Computational Physics,
A Path for Physics Ed?

Rubin H Landau

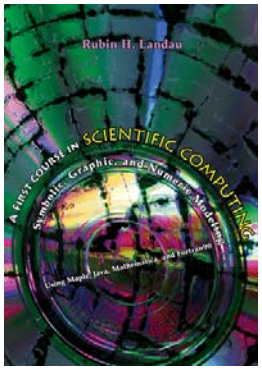
Computational Physics for Undergraduates
BS Degree Program: Oregon State University

Thanks Wolfgang, Nancy, Davidson; dream come true
Daunting Task: What new left to say?
Yesterday: Thanks Amy: L & Paez (1997) = "Ancient"

Supported by NSF (CCLI, CI-Team) & OSU
"Engaging People in Cyber Infrastructure"

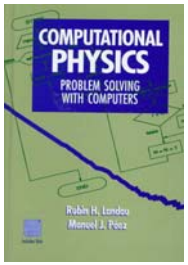
Awkward Beginning

(PUP 2005)

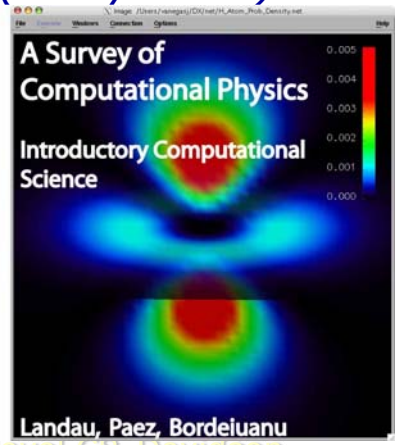


- Bragert or fool? Doing CP since 1966, Ed 1988
- Introduced 4 courses in CP ⇒ BS degree in CP
- Co-author 4-5 book scientific computation (P)
- Not brag, peddle books; *contribute develop CP*
- More fun to *do* than talk about
  - 15 years content provider ⇒ model
- 1 approach not best for all
  - all politics is local
- *Yet,* books + courses = ∑ thought (fool not to)
  - works for *us,* and pieces for others
  - fool not to present my views, know best

D of SC



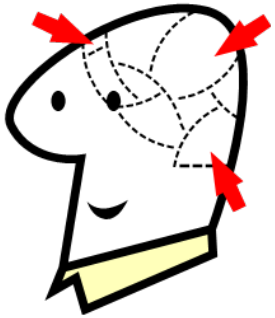
(Wiley 2007)



(PUP, 2008)

Why? Need Δ (Physics Ed)

- Historical Δ in how/what do science
  - ↑ computer power & pervasiveness
- Premise: ⇒ Δ future undergrad physics Ed
  - *content, more C*
- P Choice: like *Classic Greek,* or living?
  - others *do* much P; MD, CFD, NL…
- P's strength: = problem via basic prin's & math; now +C
- Proper for P Ed: C + P & understand C + P (CSE)?
- ≠ Computation + "Physics-Education" (tool)
- CP Ed ⇔ research (creative) = Hi Q
  - = PE+R ≠ PER



Evidence for Δ (Physics Ed) 1

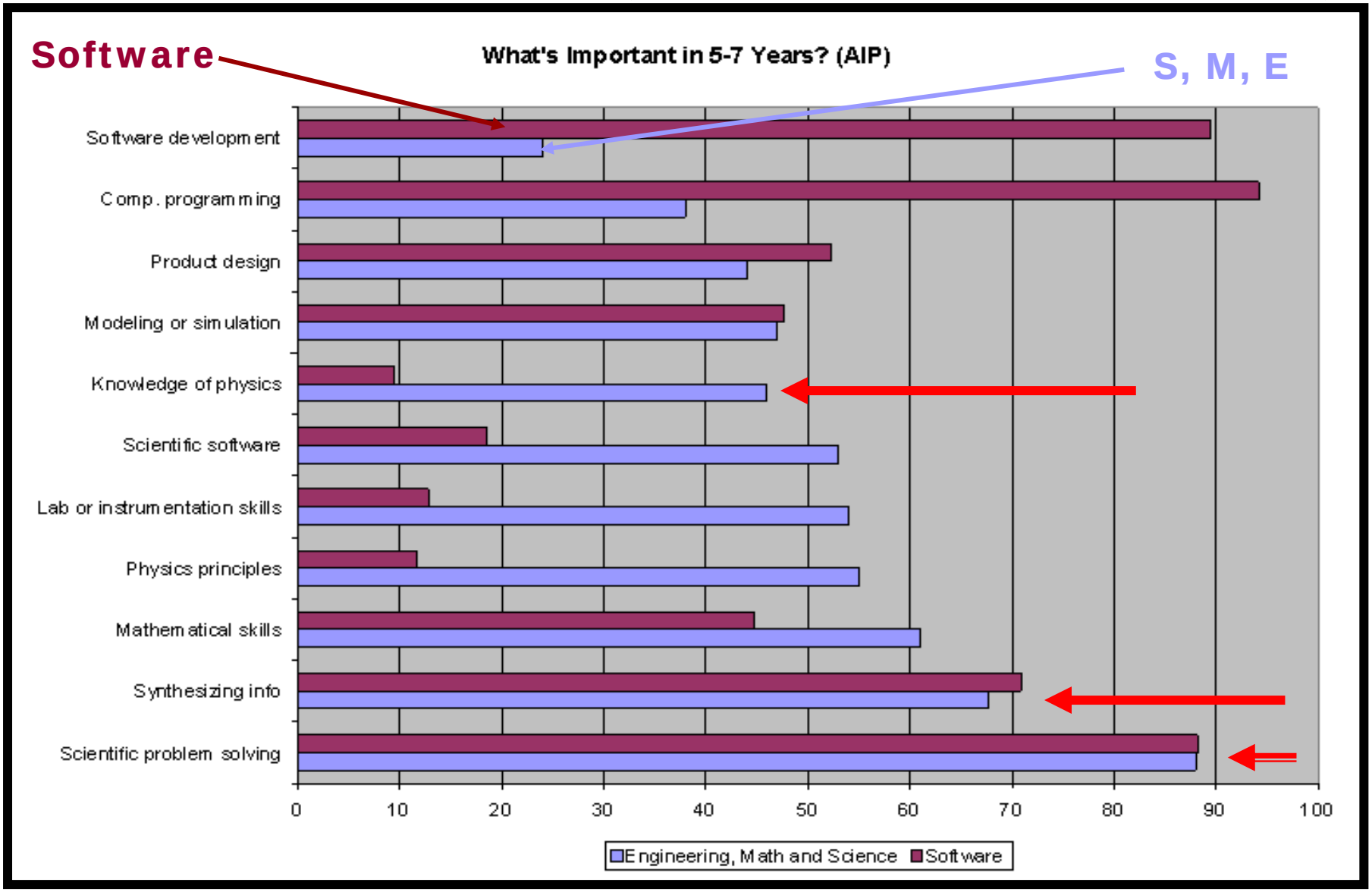
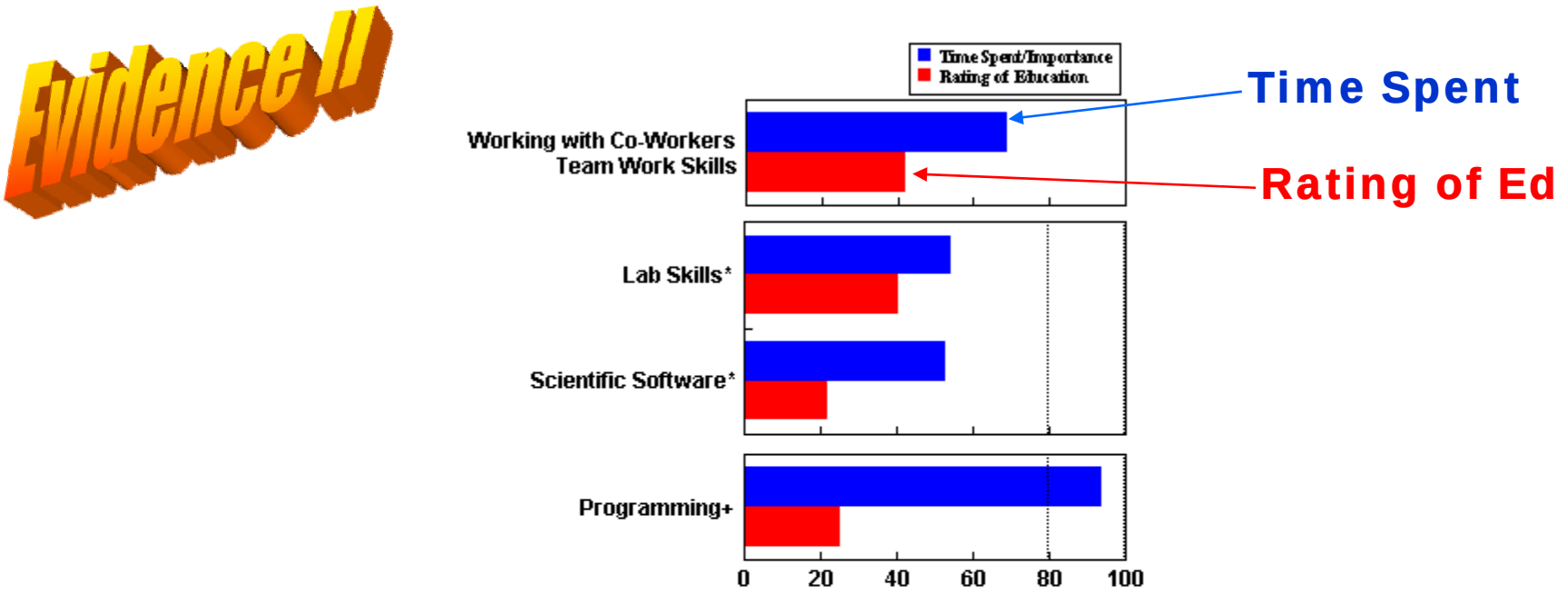


