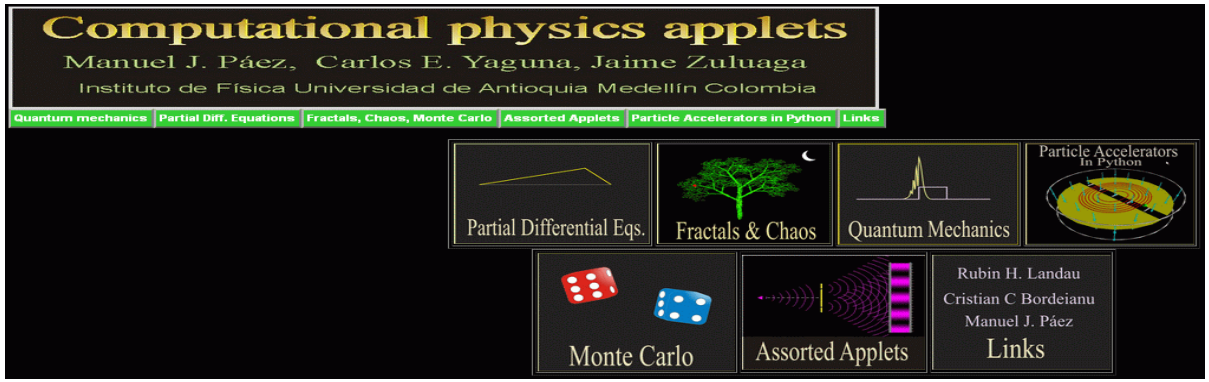
Computational Physics
An Improved Model for Physics Education

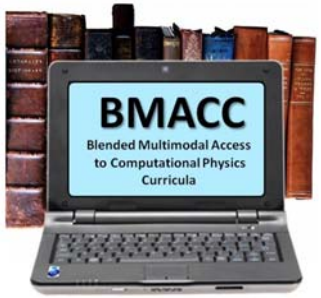
Rubin H Landau

1st = Computational subatomic few-body systems (1966-2003)

2nd = Research developments (1988-) → broaden, education



Computational Physics for Undergraduates Degree Program
Supported by NSF (CCLI. CI-Team/EPIC), OSU, MSR



Contributing Group

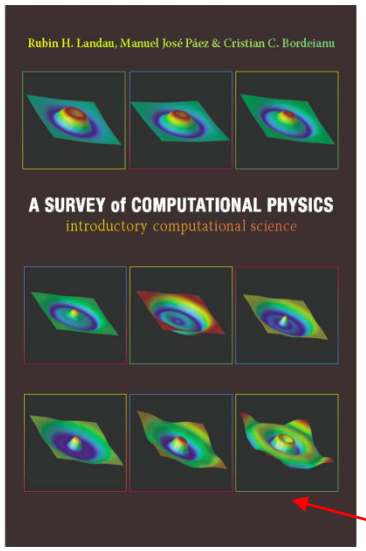
- Manuel J Paez, University of Medellin, Colombia, SA, CoAuthor
  - C. E. Yaguna, J. Zuluaga, Oscar A. Restrepo, Guillermo Avendano-Franco
- Cristian Bordeianu, University of Bucharest, Romania, CoAuthor
- Paul Fink, Robyn Wangberg, CoAuthors
- Justin Elser, Chris Sullivan (system support)
- Sally Haerer, Saturo S. Kano (consultants, producers)
- Melanie Johnson (Unix Tutorials)
- Hans Kowallik (Computational Physics text, sounds, codes, LAPACK, PVM)
- Matthew Ervin Des Voigne (tutorials)
- Bertrand Laubsch (Java sound, decay simulation)
- Jon J Maestri (vizualizations, animations, quantum wave packets)
- Guenter Schneider, 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)
- Pat Cannan, Don Corliss, Corvallis High School (N-D Newton Raphson)
- Brian Schlatter
- Daniel Moore, (REU, Summer 98; Whitman College, WA)
- Justin Murray, (REU, Summer 98; Weber State University, Ogden, Utah
- 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!

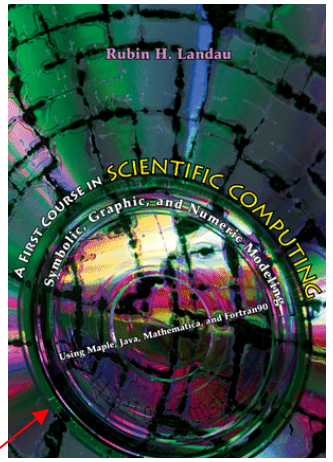
Preview (CP-2 Resource Letter, AJP)

D of SC

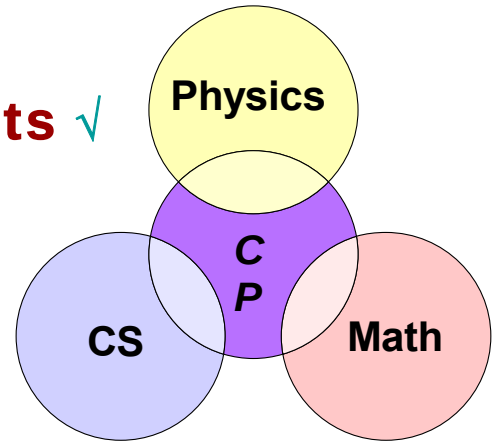
1. CSE Courses and Programs (data) √
2. Need Comp Science & Engr (data) √
3. Comp Phys as CSE , CP Contents √
4. Journals
5. Conferences & Organizations
   - b. SC Center & Grids
   - c. CSE Ed Focus Groups √
6. Books √
   - a. CP
   - b. Applied Math & CSE
7. Tools, Languages, Environments √
8. Parallel Computing
9. Digital Libraries, eTexts √
   - a. Subroutine libes
   - b. General DLs



(PUP, 2008)



(PUP, 2005)



Changing the Status Quo?

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Computational Degree Programs

Swanson (follow up), Epic, Mariasingam, L

≈ 4x(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. 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

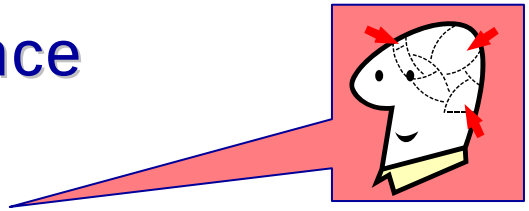
What's in a name? That which we call a rose By any other name would smell as sweet

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)	

(NY Botanical)

Why Need Δ (Phys Ed)?



- Historical rapid Δ in how/what do science
  - ⇑ computer power & pervasiveness
- Premise: ⇒ Δ undergrad Ph Ed > *delivery (C tool)*
  - Proper for P Ed Δ *content: more C, Understand C*
  - CSE view*; Toolset freedom, Compt Thinking (CMU)*
- 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 *e.g.,* CSE *do* FD, MD, NLinear, Combustion…
  - Simulation: Solitons, QCD, Stars, Black hole, Particle Expt
- Phys = solve problem: basic prin's + math tool; now + C
- CSE Ed view ⇔ research (creative) = Hi Q
  - = P Ed+R ≠ PER (inward)

