
- ⇒ Δ undergrad Ph Ed > *delivery (C tool)*
  - Proper for P Ed Δ *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"

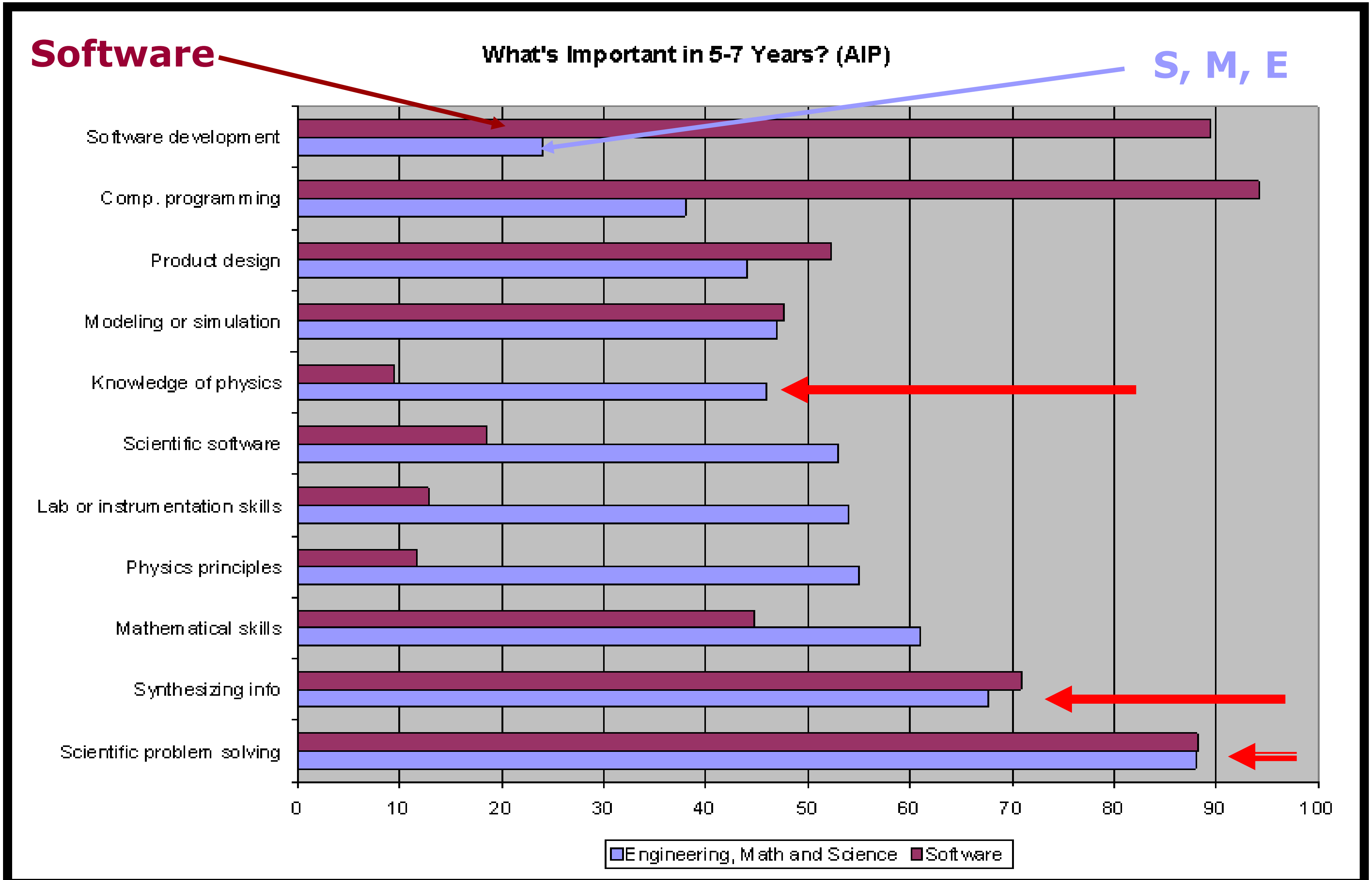
    (APS/AAPT Taskforce on Grad Ed., R Diehl)
- PH(t) narrows, CSE *do* Fluids, MD, NLinear, data mining
- Simulation: Solitons, QCD, Stars, Black holes, Particle-Astro

Premise (cont): Need Δ (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)