Figure 6. Time spent on or importance of activities compared to rating of physics bachelors' education.



* Engineering, math, and science jobs (but not teachers).
+ Software jobs.

These data reflect the percentage who chose 4 or 5 on a 5-point scale. Based on physics bachelors with no additional degrees who are not primarily students, 5 to 8 years after graduation.

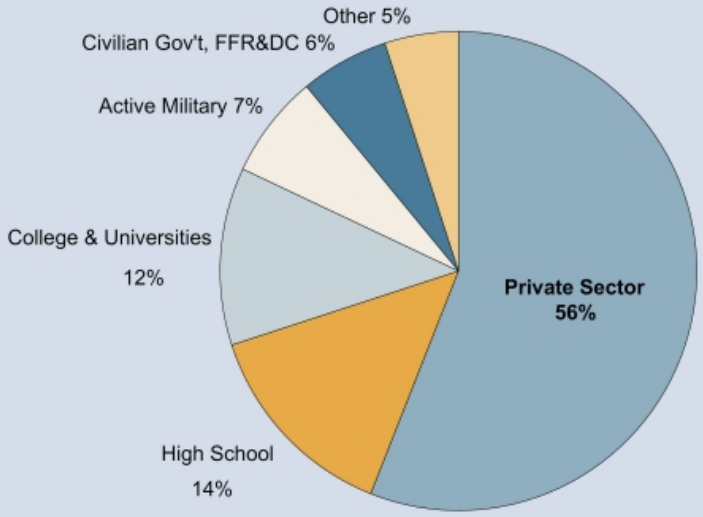
AIP Statistical Research Center, 1998-99 Bachelors Plus Five Study.

Evidence for Δ (Physics Ed) 3

- National Science Board: remain in field
  - 35% of CS, math BS (74% PhD)
  - 22% of physical, biological (52%)
  - UG P ⇒ overemphasize P = weaker preparation
- Employment in STEM ↑ 3 X *wrt* others (5X CS)
- Number of STEM BS
  - 35% (1966) ↓ 31% (2000) [46% China]
- President's Info Technology Advisory Comm
  - CS depts can't meet need, and not diverse, (prev)
  - "computational science indispensable in every sector, ... need be recognized by govts & universities" (recent)

⇑ level CP, Davidson

Figure 8. Initial employment sectors of physics bachelor's, classes of 2003 & 2004.



AIP Statistical Research Center, Initial Employment Report.

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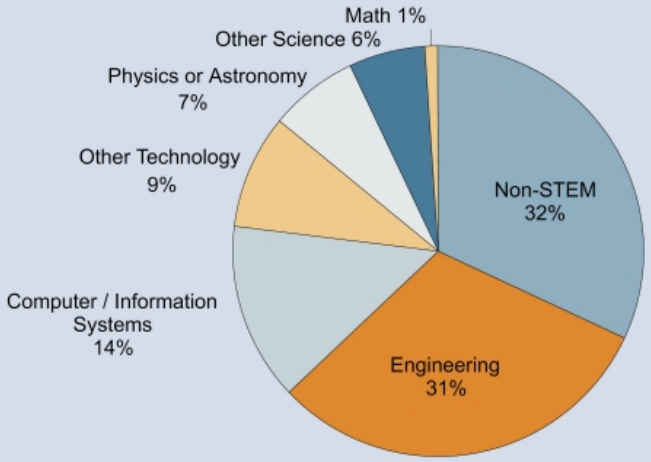
Figure 9. Field of employment for physics bachelors in the private sector, class of 2004.



STEM: Science, Technology, Engineering and Math

AIP Statistical Research Center, Initial Employment Report.