Evidence for Δ (Physics Ed) 1

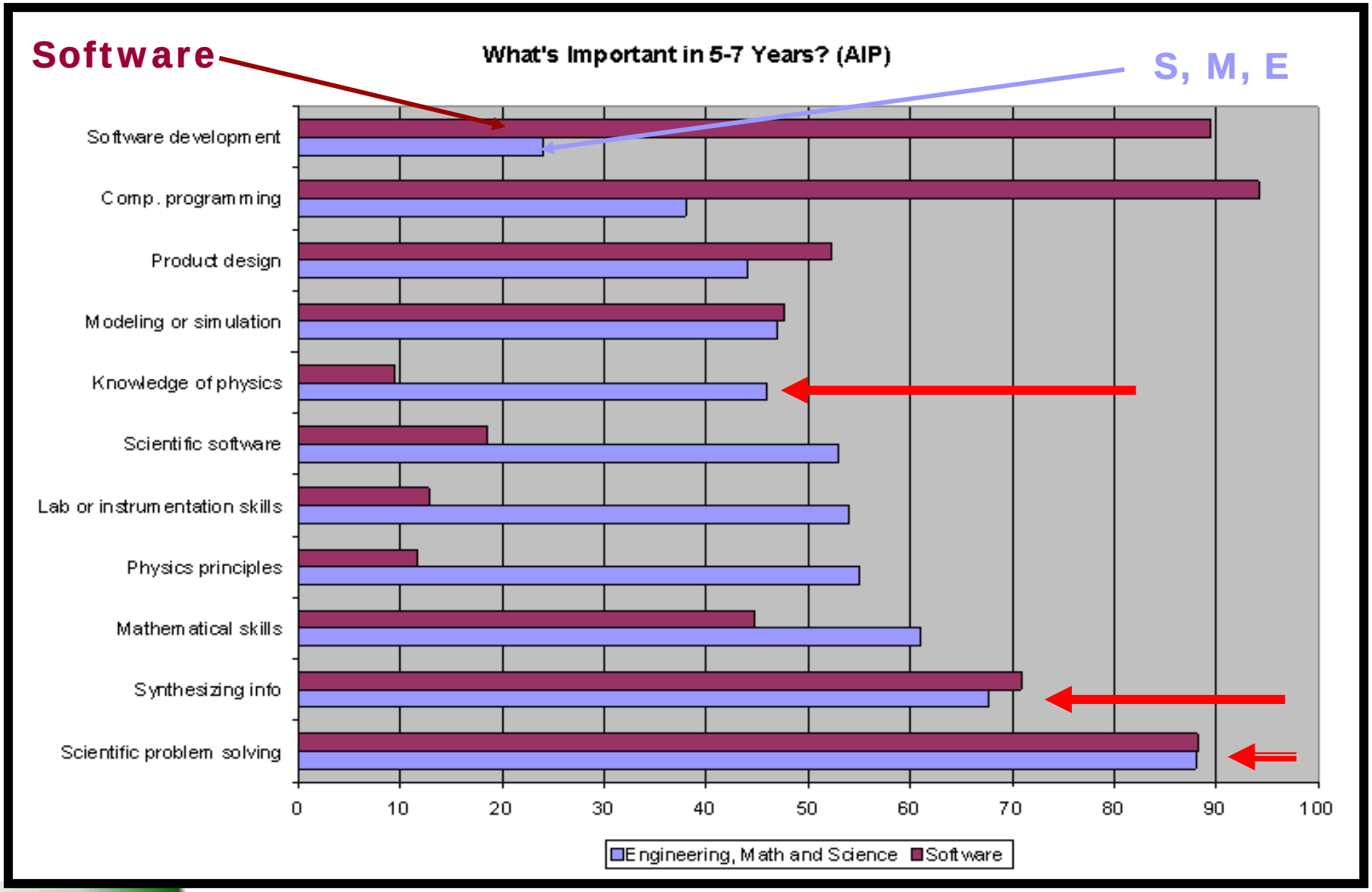
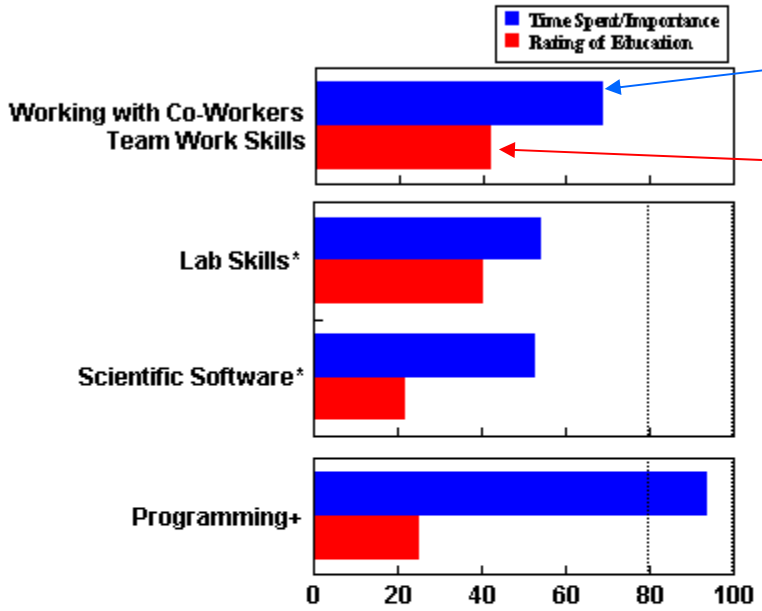


Figure 6. Time spent on or importance of activities compared to rating of physics bachelors' education.

Evidence II



Time Spent

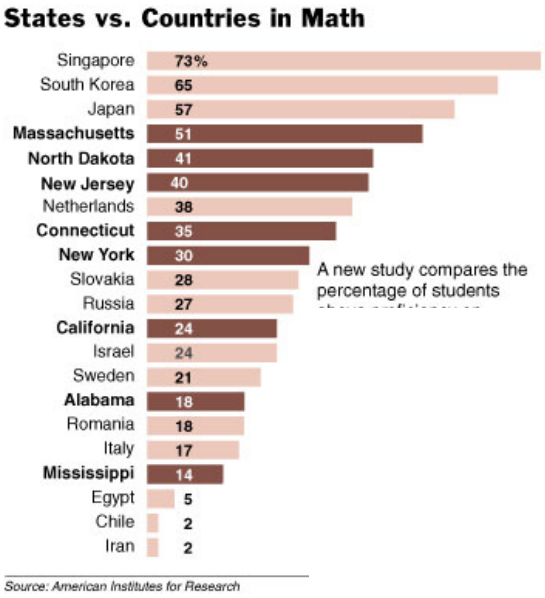
Rating of Ed

* 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%)
  - ≠ *bad thing!*
- ⇒ UG P overemphasize P = weaker prep

NYT 14Nov07

- Number of STEM BS (“nerds’’)
  - 35% (1966) ⇓ 31% (2000) [46% China]
  - 57% Physics PhD (2006) non-US citizen
  - Yet number ≠ issue! *Death of Distance*

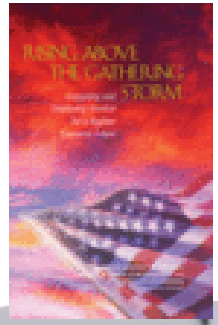
Words of the Wise Men/Women

- President's Info Tech Advisory Comm
  - CS depts can't meet need, not diverse,
  - "computational science indispensable in every sector,… need be recognized by govts & universities" (recent)

- B Labor (2009): decade IT shortage

- Gathering Storm Report, 2005

  (Steve Chu, Bob Richardson: Nobles, Sec E, VPR CU)
  - Serious, intensifying challenge competiveness & Stnd of Living
  - On losing path
  - US entitled to better Q of life



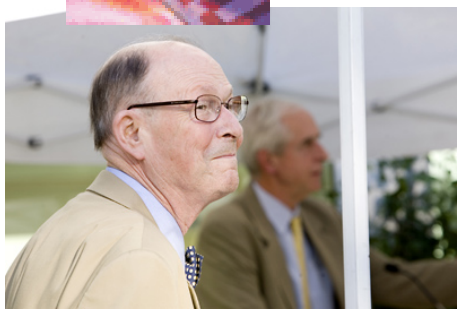
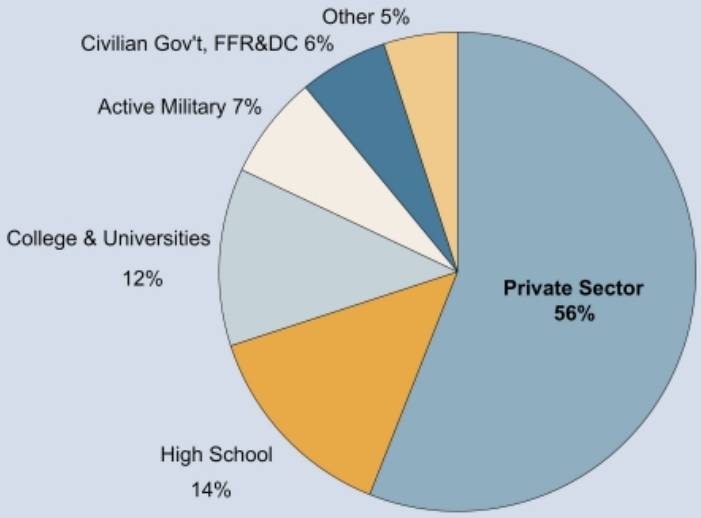


Figure 8. Initial employment sectors of physics bachelor's, classes of 2003 & 2004.



AIP Statistical Research Center, Initial Employment Report.