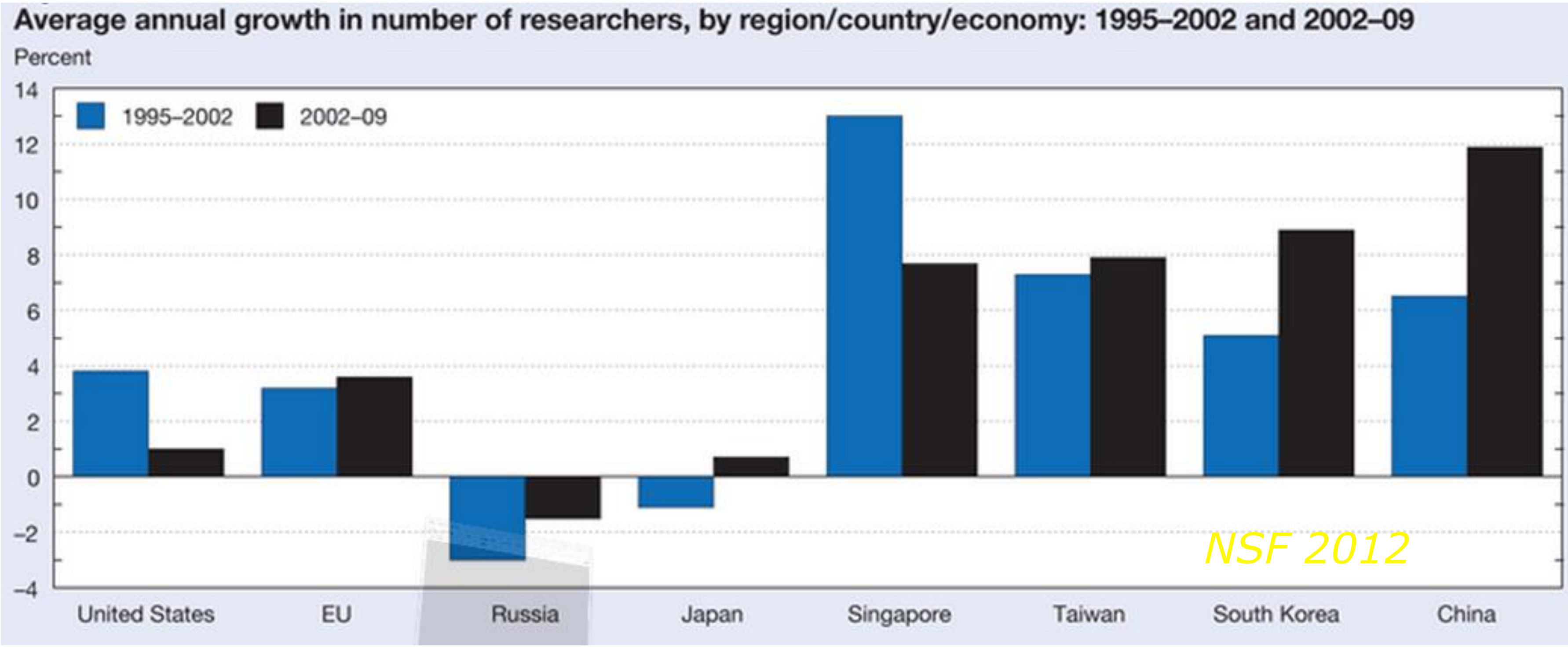
Evidence for Δ (Physics Ed) 1



Evidence for Δ (Physics Ed) 2

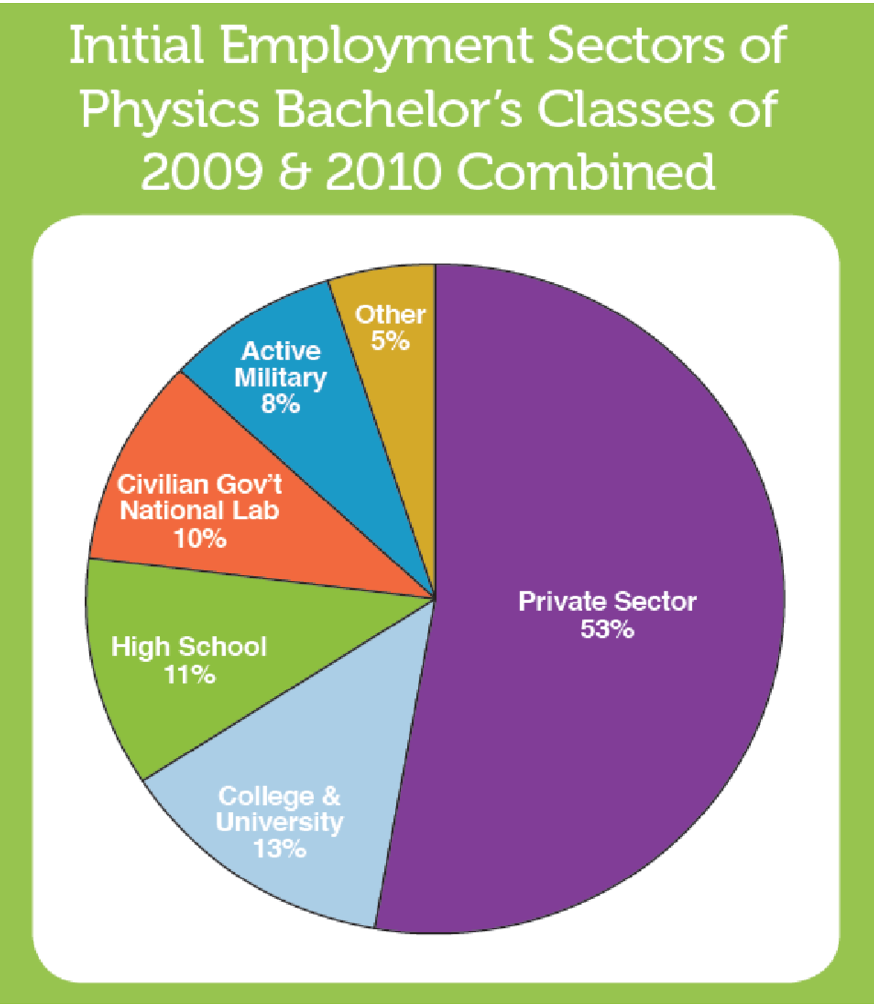
- National Science Board: remain in field
  - 35% of CS, math BS (74% PhD)
  - 22% of physical, biological (52%)
  - ≠ *bad thing!*
- ⇒ Undergrad Physics overemphasize Physics!
  - = weaker preparation for career
  - *"In the new economy, computer science isn't an optional skill"* B. Obama, 2016

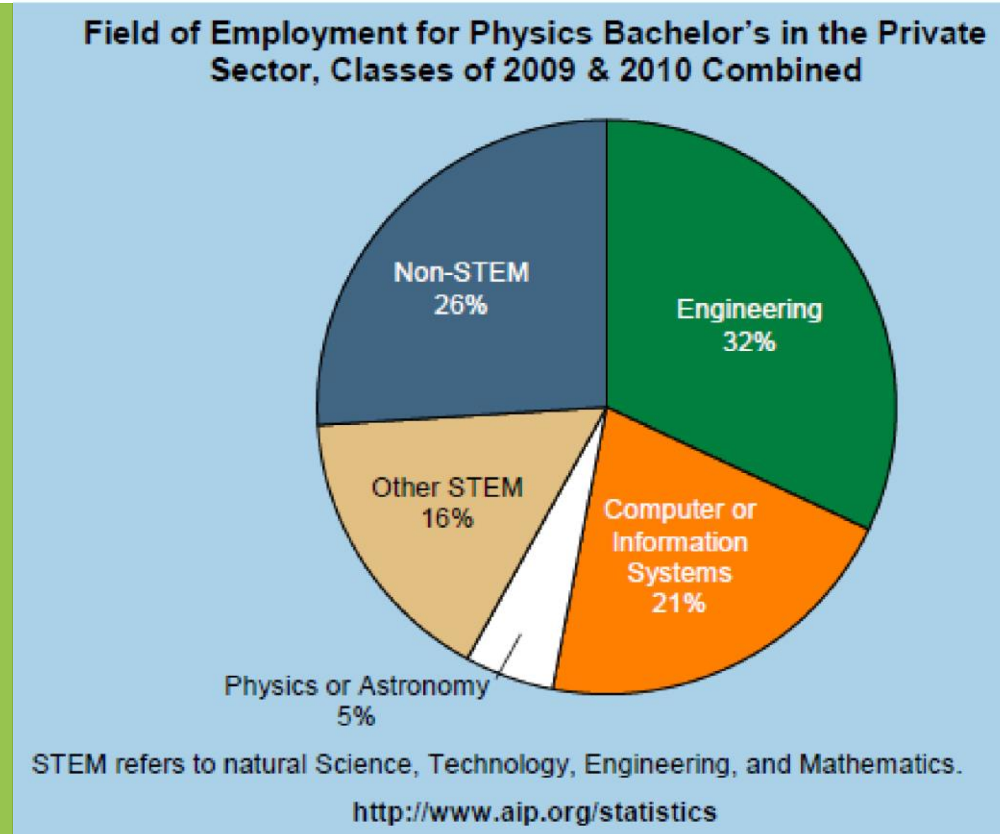
Evidence for Δ (Physics Ed) 3



- Number US STEM grads decreasing
- Yet Numb ≠ issue!, t_{HW}=24hr (1961) → 15 hr
- Bristol Comp Ph Exam: 75% (1990) → 50% (2000)
- Though entrance grades increased (B → A)

Evidence for Δ (Physics Ed) 4





Where Do Physics BS's Go?