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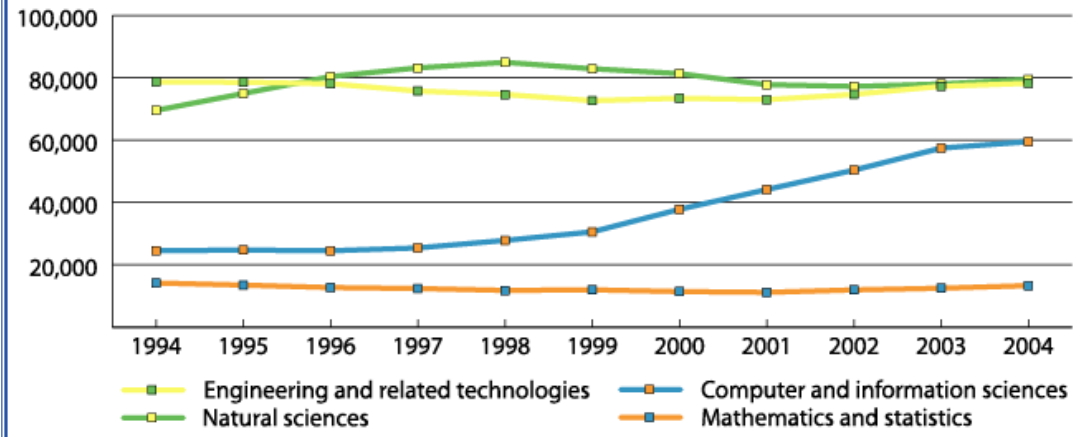
Done

Where Do Physics BS's Go?

Chart 3
Bachelor's degrees in STEM subjects, 1994-2004



Source: U.S. Department of Education

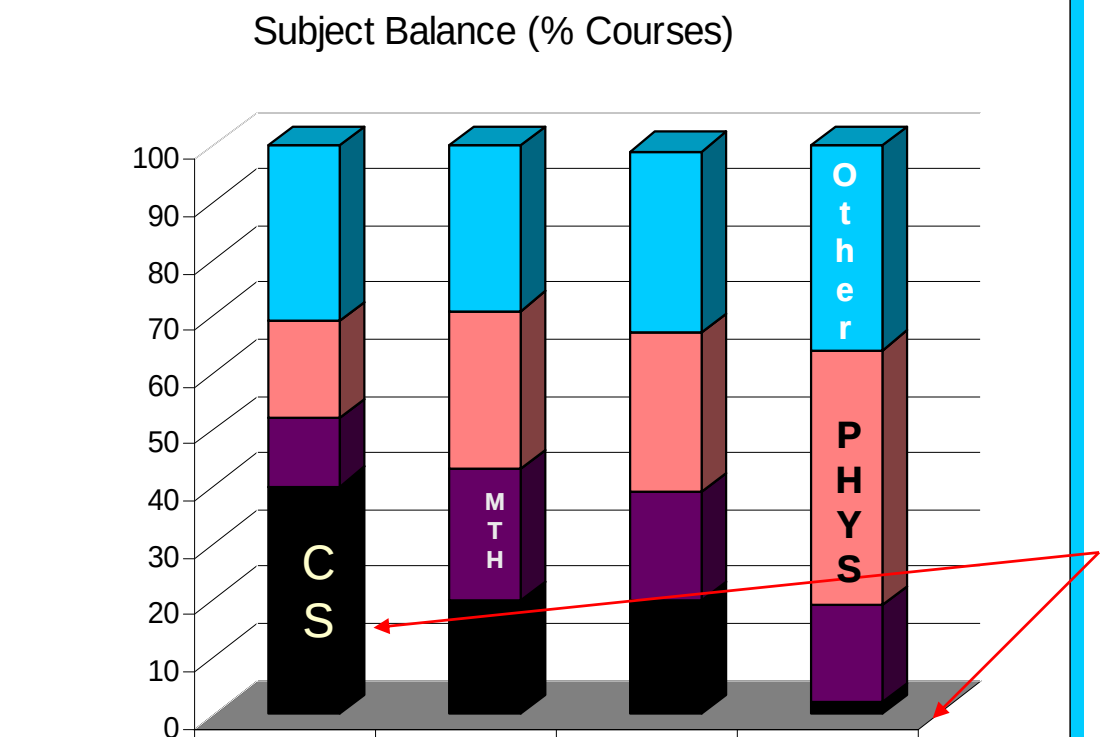
Broad View

Table 2
Employment growth and job openings in STEM occupations, projected 2004-14

Occupational group	Employment		2004-14 change		Job openings due to growth and net replacement, 2004-14
	2004	2014	Numeric	Percent	
Science occupations, natural*	**806,330**	**931,027**	**124,697**	**15%**	**315,000**
Life scientists	231,723	279,890	48,166	21	103,000
Physical scientists	250,417	280,913	30,496	12	94,000
Natural science technicians	324,190	370,224	46,034	14	118,000
Technology occupations (computer specialists)	**3,045,836**	**4,002,547**	**956,711**	**31**	**1,350,000**
Engineering occupations	**2,299,778**	**2,576,906**	**277,128**	**12**	**798,000**
Engineers	1,448,871	1,643,500	194,629	13	507,000
Drafters, engineering, and mapping technicians	850,906	933,406	82,500	10	291,000
Mathematical science occupations	**106,965**	**117,297**	**10,332**	**10**	**39,000**
STEM occupations, total	**6,258,909**	**7,627,777**	**1,368,867**	**22**	**2,503,000**

* This group may include a small number of social science technicians, who are counted among life, physical, and social science technicians, all other.

Evidence for Δ (Physics Ed) 4

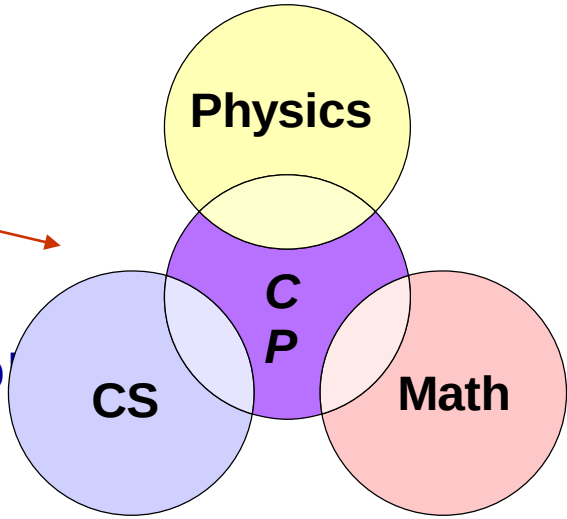


	CS	CSE	CP	PH
Other	31	29	32	36
Application	17	28	28	45
Math	12	23	19	17
Comp	40	20	20	2

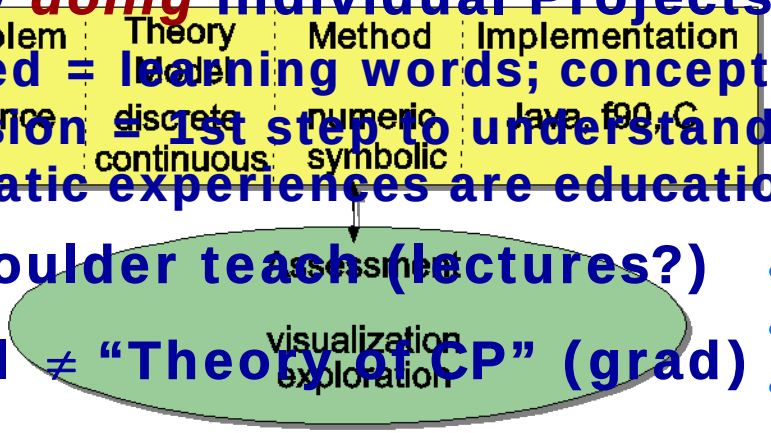
- RHL Survey (O&L)
- CSE, CP ~ balance
- Small sample
- Stereotypes √
- PH: ⇑ imbalance?