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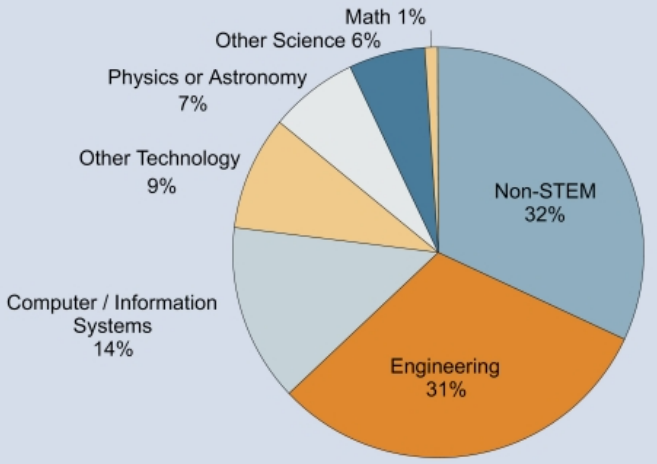
Figure 9. Field of employment for physics bachelors in the private sector, class of 2004.



STEM: Science, Technology, Engineering and Math

AIP Statistical Research Center, Initial Employment Report.

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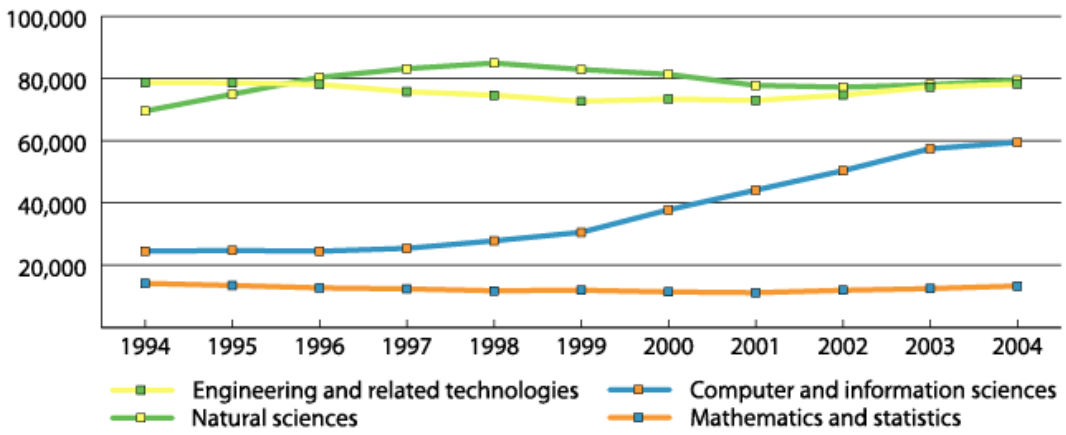
Done

Where Do Physics BS's Go?

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



Source: U.S. Department of Education

Broad View

Employment in STEM
⇑ 3 X *wrt* others
(CS 5X)

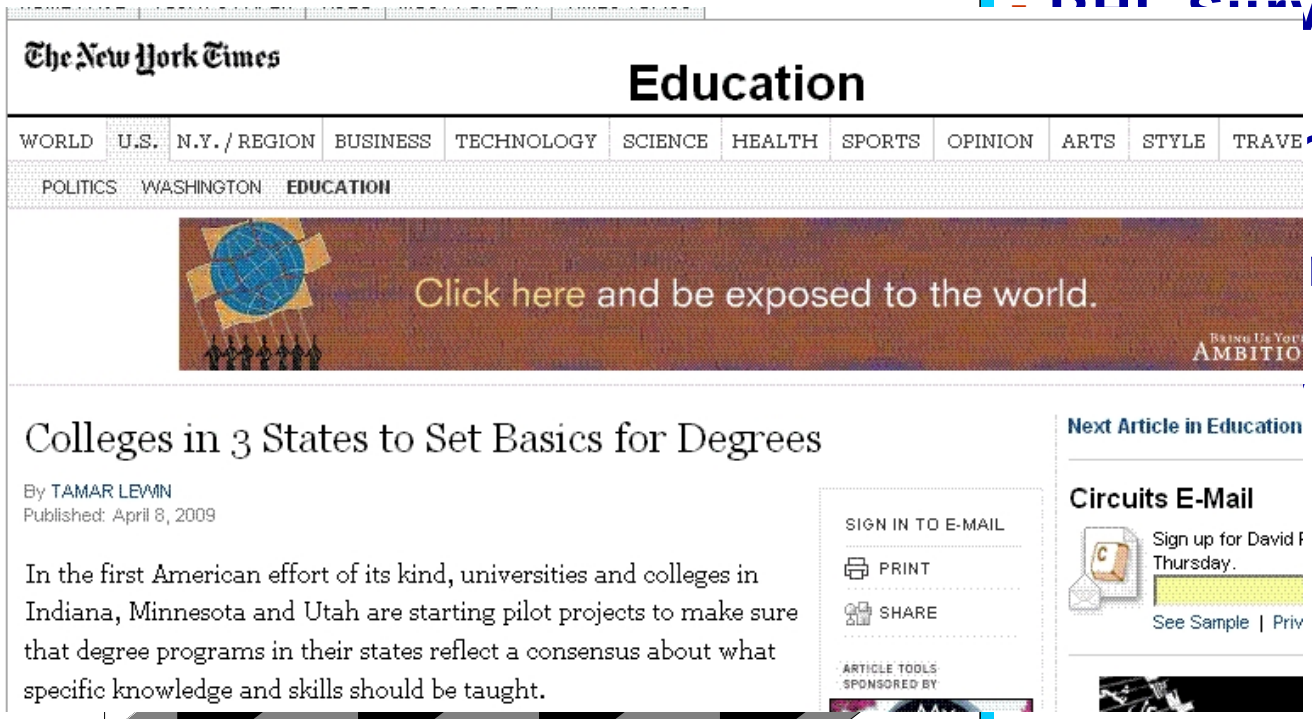
Table 2
Employment growth and job openings in STEM occupations, projected 2004-14

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 (Science Ed) 4

- PHL Survey (Y&L)
- ~ balance
- mple
- pes √
- imbalance?



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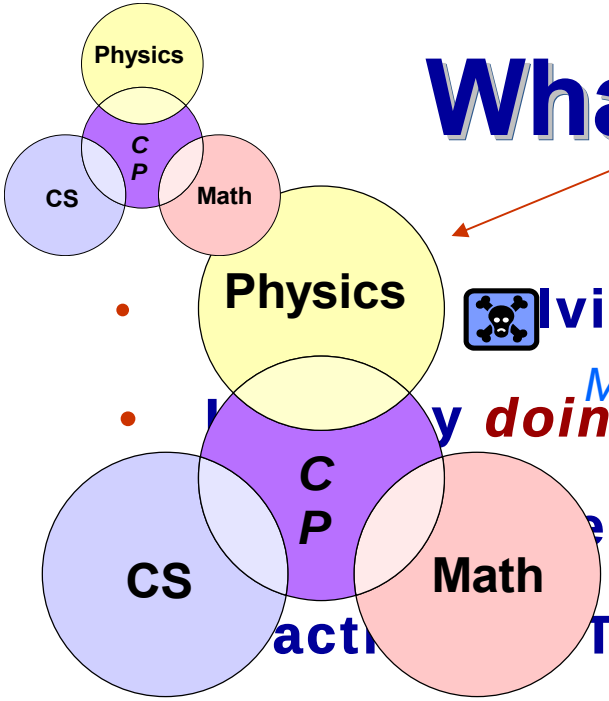
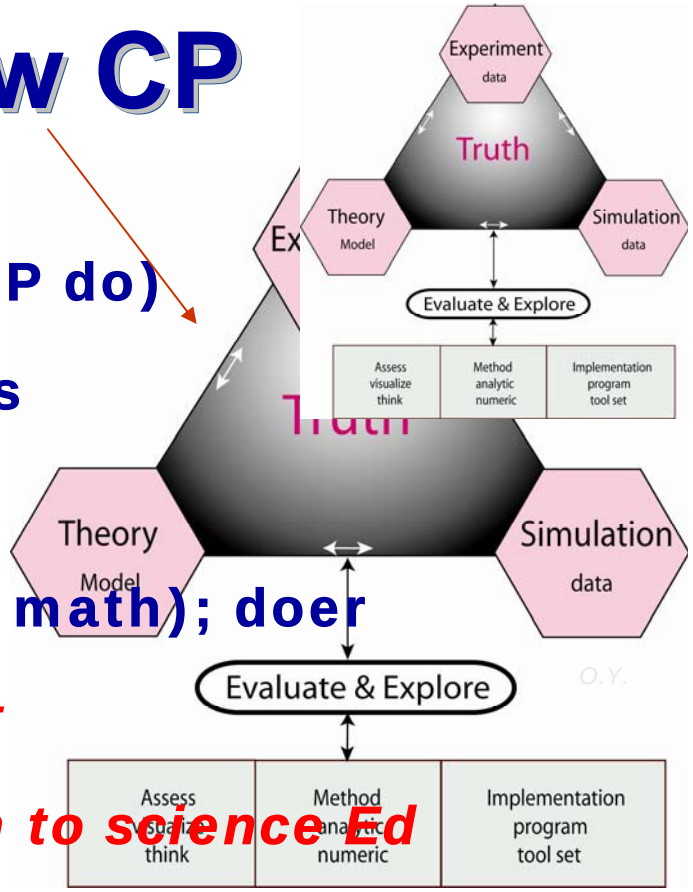
	CS	CSE	CP	PH
Other	31	29	32	36
Application	17	28	28	45
Math	12	23	19	17
Comp	40	20	20	2