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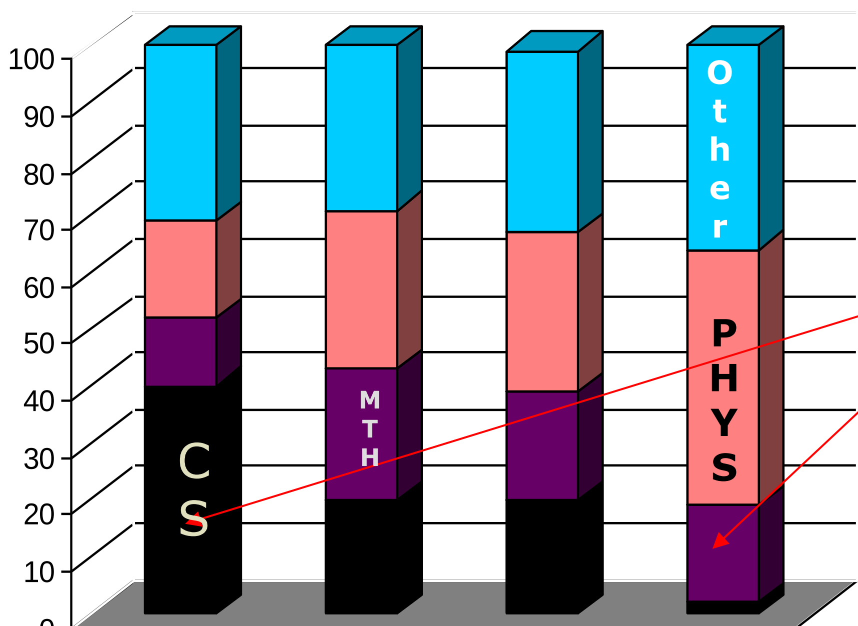
Evidence for Δ (Science Ed)

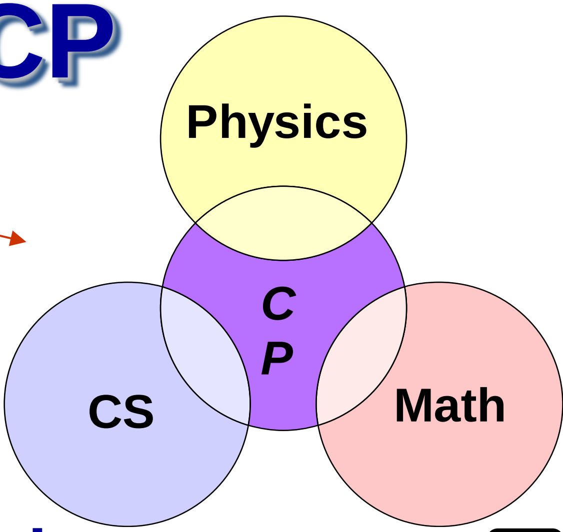
Subject Balance (% Courses)



	CS	CSE	CP	PH
Other	31	29	32	36
Application	17	28	28	45
Math	12	23	19	17
Comp	40	20	20	2

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

What = CP, How CP



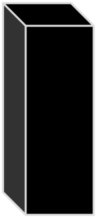
- **Problem solving (why do P, what P do)**
- **Learn by *doing* individual Projects**
- **Over-shoulder teach (lectures?)**

Problem	Theory Model	Method	Implementation
science	discrete continuous	numeric symbolic	Java, f90, C

Assessment

visualization exploration

- **Practical ≠ "Theory of CP" (grad, math); doer** *Multi ≠ Inter*
- ***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)**



O.Y.

Changing Physics Courses May help

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"

BOOK SERIES

Series in Computational Physics

Series Editors

Steven A. Gottlieb

Rubin H. Landau

About the Series

This textbook series is aimed at the modern physics curriculum, presenting teaching and learning resources at the advanced undergraduate and graduate levels. It covers all areas of physics in which computation is now an integral component as well as new, cross-disciplinary topics of modern computational sciences. The presentation is concise and practical, often including solved problems and examples. Among subject areas addressed are condensed matter physics, materials science, particle physics, mathematical methods of computational physics, quantum mechanics, plasma physics, fluid dynamics, statistical physics, optics, and biophysics. These books highlight the importance of numerical methods and computational tools, giving essential foundational materials for students and instructors in the physical sciences as well as academic and industry professionals in physics, engineering, computer science, applied math, and biology.

Want to Publish with Us?

If you are interested in proposing a book for the series, please contact one of the series editors or one of our acquisitions editors.

Book Proposal Form

BS in CP @ OSU

	Fall	Winter	Spring
Fresh (46)	Diff Calculus (Mth) Writing/fitness Gen Chem I Perspective CP Seminar	**Scientific Comptng I** (PH/MTH/CS) Intgl Calculus (MTH) Perspective - 2 Gen Chem II	**Intro CS I (CS)** Vector Calc (MTH) Gen Phys I Writing/fitness
Soph (45)	**Intro CS II (CS)** Vector Calc II (MTH) Gen Phys II Writing II	**Discrete Math (MTH)** Infinite Series (MTH) Gen Phys III Perspective	**Scientific Comptg II** (PH) App Diff Eqs (MTH) Intro Mod Phys **Linear Algebra (MTH)**
Jr (44)	**CP I (PH)** Symmetries (PH) Oscillations (PH) Vector Fields (PH) Writing III **CP Seminar**	**CP II** (PH) **Data Structures (CS)** 1D Waves (PH) Quantum Measures (PH) Central Forces (PH) Elective	Class Mech (PH) Quantm Mech (PH) Perspective **Statistics (MTH)** Biology
Sr (45)	E & M Math Methods **Num Lin Alg (MTH)** Electives - 2	**Adv CP Lab (PH)** Social-Ethical CS Elective - 2 Synthesis	**Adv CP Lab -Thesis** **CP Seminar** Elective –2 **Multi Media, Web (CS)**

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

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Computational Degree Programs

Abbassi, Swanson, Epic, Mariasingam, L $\approx$ 5x(2001)

Computational Physics	**Computational Mathematics**
1. Houghton C	1. Arizona State
2. Illinois State	2. CUNY Brooklyn
3. Oregon State	3. Michigan State
4. SUNY Buffalo	4. Missouri So State
5. Chris Newport (BS/MS+CS)	5. Rice
Computational Science	6. Rochester Inst Tech
1. Stanford (+Math)	7. Seattle Pacific
2. SUNY Brockport	8. Saginaw Valley State
3. Stevens Inst Tech	9. San Jose State
4. UC Berkeley	10. U Chicago
Computational Biology	11. U Illinois Chicago
1. Carnegie Mellon	
2. U Pennsylvania	

Foreign	**Programs**
1. Australian National University	5. 6. U Calgary (CSE) , Waterloo
2. Kanazawawa U Japan (CSE)	7. U Erlangen-Nurnberg (CSE)
3. National U Singapore (CSE)	8. U Waterloo (CSE)
4. Trinity C, Dublin (CP)	9. Utrecht U (CSE)

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)