⇑ level CP, Davidson

What & How?



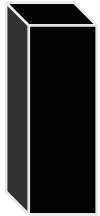
- Problem solving (why became P's)
- Learn by *doing* individual Projects
  1. most ed = learning words; concept simpl
  2. confusion = 1st step to understanding
  3. traumatic experiences are educational
- Over-shoulder teach (lectures?)
- Practical ≠ "Theory of CP" (grad)
- CS + Math + P in context
- *More efficient approach to Physic Ed*
  - ok ↓ # "physics" courses
- Compiled language
  - see algorithm (eqtns)
  - bare bone codes given
  - "I am not a bigot!" (packages)



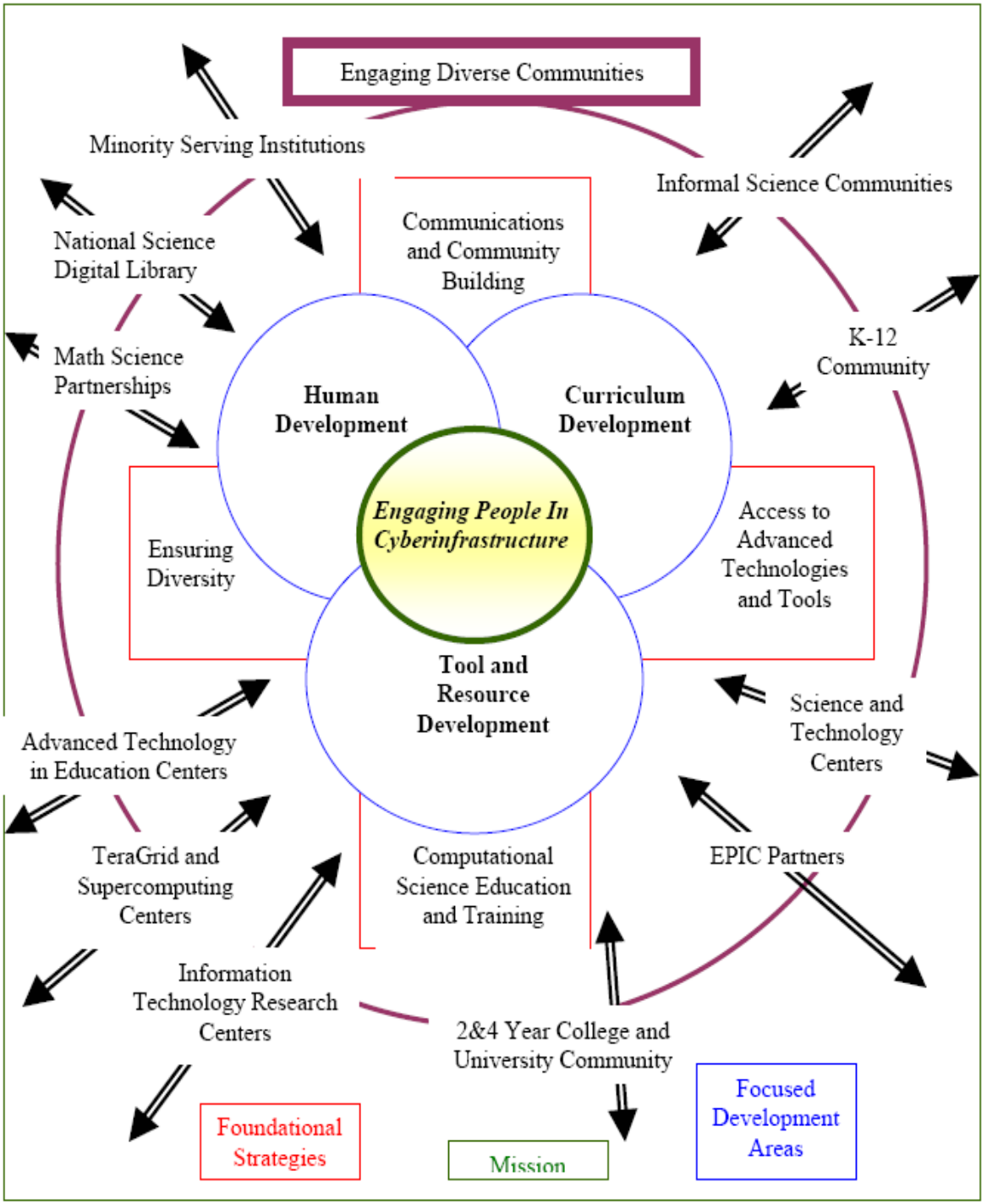
Multi ≠ Inter

- *equation solved (math)*
- *numerical method used*
- *code listing*
- *results (graph / table)*
- *discussion*

(meet the boss)



UCES Award
(DOE)

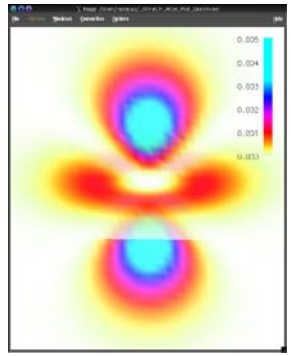


CSE COMMUNITY

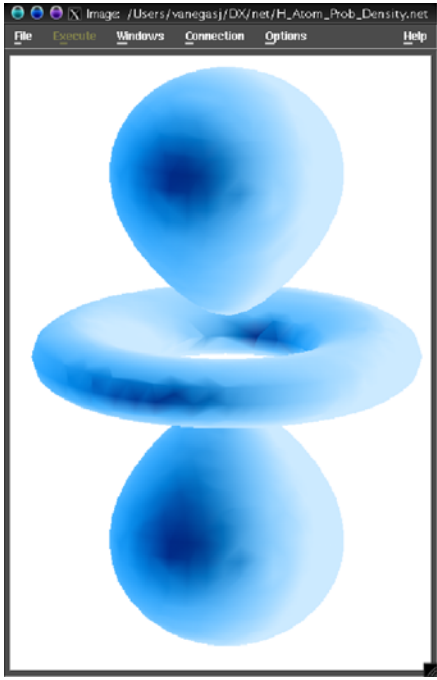
Intellectual Content of CP
Student Learning Outcomes (SLO)

- *Elements of Computational Science & Engineering Ed*
  Yasar & Landau, SIAM Review, 45, 4, 787-805 (2003)
- Prerequisite establish CP courses, program
- Easy (too) expect 1 course teach entire subject
- Historically guided by research needs; grad study
- *See handout* for specifics
- Not pie in the sky *(Norman!)*
  - Don't have to buy entire curriculum