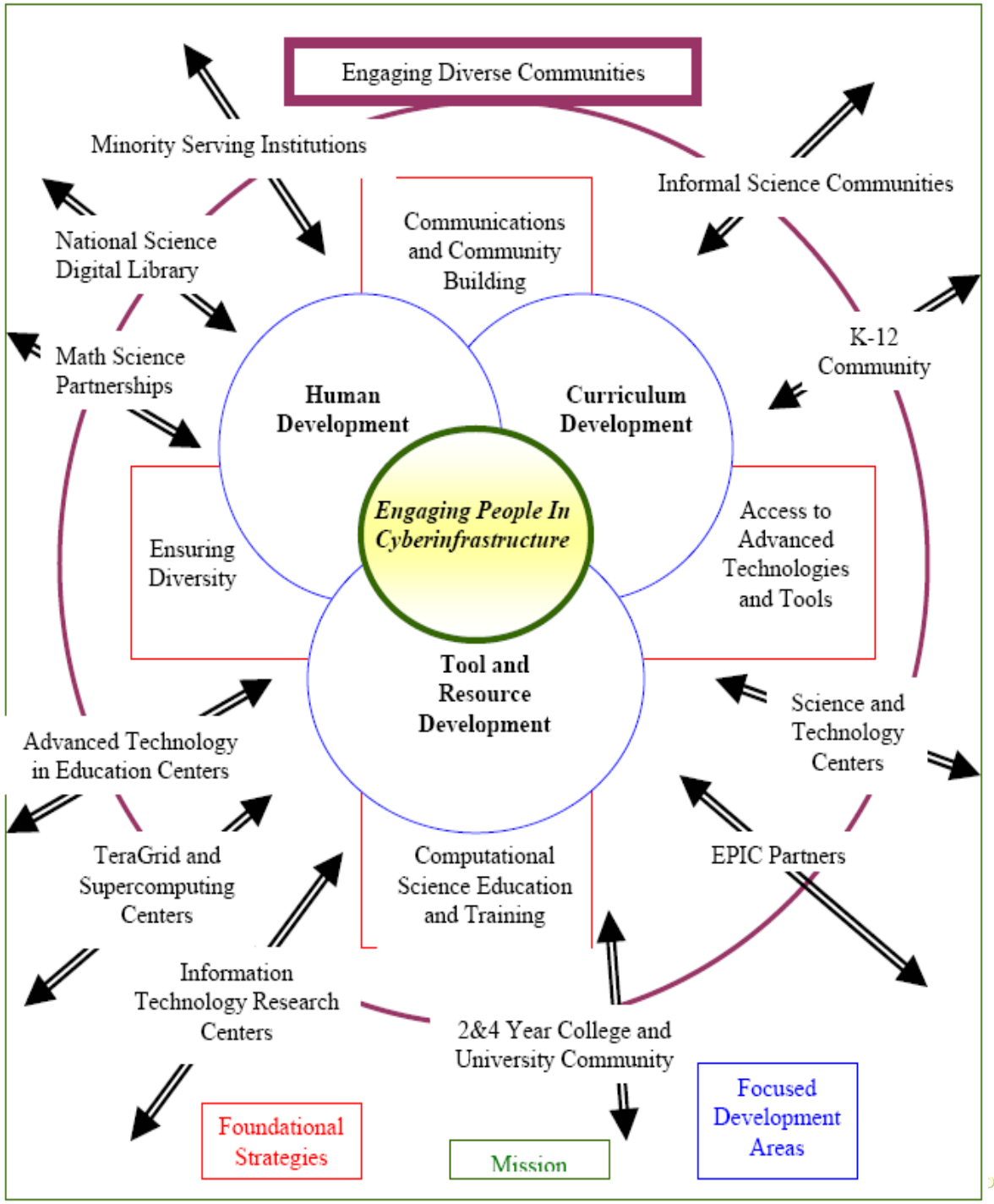
What = CP, How CP



- Physics
- lving (why do P, what P do)
- *Multi ≠ Inter*
- y *doing* individual Projects
- er teach (lectures?)
- acti 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!" (packages)



UCES Award
(DOE)



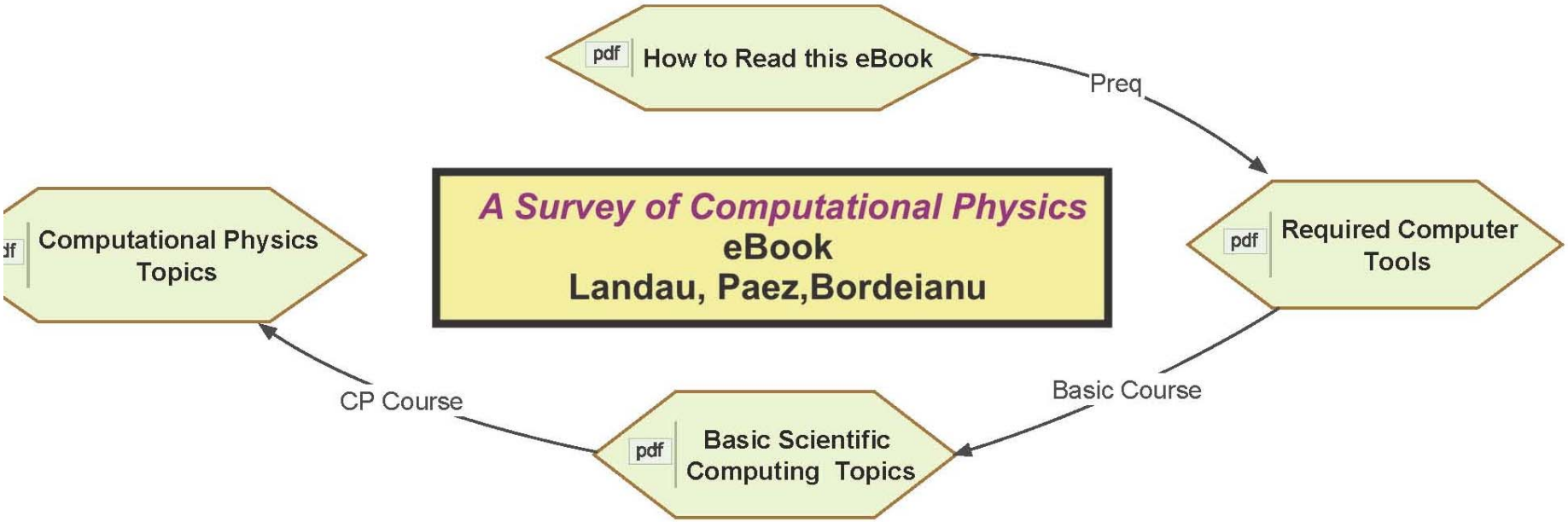
CSE COMMUNITY

Intellectual Content of CSE Ed

Student Learning Outcomes (SLO)

- ***Elements of Computational Science & Engineering Ed***
  Yasar & Landau, SIAM Review, 45, 4, 787-805 (2003)
- **Prerequisite establish CX courses, program**
- **Easy (too) expect 1 course teach entire subject**
- **Historically guided by research needs; grad study**
- ***See SLOs* for specifics**