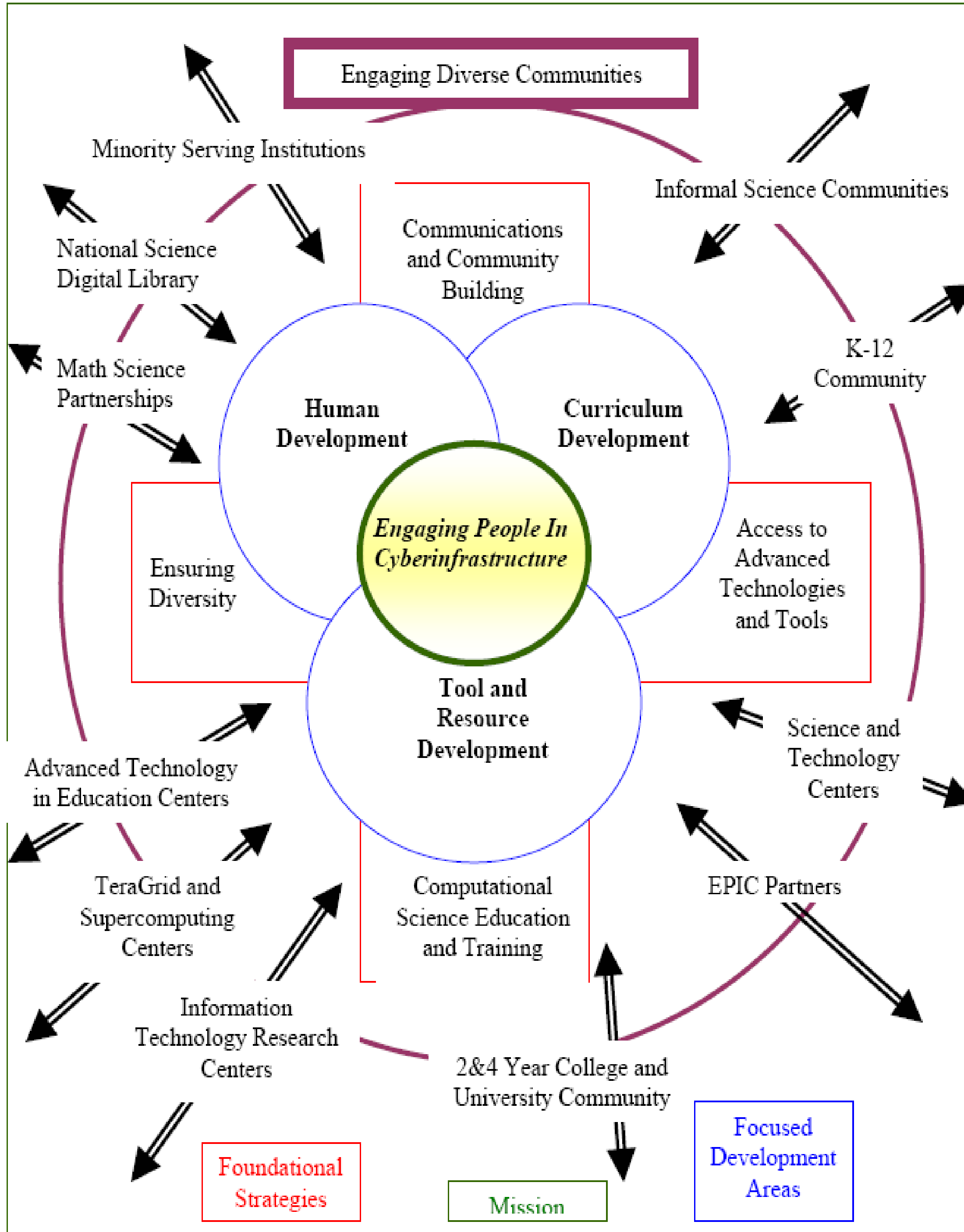
Computational Physics	**Computational Science**
1. Carnegie-Mellon, 2. Abilene Christian	1. Capital
3. North Carolina State, Chapman	2. Clark
4. Penn State Erie	3. Old Dominion
5. U Arkansas	4. RPI
Computational Mathematics	5. Salve Regina
1. Princeton (App & CM)	6. Syracuse
2. San Diego State (App & CM)	7. U Wisconsin Eau Claire
3. U Central Florida	8. U Wisconsin LaCrosse
4. U Nebraska-Lincoln	9. U Wisconsin Madison
Computational Biology	10. Wittenberg
1. UC Merced	11. Wofford C
2. Center CB (Colo)	

(NY Botanical)