Typical SLO, Student Perspective



- High-level computer languages
- High-performance computing (HPC)
- Applied math & computational methods
- Simulation & modeling basics
- Interpret & analyze data visually
  - during & after computation
- Apply computing skills to physics
- Communicate process effectively



e.g.: 1. Computational Tools

a) Ability to work with UNIX & WINDOWS OS

b) Compiled language programming; Fortran95, C, C++, Java, Python

c) Familiarity with problem-solving environments

   i. MAPLE, MATLAB, MACSYMA, MATHEMATICA (numeric & symbolic)

d) Familiarity with floating-point computations

e) Familiarity with numerical methods

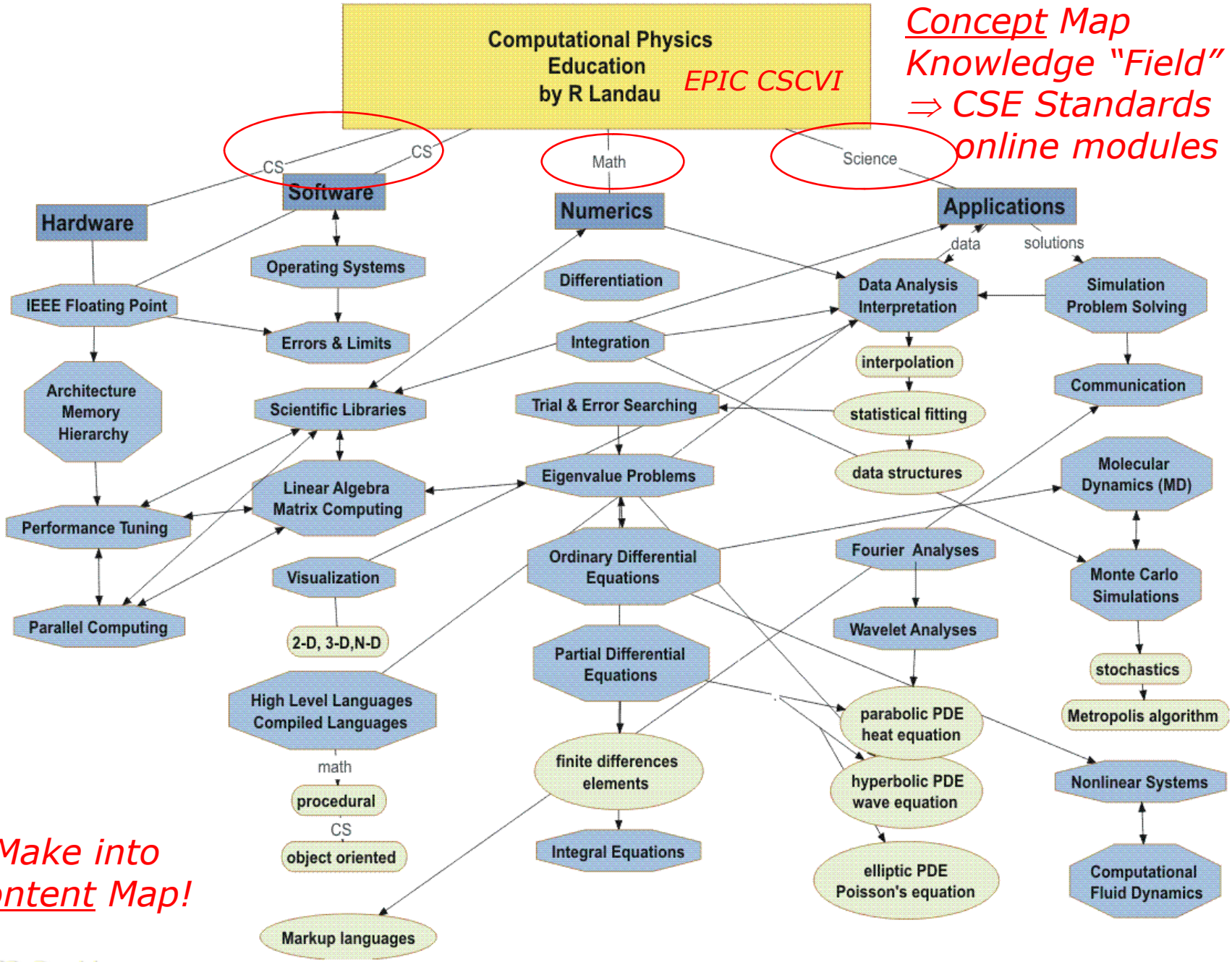
   i. integration, differentiation, ODE & PDE solutions, Monte Carlo