- **≠**  **, don't need CP BS**
- **Don't have to buy entire curriculum (AAPT, CiSE, MS, OH, UC, CSU, CCLI)**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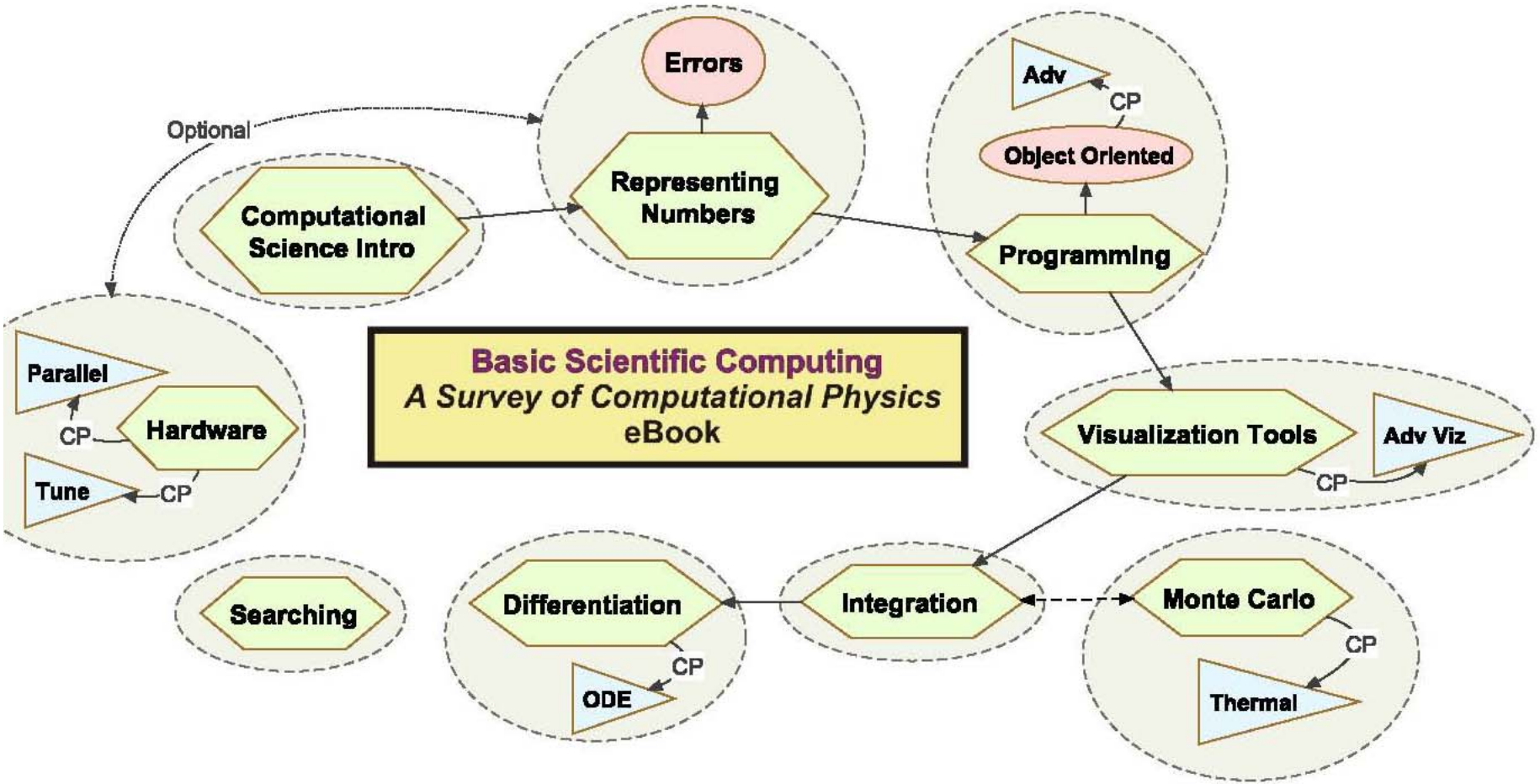
Preq
A Survey of Computational Physics
eBook
Landau, Paez,Bordeianu
pdf Required Computer Tools
Computational Physics Topics
CP Course
Basic Course
pdf Basic Scientific Computing Topics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Computational Science Intro
Adv
CP
Object Oriented
Programming
Basic Scientific Computing
A Survey of Computational Physics
eBook
Parallel
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Integration
Monte Carlo
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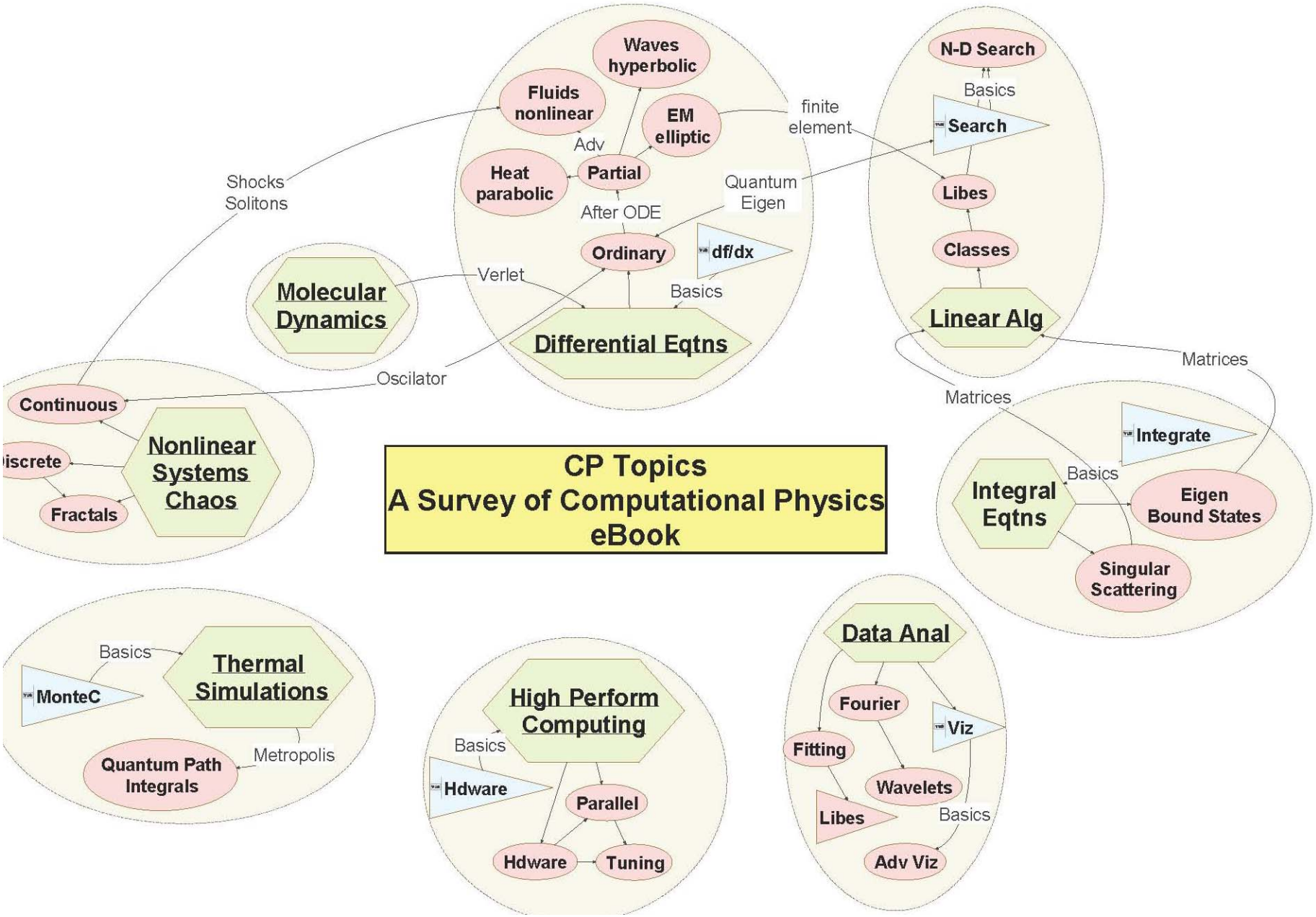
CP Topics
A Survey of Computational Physics
eBook
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Fluids nonlinear
EM elliptic
Adv
Heat parabolic