It Takes a Village

DOE Awards, Fellowship

XSEDE (NSF)
(Extreme Sci & Engr Discovery Environ)
= Σ SuperComputer Centers

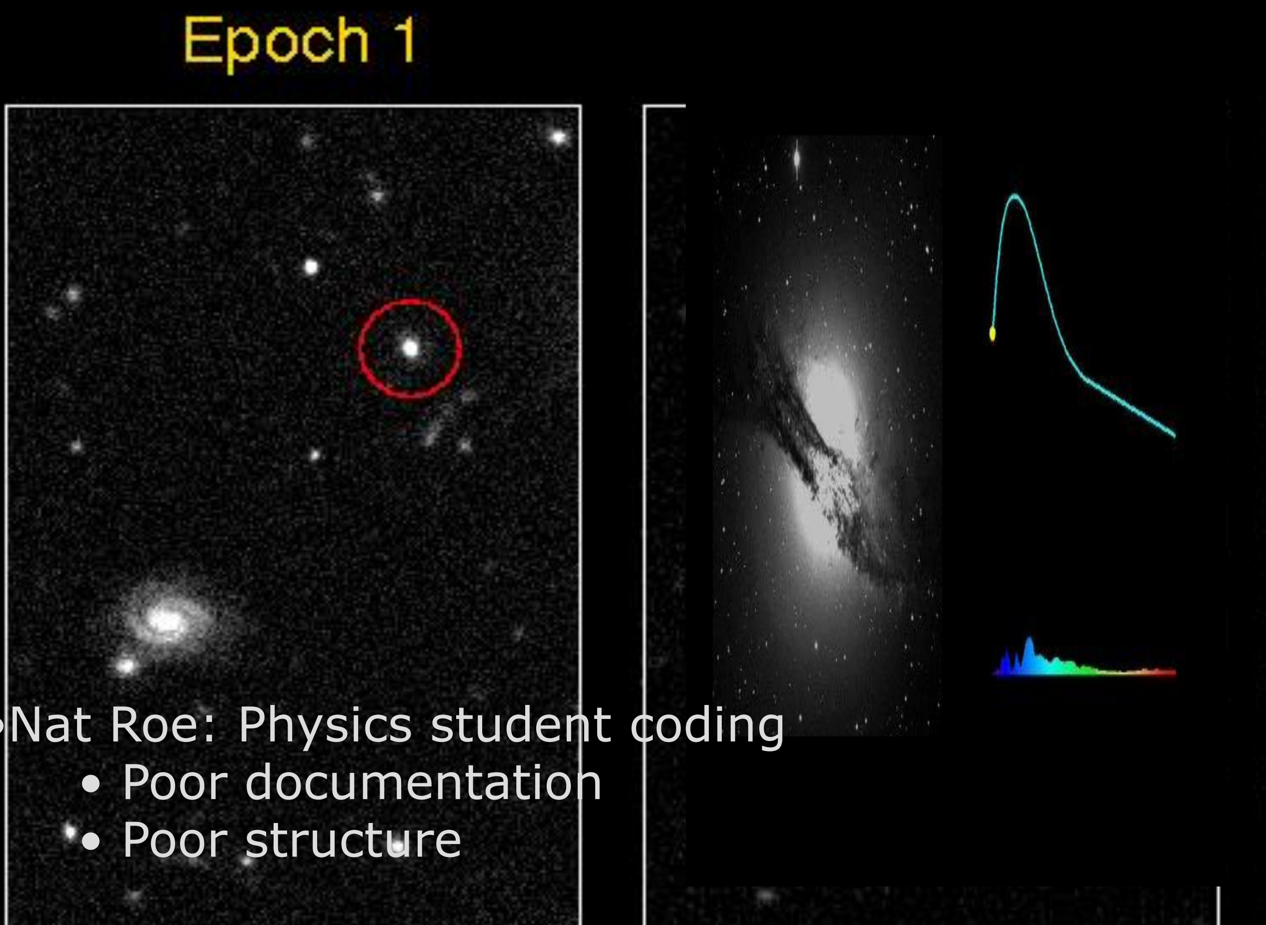


CSE COMMUNITY

UG

CP Research, eg 7 Supernova on Demand

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



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

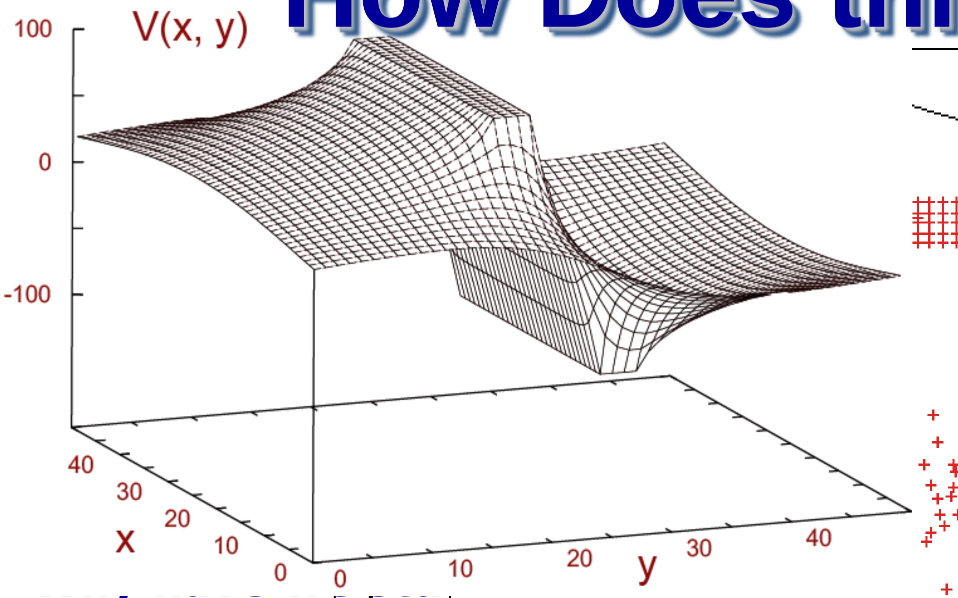
Intellectual Content Computational Physics Ed

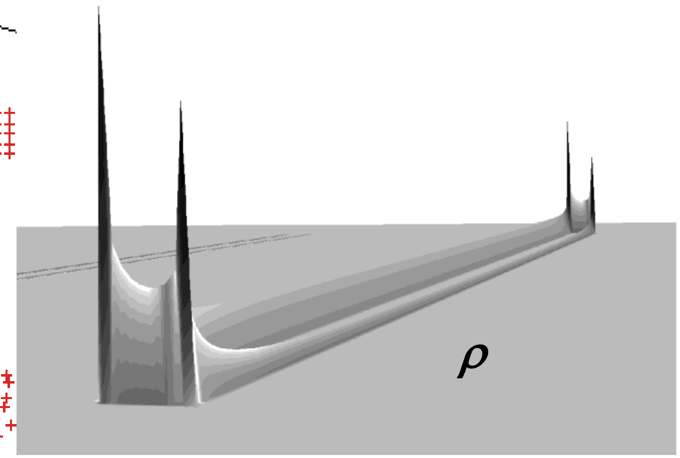
- *Elements of Computational Science & Engineering Ed, Yasar & L (SIAM)*
- **Prerequisite establish Computational Physics course**
- **Include CP Examples in classes**
- **Easy (too) expect 1 course teach entire subject (programming?)**
- **Historically guided by research needs; grad study = easy**
-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

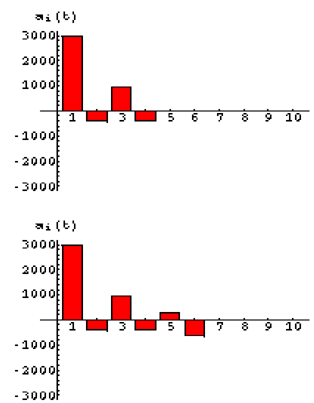
Examples for Physics Courses

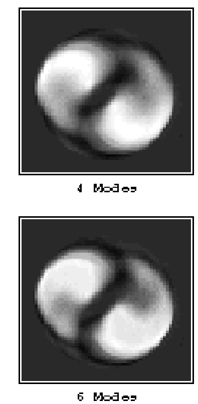
- Spontaneous Decay Simulation
- Classical Chaotic Scattering
- Proper ODE Solution
- Double & Chaotic Pendula
- Nonlinear Dynamics, Bifurcation
- Fractals & Statistical Growth
- Laplace & Possion Equations
- Realistic PDE Solutions
- Molecular Dynamics
- Quantum Wave Packets
- Realistic Waves
- Shock Waves
- Solitons
- Sonifications
- Fluid Dynamics
- DFT, Wavelet Analysis
- Feynman Path Integrals
- Wavelet Analysis
- Prin Component Analysis
- Data Intensive

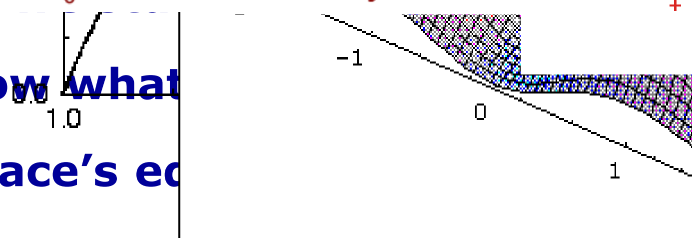
How Does this Work?