f) Use of math subroutine libes & repositories

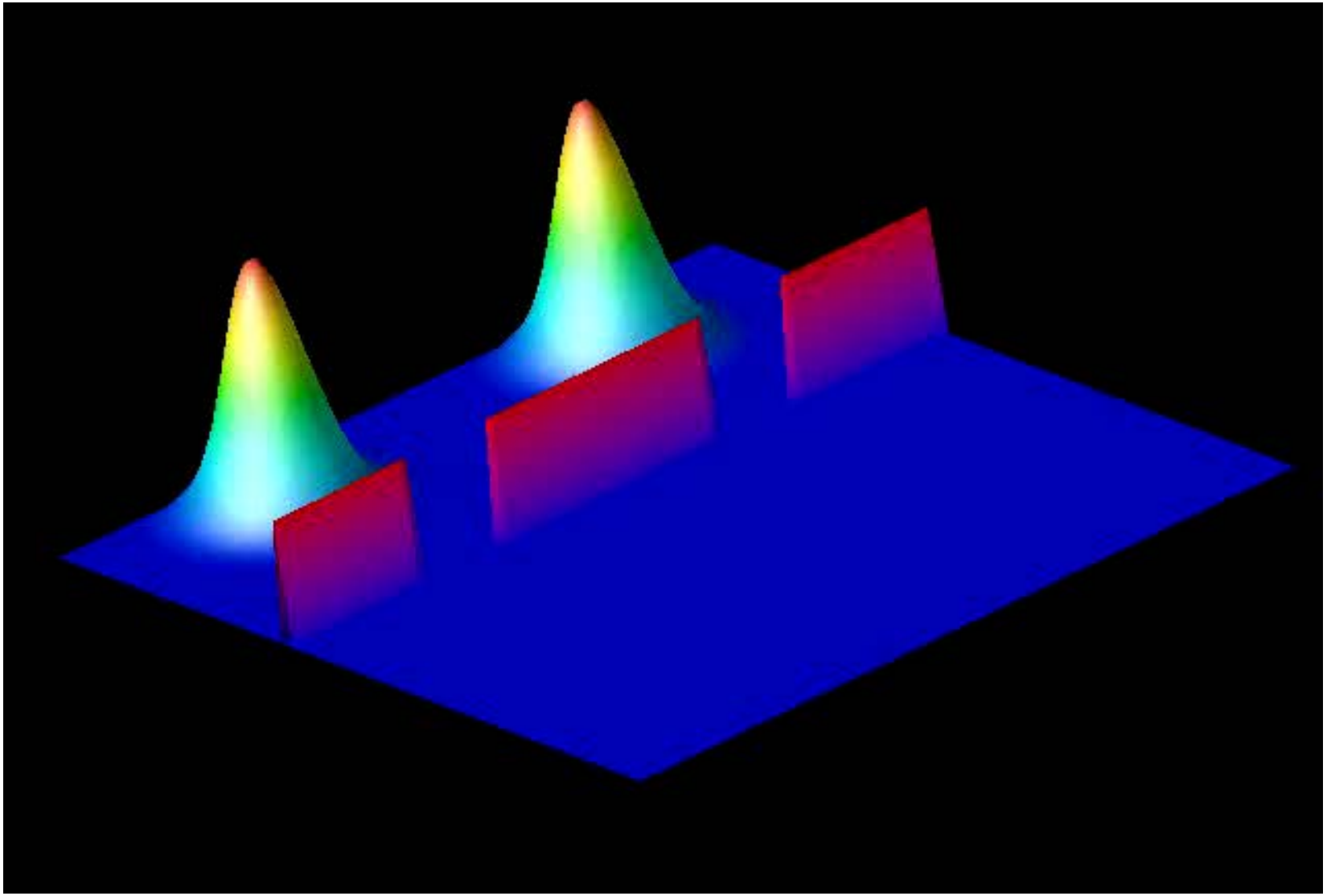
   i. Netlib, BLAS, scaLAPACK, JAMA

g) Use of 2-D and 3-D visualization software packages

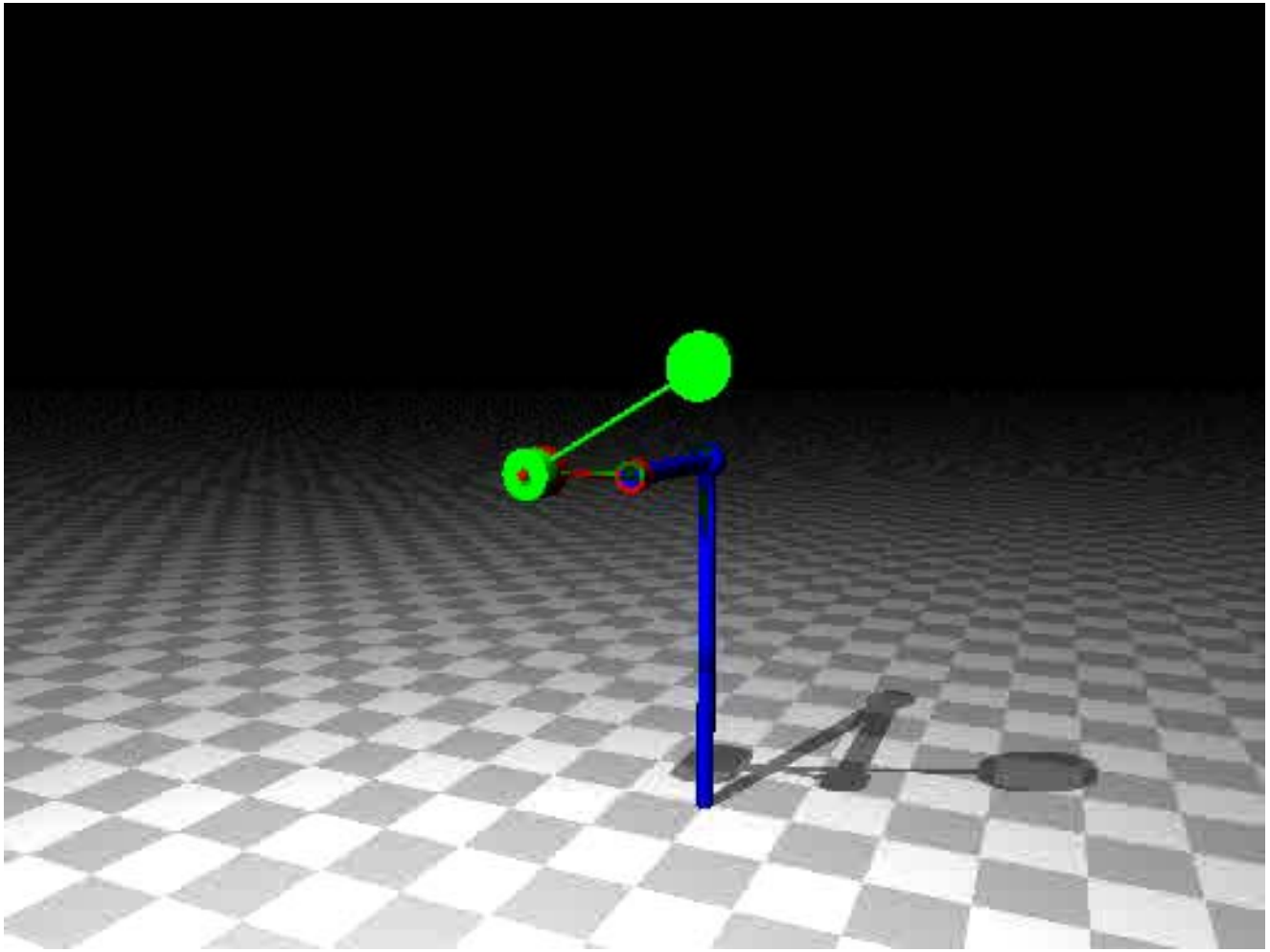
   i. AVS, OpenDX, gnuplot, Grace, Ptolemy (PtPlot), VisAD


Computational Physics
Education
by R Landau
EPIC CSCVI
Concept Map
Knowledge "Field"
⇒ CSE Standards
online modules
CS
CS
Math
Science
Hardware
Software
Numerics
Applications
data
solutions
IEEE Floating Point
Operating Systems
Differentiation
Data Analysis
Interpretation
Simulation
Problem Solving
Errors & Limits
Integration
interpolation
Communication
Architecture
Memory
Hierarchy
Scientific Libraries
Trial & Error Searching
statistical fitting
Molecular
Dynamics (MD)
Linear Algebra
Matrix Computing
Eigenvalue Problems
data structures
Performance Tuning
Fourier Analyses
Ordinary Differential
Equations
Monte Carlo
Simulations
Visualization
Parallel Computing
Wavelet Analyses
2-D, 3-D,N-D
Partial Differential
Equations
stochastics
High Level Languages
Compiled Languages
parabolic PDE
heat equation
Metropolis algorithm
math
finite differences
elements
hyperbolic PDE
wave equation
Nonlinear Systems
procedural
CS
object oriented
Integral Equations
elliptic PDE
Poisson's equation
Computational
Fluid Dynamics
Markup languages
Make into
Content Map!
© Rubin Landau, CPUG