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Basics
Differential Eqtns
Quantum Eigen
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Molecular Dynamics
Verlet
Oscilator
N-D Search
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Search
Libes
Classes
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Matrices
Matrices
Continuous
Nonlinear Systems Chaos
Fractals
Integrate
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Eigen Bound States
Singular Scattering
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MonteC
Thermal Simulations
Quantum Path Integrals
Metropolis
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High Perform Computing
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Libes
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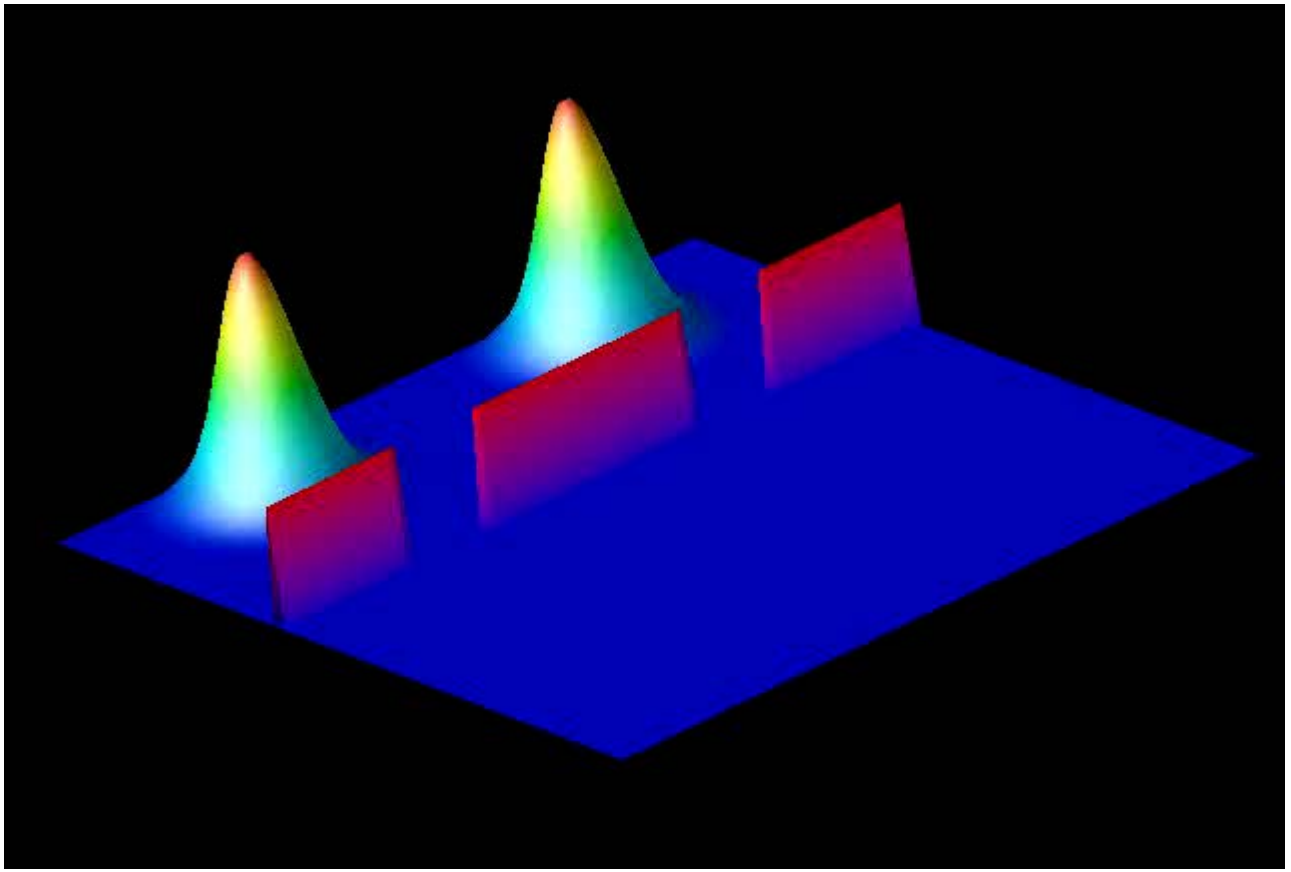
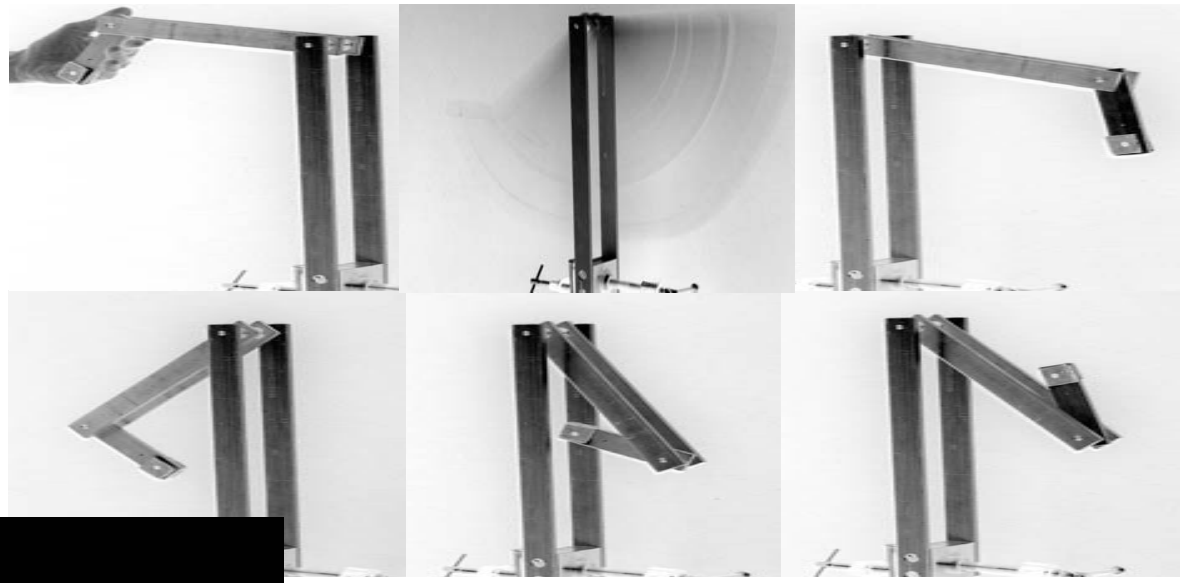
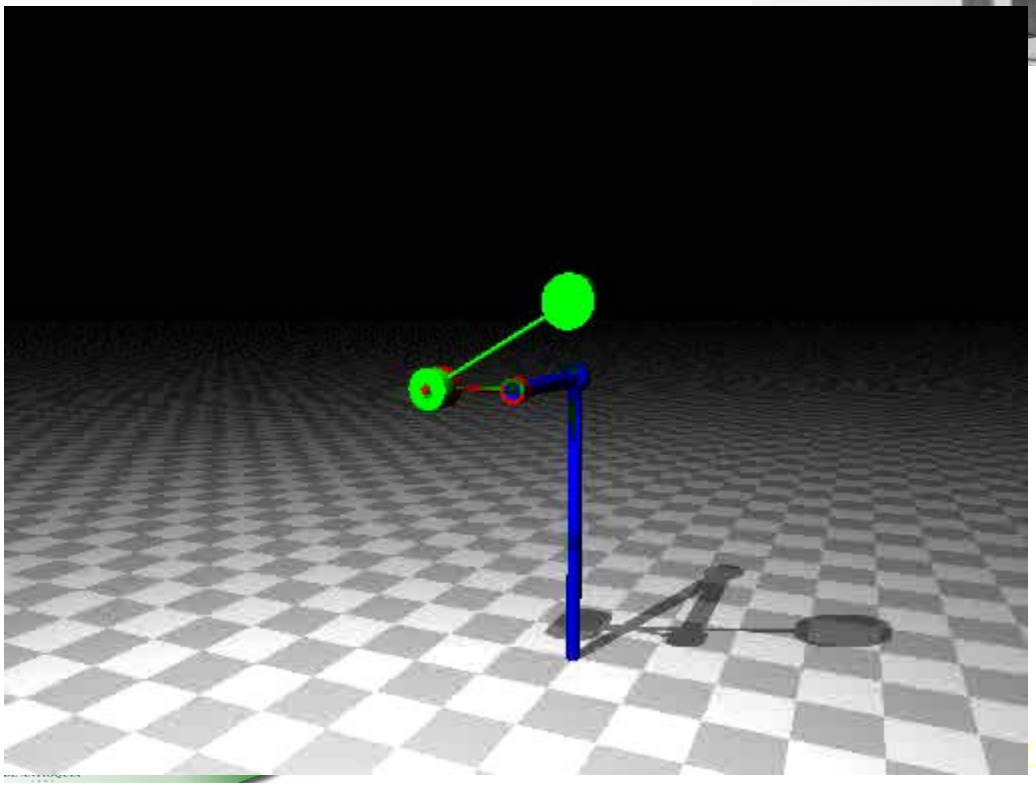
Adv Viz