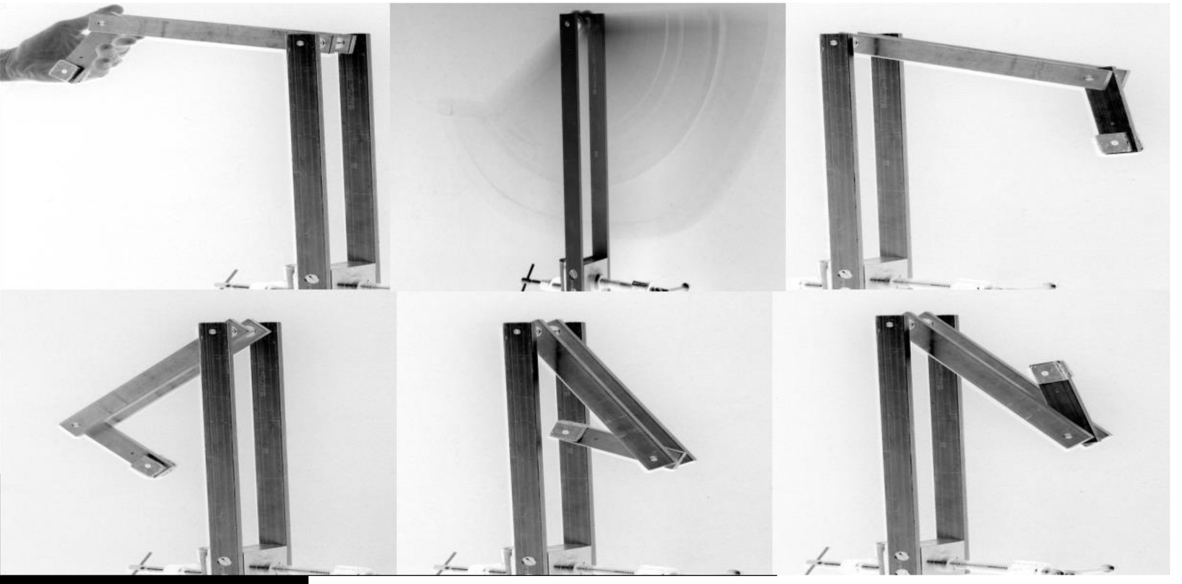


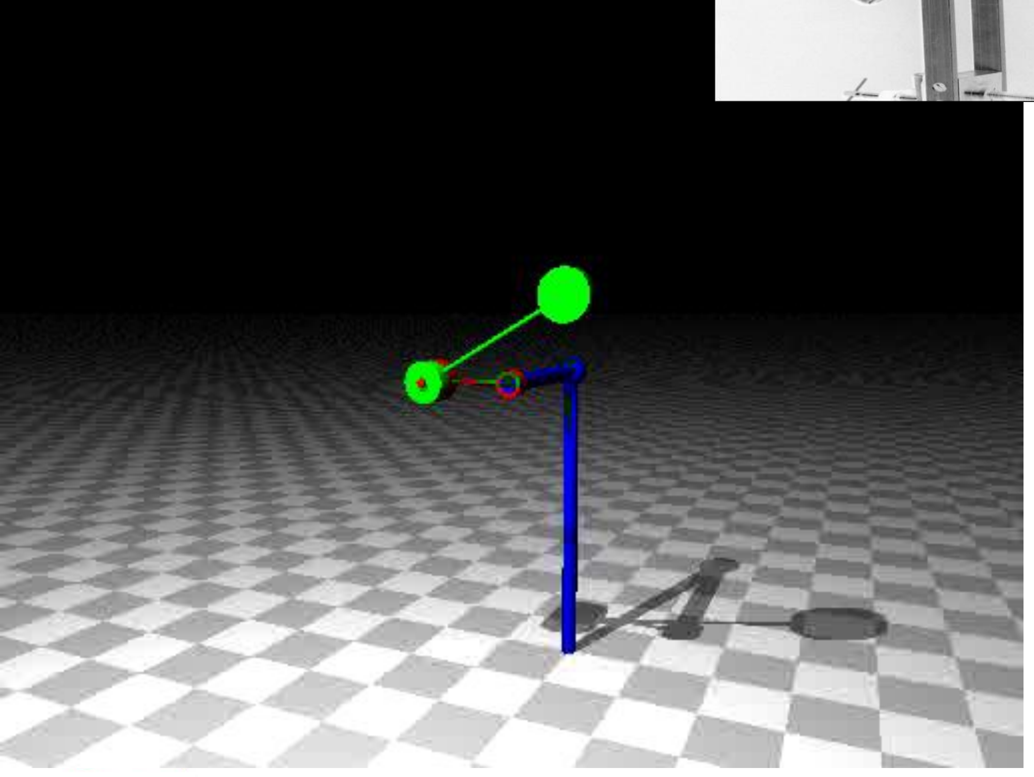




1.
2.
3.
4.
5.
6.
7. "Now I know what
8. "Now Laplace's ec
9. "I was up all night.
10. Chaotic scattering: several MS, 1 Ph D t
11. "MD: way I thought simulations should
12. Great prep physics, astroP, CS, ocean, bioP, brain
13. Women: didn't know liked C, problem solving