Visualizations, 2 Slit Diffraction

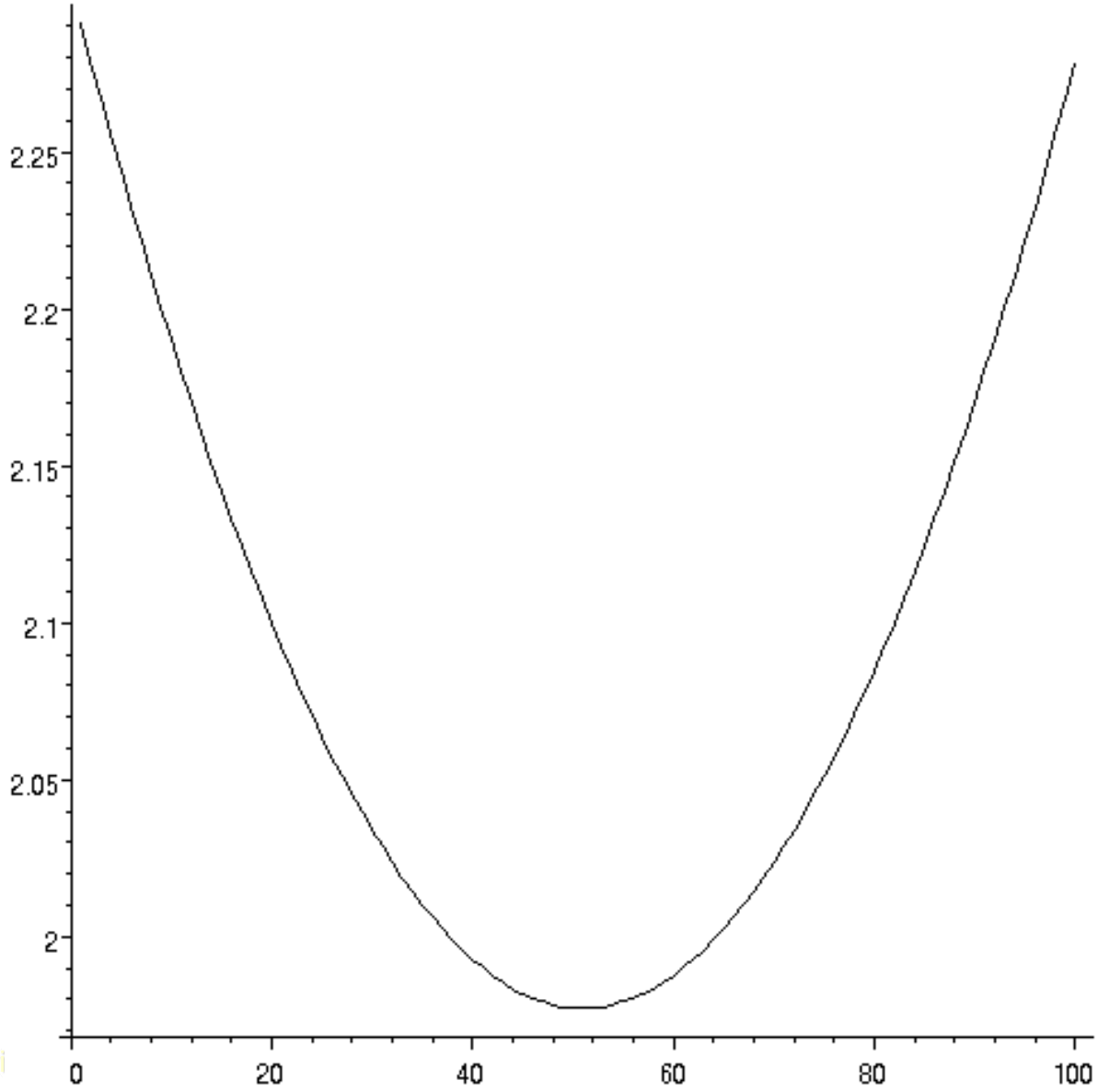


Double Pendulum



Fractal Growth

Catenary Wave + Friction



BS in CP @ OSU

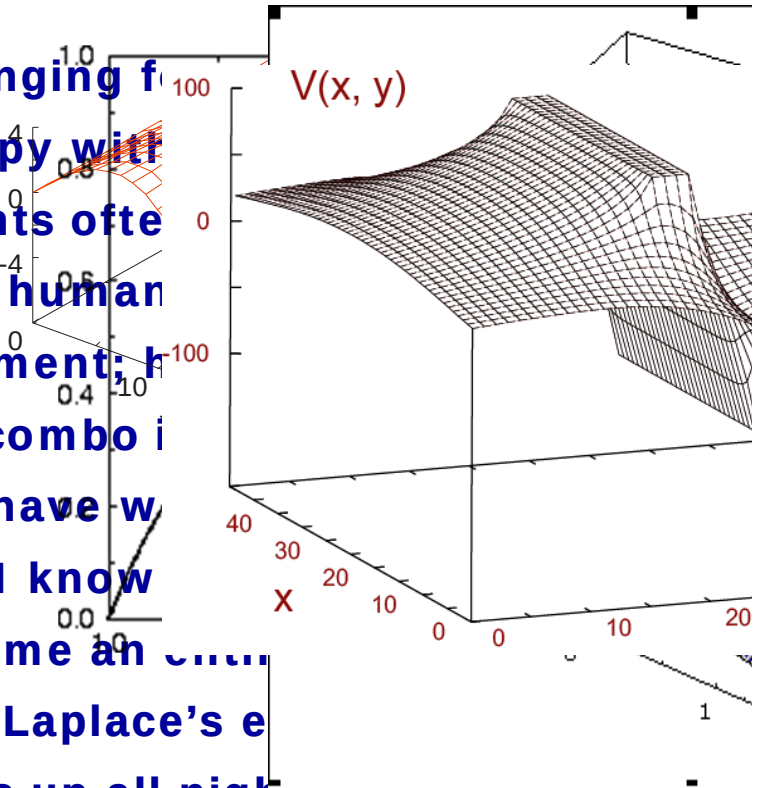
	Fall	Winter	Spring
Fresh (46)	Diff Calculus (Mth) Writing/fitness Gen Chem I Perspective CP Seminar	**Scientific Comptng I** (PH/MTH/CS) Intgl Calculus (MTH) Perspective - 2 Gen Chem II	**Intro CS I (CS)** Vector Calc (MTH) Gen Phys I Writing/fitness
Soph (45)	**Intro CS II (CS)** Vector Calc II (MTH) 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 Quantum Mech **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)**

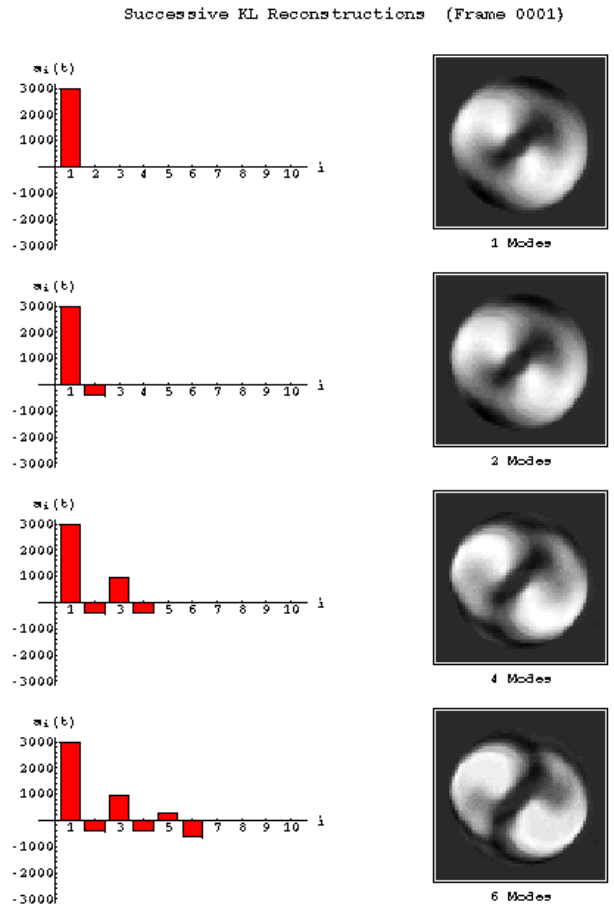
Real computation across the curriculum

Not 1 course, not just our view

Use what's available

How Does this

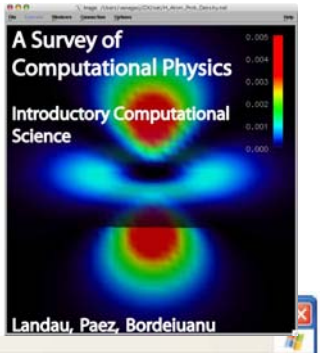




1. Challenging f
2. Unhappy with
3. Students ofte
4. Tears; human
5. Excitement; h
6. "This combo i
7. "Why have w
8. "Now I know
9. "Gave me an
10. "Now Laplace's e
11. "I was up all night making bifurcation
12. Chaotic scattering: several MS, 1 Ph D
13. "MD: way I thought simulations shou
14. Great prep ⇒ physics, astroP, CS, ocean, bioP, brain
15. Women: didn't know liked C, problem solving