Visualizations, 2 Slit Diffraction

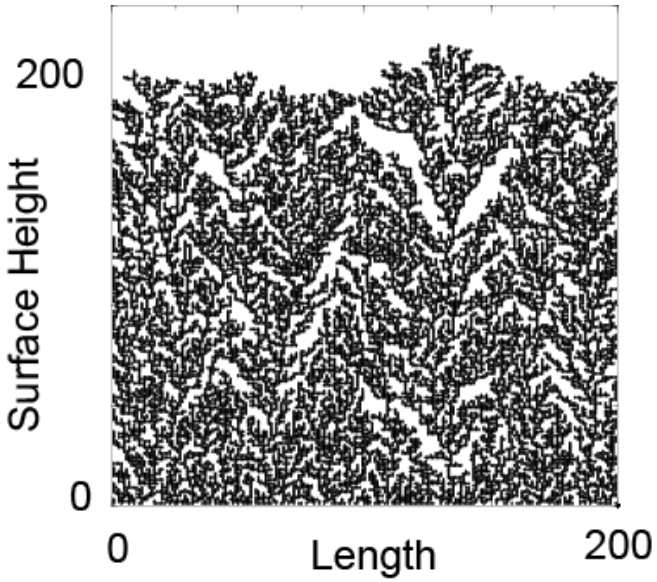


Double Pendulum





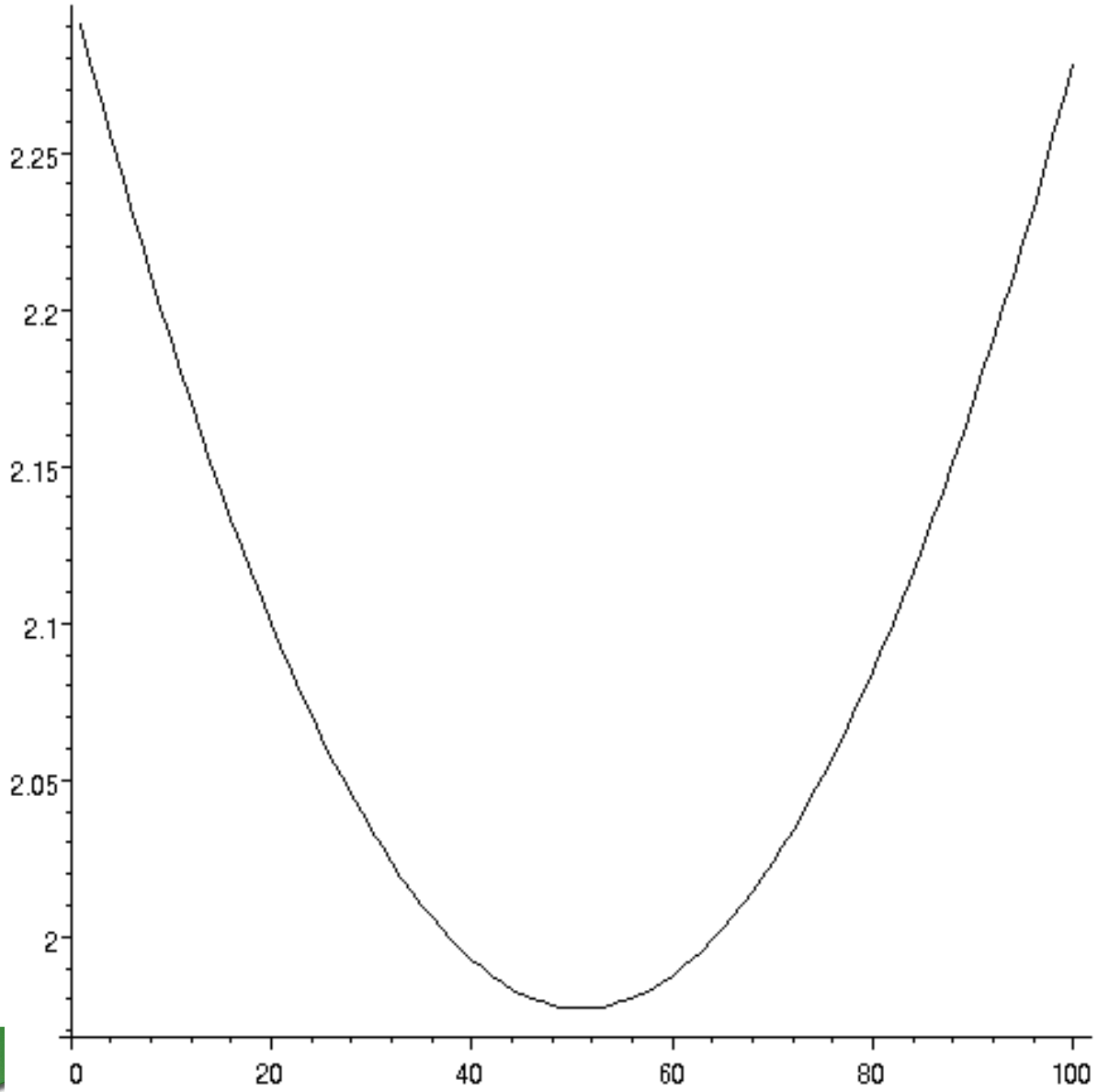
Fractal Growth



Jackson Pollock

(Richard Taylor, UofO, NYT)

Catenary Wave + Friction



BS in CP @ OSU

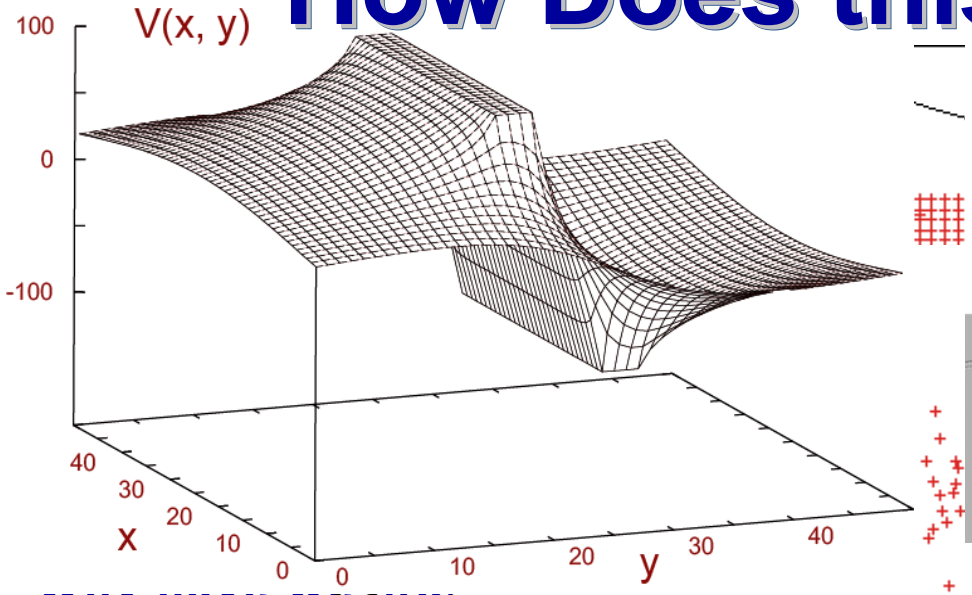
	Fall	Winter	Spring
Fresh (46)	Diff Calculus (Mth) Writing/fitness Gen Chem I Perspective CP Seminar	**Scientific Comptng I** (PH/MTH/CS) Intgl Calculus (MTH) Perspective - 2 Gen Chem II	**Intro CS I (CS)** Vector Calc (MTH) Gen Phys I Writing/fitness
Soph (45)	**Intro CS II (CS)** Vector Calc II (MTH)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

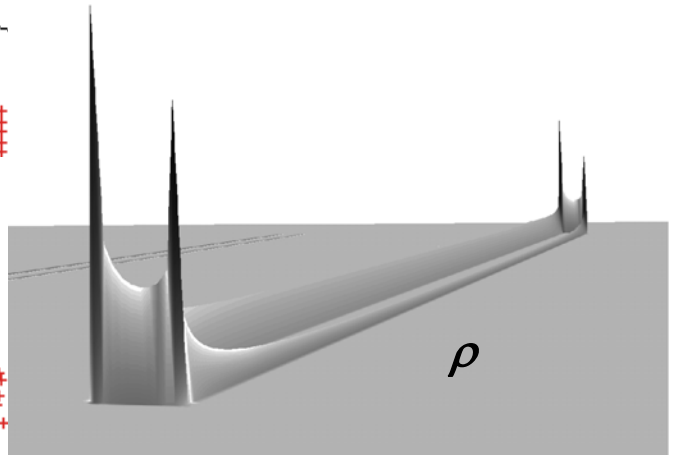
Real computation across the curriculum

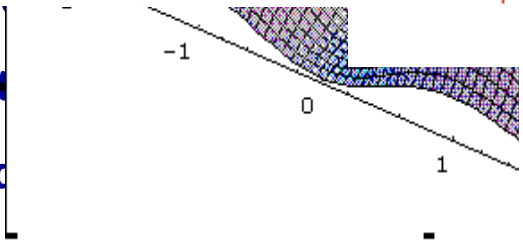
Not 1 course, not just our view

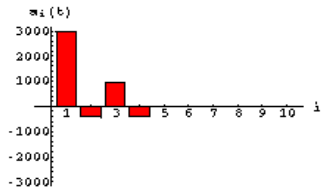
Use what's available

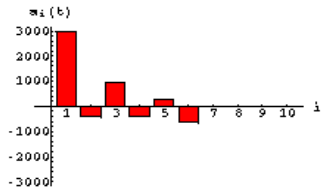
How Does this Work?