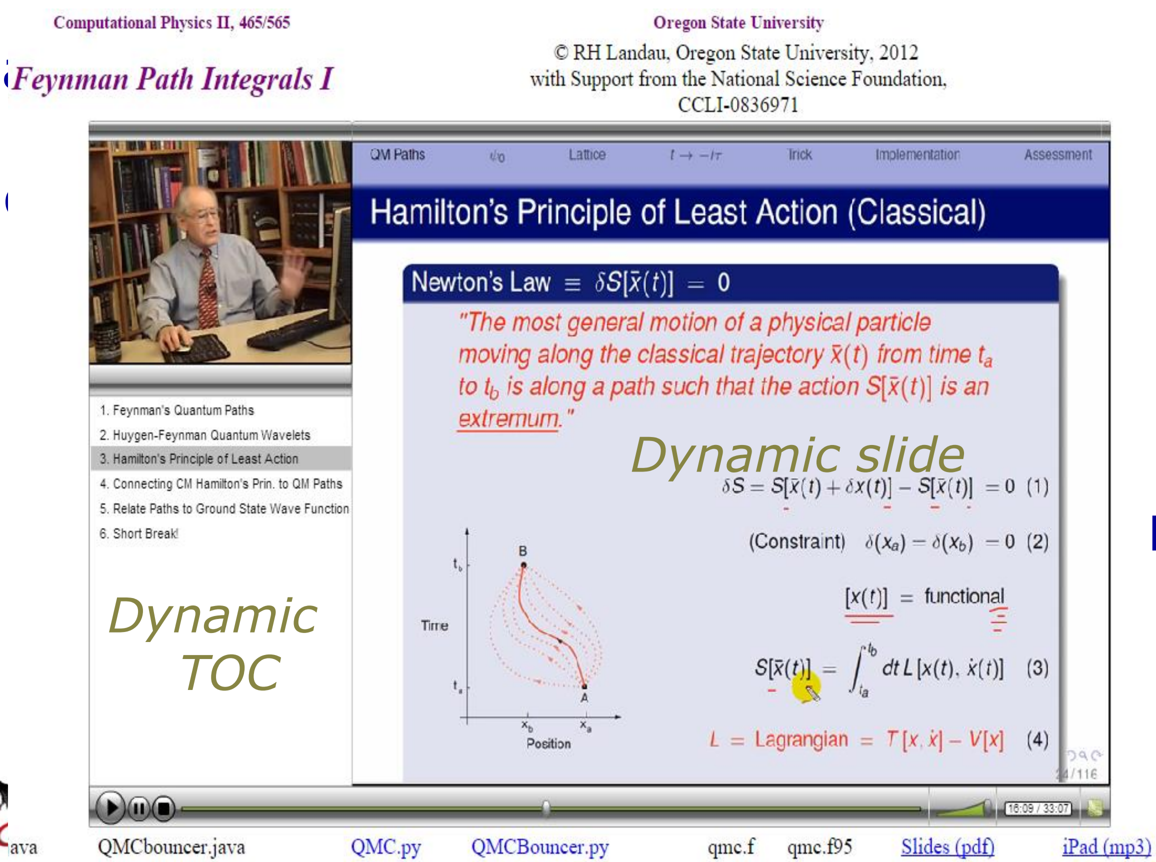
Double Pendulum





Online Courses

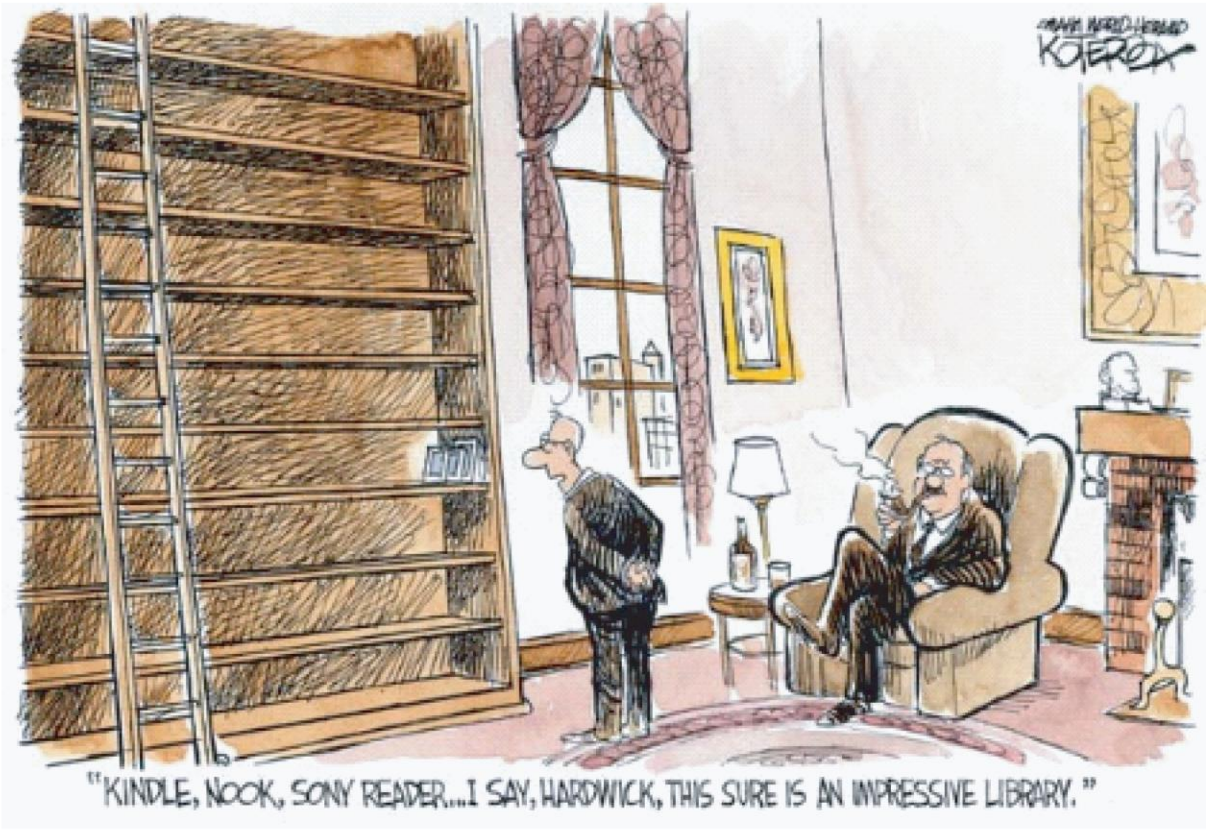
- Web N is here to stay & grow
- Challenge use it well for Education
- Not: general ed, weak discipline, motivation
- N
- G

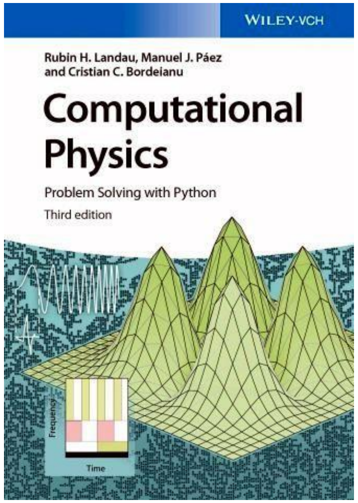


*Free Online Lecture **and** Slides* *(N-D Search)*

RHL: Hybrid Course
Online Lectures
Lecture time → Lab time

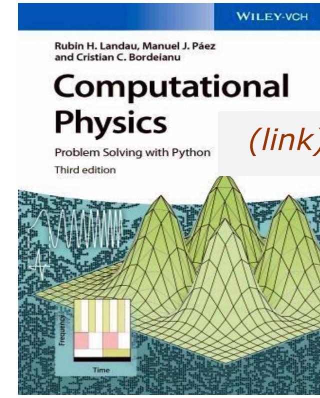
Digital Book





[Python (link)]

Digital Book



(link)

Technology Catching Up

- Exploring since 1996 WWW
- Multiple senses
- High accessibility potential
- Δ learning approaches
- Students: integrated package
- Vision: Interactive eqns, figs
- Html1, Java Applets, XML, ePub, Ibook, Kindle, Pdf-href, Html5-wiley?
- Python notebook (TOC -8 euler, abm)

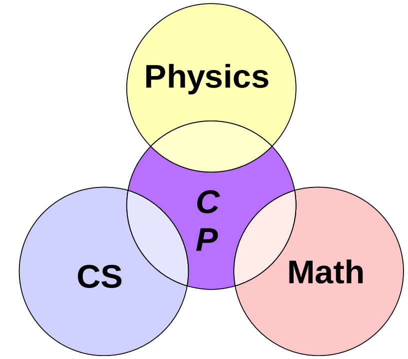
~rubin/Books/CPbook/eBook/Notebooks

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

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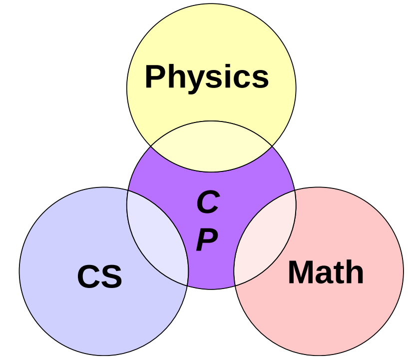
Conclusions & Summary



- Suggest: rejuvenate Phys Ed with modern Res (+CP)
- Need Δ 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