Digital Books & Online Courses

- Web here to stay, challenge: use it well
  - Not: general education, weak discipline, motivation
  - Natural (best) for computing



- Digital book (MathML);
  live equations &
  figures (SVG),
- Digital Libe
- Online courses
  - S. Haerer & S. Clark
  - national CSE
  - repository (EPIC)

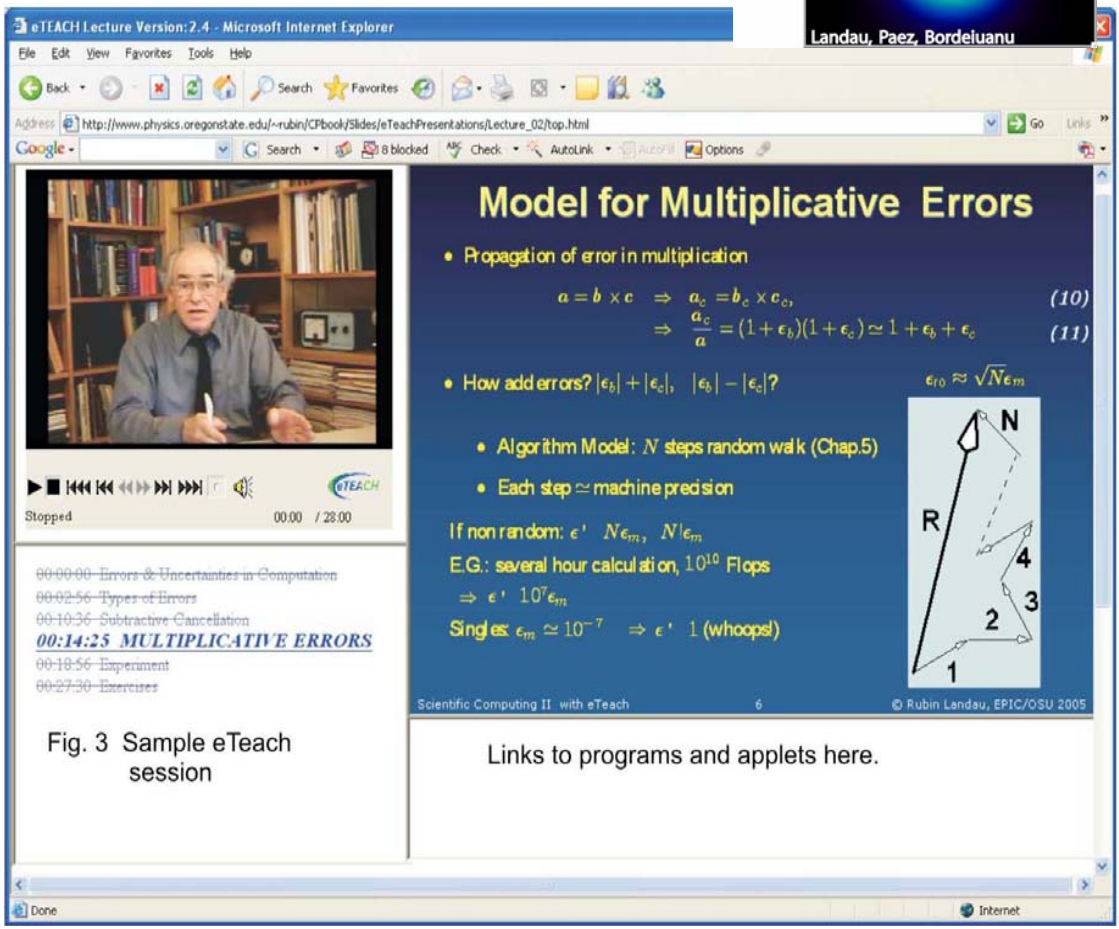


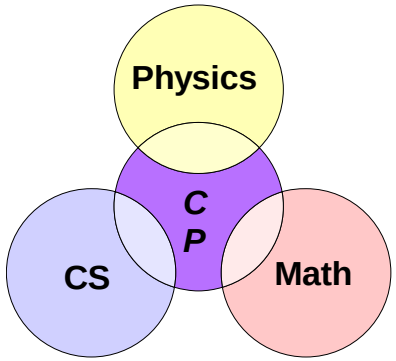
Fig. 3 Sample eTeach session

CP Applets, Web Enhancements

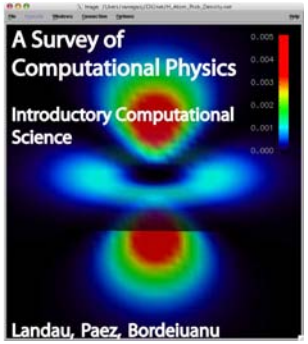
Multimodal views: abstract concept formation
Free: www.physics.oregonstate.edu/~rubin

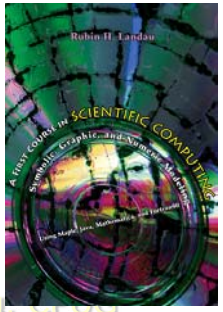
- Coping with Unix (early Web tutorial)
- Spontaneous Decay Simulation (cgi, sound, java)
- Chaotic Pendulum with Java (old: animated gif)
- Solving Simultaneous Nonlinear Equations (HS, libes)
- Visualizing Physics With Sound (Sonification)
- Wavepacket-Wavepacket Collision Movies
- The CP Applet Collection (Paez, Medellin)

Conclusions & Summary



- Let's connect P E with modern R
- Need for change in P BS curriculum
- CP courses, materials: More efficient *Model*
  - learning within problem solving
  - learn P + CS + math in context
  - learn all 3 better
  - toolset: common to CSE
  - Dissemination: 2 new books (Princeton)
  - Digital library materials?
  - Thank you, please carry on!





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

Computational Degree Programs

Swanson (follow up), Epic, Mariasingam, L

= 3x(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. Stevins 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. U Calgary (CSE)
2. Kanazawawa U Japan (CSE)	6. U Erlangen-Nurnberg (CSE)
3. National U Singapore (CSE)	7. U Waterloo (CSE)
4. Trinity C, Dublin (CP)	8. 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 (21)
(all politics are local)

Computational Physics	Computational Science
1. Abilene Christian	1. Capital
2. North Carolina State	2. Clark
3. Penn State Erie	3. Old Dominion
4. 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)	