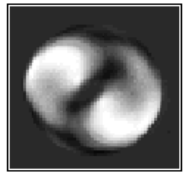


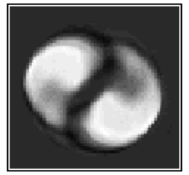












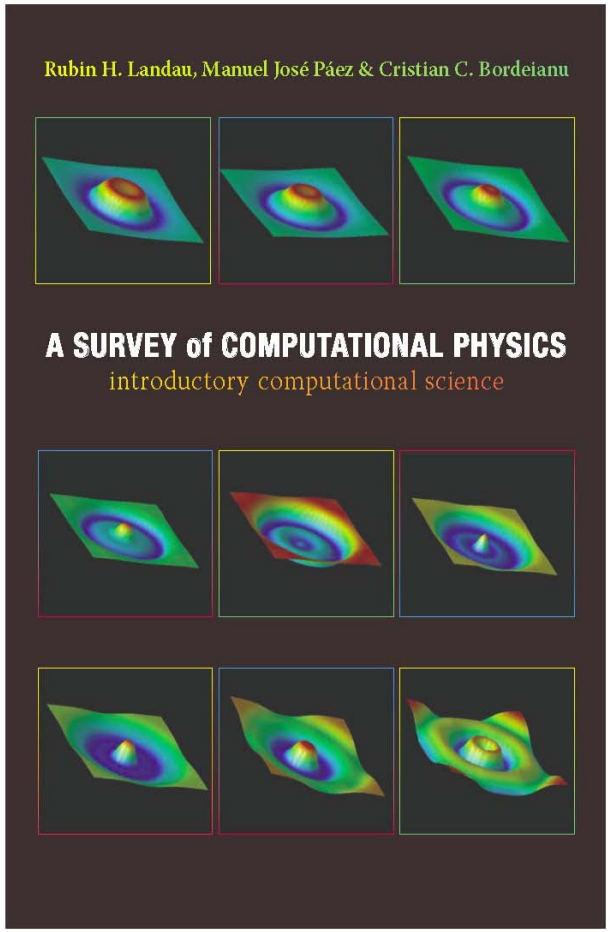
1.
2.
3.
4.
5.
6. [illegible]
7. "Now I know what
8. "Now Laplace's eq
9. "I was up all night."
10. Chaotic scattering: several MS, 1 Ph D t
11. "MD: way I thought simulations should
12. Great prep physics, astroP, CS, ocean, bioP, brain
13. Women: didn't know liked C, problem solving

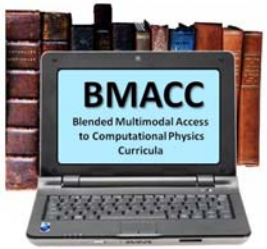
Digital Books & Online Courses

- Web N is here to stay & grow; challe
- Not: general ed, weak discipline, mo
- Natural (best) for computing educati

- Digital book (MathML)
  - Now hot topic (slates)
  - Live/search eqns, figs
  - Compadre
  - Nat Science Digital Libe
  - RHL: package lectures
  - Sally Haerer

Fig. 3 Sample eTeach session



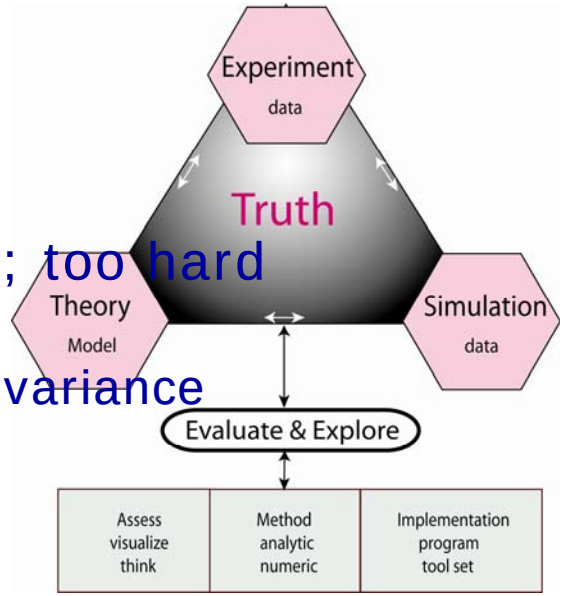


Computational Physics Thinking *(RHL War Story)*

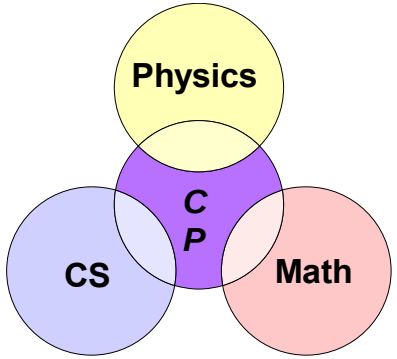
center for Computational Thinking
Carnegie Mellon

NSF: Cyber-Enabled Discovery & Innovation

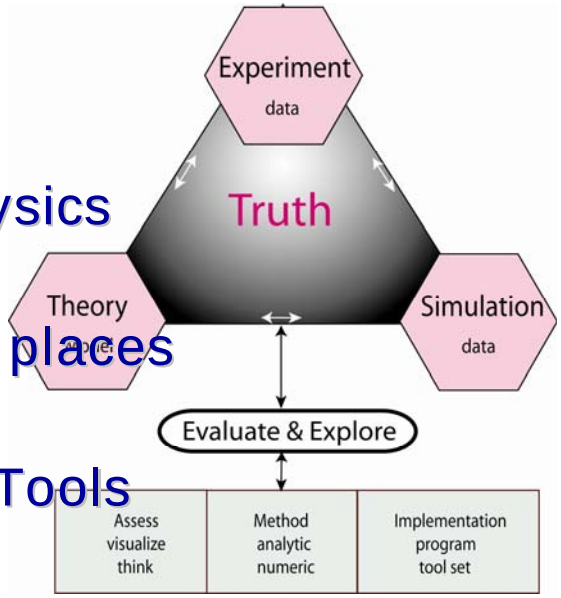
- Δ approach physics, understand problems + Compute in mind
  - Other sciences, multiscale & multiphysics
- Approach: predictions otherwise unattainable; too hard
- $\Uparrow$ realism, complexity, $\Uparrow$ experiment, mean $\rightarrow$ variance
- Computing too important to leave to CS
- CS: multiple multiple-layers abstraction; scaling
- Δ Ed: PH + CS + Math in problem solving *context* (cut CS, math)

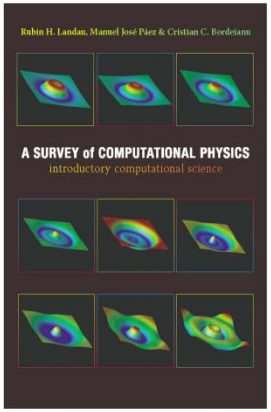


Take Home Lessons



- Computing essential most forefront research
- Exciting research + significant computation
- Multiscale & Multiphysics; broader view of physics
- CyberInfra world: big science in small distant places
- Rejuvenate Physics Ed + Modern Research & Tools
- Ph + CS + Math in problem/research context
  - Learn all 3 better, frees time for C, App Math
- Teach C: do it right; ⇒ right PH, right questions





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

Physics 467/567 Advanced Computational Laboratory

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