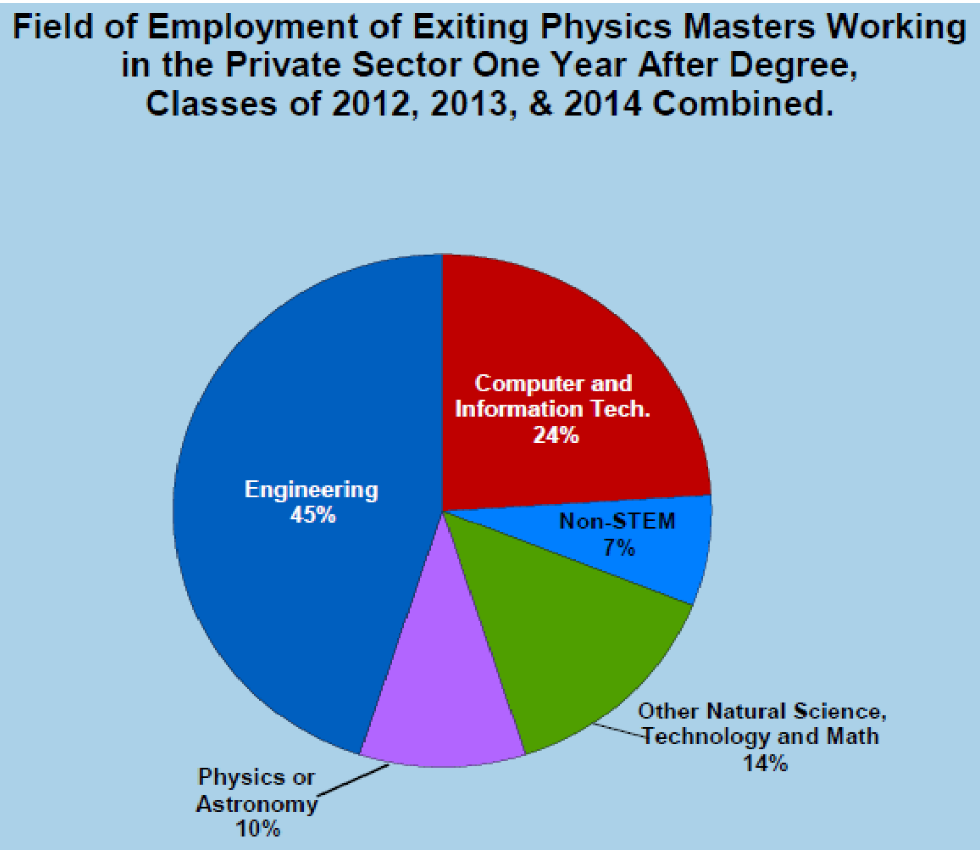
Statistics, data fitting

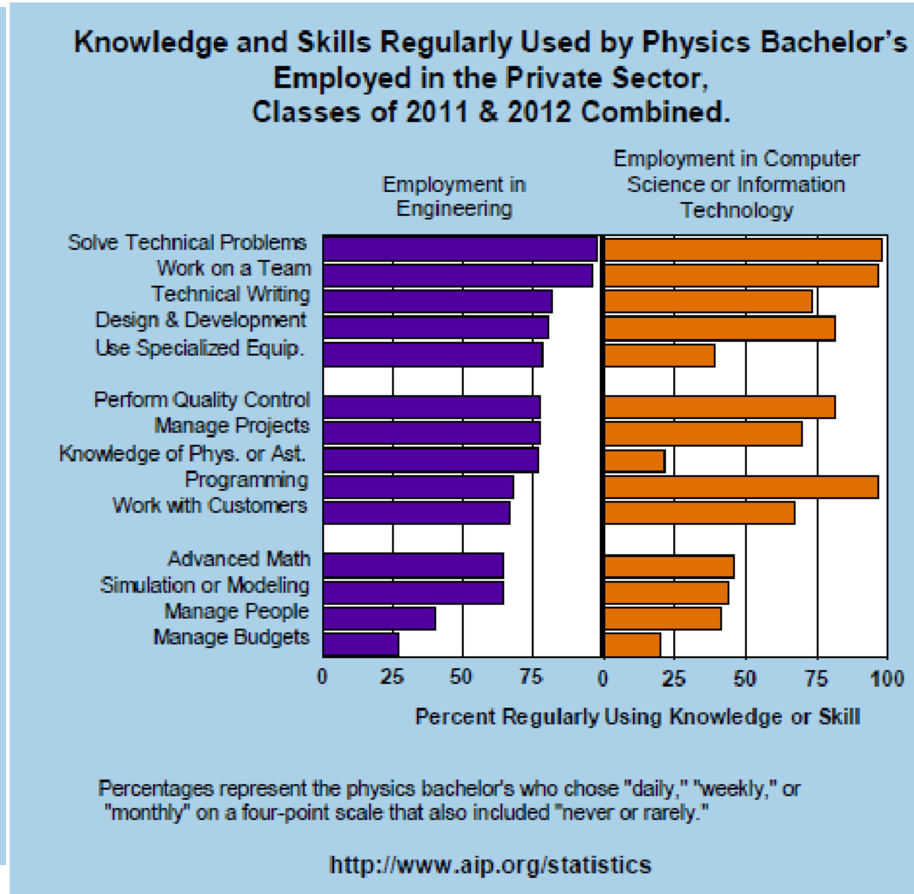
Computational thinking

Symbolic programming

LATEX

Evidence for Δ (Physics Ed) 5





Two Lower-Division Courses

Physics/Math/CS 265, Scientic Computing I (*A First Course*, Princeton)

OS, Basic Maple, Number Types	Logical control, plotting
Maple Functions, Number types, Symbolics	Visualization, Loops, Integration
Calculus, Equation Solving	Objects, Complex Arithmetic
Introductory Java	Web Computing: Applets
Limits, Methods (functions)	Arrays, File I/O

Physics 464/564, Intro Computational Science (*Computational Physics*, Wiley)

Unix Editing and Running*	Monte Carlo Techniques
Floating Point Errors & Uncertainties	Random Walk, Decay Simulation*
Limits: precision, under/overo ws	Interpolation, cubic spline
Matrix Computing with JAMA libe	Least-squares t, Quadrature
Differentiation, ODEs, ODE Eigenvalues	Hardware: Memory, CPU, Tuning

Contents of Upper-Division Courses

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

- Realistic, Double Pendula*
- Fourier & Wavelet Analyses
- Predators & Prey: Nonlinear Mappings*
- Chaotic Pendulum/Scattering*
- Fractals, Aggregation, Trees, Coastlines*
- Bound States via Integral Eqtns
- Quantum Scattering, Integral Equations
- Thermodynamics: The Ising Model
- Quantum Path Integration*
- Fluid Dynamics
- Electrostatic Potentials
- Parallel Computing (MPI), Heat Flow
- Waves on a String
- Shock Waves & Solitons
- Molecular Dynamics Simulations
- Electronic Wave Packets

Physics 467/567 Advanced Computational Laboratory

- Radar Maps of Archaeological Tells
- Molecular Dynamics Simulations
- Meson-Nuclei p-Space Scattering
- Wavepacket-Wavepacket Interactions
- Serious Scientic Visualization
- Earthquake Analysis
- Density Functional Theory
- Gamow States of Exotic Atoms
- Pion Form Factor Data Analysis
- Particle Hydrodynamics
- Brain Waves Principal Components
- Quantum Chromodyanmaics