Computational Problems for Physics Courses
Motivation & Examples

Rubin H Landau

http://physics.oregonstate.edu/~landaur/

CP Author, Founder CP Degree Program

Computational subatomic few-body systems (1966-2003)
CP Education (1988-)

Grad School: How creative? Plenty smarts; Exact Compute

DCOMP Boston, March 2019
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# Contributors

**Coauthors:** Manuel Paez & Cristian Bordeianu-d

## In Addition: Suffering Students & Collaborators

<table>
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<tr>
<th>Names</th>
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<tbody>
<tr>
<td>C. E. Yaguna, J. Zuluaga, Oscar A. Restrepo, Guillermo Avendano-Franco</td>
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<tr>
<td>Sally Haerer, Saturo S. Kano (consultants, producers)</td>
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<tr>
<td>Melanie Johnson (Unix Tutorials)</td>
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<tr>
<td>Hans Kowallik (CP text, sounds, codes, LAPACK, PVM)</td>
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<tr>
<td>Matthew Ervin Des Voigne (tutorials)</td>
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<td>Bertrand Laubsch (Java sound, decay)</td>
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<td>Jon J Maestri (vizualizations, animations, quantum wave packets)</td>
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<td>Juan Vanegas (OpenDX)</td>
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<td>Al Stetz, David McIntyre (First Course)</td>
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<td>Connelly Barnes (OOP, PtPlot)</td>
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<td>Phil Carter, Donna Hertel (MPI)</td>
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<td>Zlatko Dimcovic (Wavelets, Java I/O)</td>
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<td>Joel Wetzel (figures)</td>
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<td>Justin Murray, (REU, Sum 98; Weber State)</td>
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<td>Kevin Wolver, (REU, Sum 96; St Ambrose)</td>
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Premise: Physics Ed: Take Computation Seriously

Why? Computation = Big Part of Physics & Much Else

- Nat Sci Bd: remain in field
  - 22% physics BS
  - 52% PhD
- Do something new (R&D)
  - Increased realism, complexity, precision

Data ⇒ Undergrad overemphasize Physics
→ weaker preparation: career, fulfillment
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Field of Employment for Physics Bachelor’s in the Private Sector, Classes of 2009 & 2010 Combined

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"We are teaching the same things we taught 50 years ago"
APS/AAPT Taskforce on Grad Ed., R Diehl, 2004

OK that’s physics (APS/AAPT Taskforce)

Do take math, then Math Mtds of Physics \implies

Teach Computation within physics

Use research-like examples

Teach: PH + CS + Math in problem-solving context

Using C when teach P \neq CP

“OK for pedagogy” \neq life
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- 1980s: CP Texts, now plenty good ones
- 1990s: CP Courses, Computational X programs, ...
- No need repeat past developments (PICCUP)
- Need integrate computation into physics courses
- CRC Press *Series in CP*; S Gottlieb, R Landau, Eds
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Computational Competencies by Comp Physicists

≒ AAPT Statement (G, T, L, C, 2011)
≒ HPC University (Ohio State) Computational Competencies

Tools All Physicists Should Know

- **Basic Numeric Tools**
  - Integration ⇒ Guassian
  - Differentiation
  - Floating Point Math [Errors]
  - Search Techniques
  - Linear Algebra [Libes]

- **Languages, Environments**
  - Program compiled (2) (≠ CS)
  - Symbolic
  - Operating sys (2)

- **ODEs Solutions ⇒ rk4**
  - Planets, 3-B Orbits
  - CM & QM Chaotic Scattering

- **Tools for Analysis**
  - Data fitting
  - Visualize functions & data
  - Document prep ($\LaTeX$)
  - Fourier, DFT, FFT
  - Wavelets*, Principal Components*
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### Computational Competencies by Phys Educators

#### AAPT Undergraduate Curriculum Task Force, 2016

- Computation ubiquitous in physics
- Deeper understanding of physics via fundamental laws
- Spreadsheets: “see exactly what’s happening”
- Mathematical computing packages: get computing over with quickly, don’t emphasize computing
- Programming language: worthwhile “in the long term”
- Special-purpose software best choice for classrooms, not empowering
- Process data
- Represent data visually
- Prepare documents and presentations

**AAPT 2016 ⇒ Don’t take computation too seriously!**
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Computational Problems for Physics Courses

2018 Book, collected problems, Projects & Demos [shameless commerce]

Chapters: Some borrowed, some new, all long overdue

- Computational Basics
- Data Analytics
- Classical, Nonlinear Dynamics
- Waves, Fluids
- E & M
- Quantum Mechanics
- Thermo, Stat Phys
- Bio Models: Population Dynamics, Plant Growth
- More Entry-Level Problems
- Python Codes
Problems to Include in Physics Courses (will demo)

Applications

- **Explore Nonlinear Dynamics**
  - Bifurcations, phase space (CM)
  - Double & Chaotic Pendula (CM)
  - Fractals, Stat Growth (StatMech)
  - Integral Equations (QM, CM)
- **Monte Carlo, Stochastic**
  - Spontaneous Decay (QM)
  - Random Walk (Thermo)
  - Thermal Simulations (StatMech)
  - Molecular Dynamics (≠ MC)
  - Feynman Path Integrals (QM)
- **PDEs (relax, t step, split t)**
  - Laplace/Possion (EM)
  - Heat [x-t diffusion] (Thermo)
  - Realistic Strings [waves] (CM)
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- **Fluid Dynamics**
  - Fluid Flow (> freshman)
  - Shock Waves (CM)
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Monte-Carlo Random Walks

- \( \Delta x_i = r_i, \Delta y_i = r_j \)
- Good to “see” a walk
- Stochastic processes & math: very interesting, \( R_{rms} \propto \sqrt{N} \)
- Random, probability, experimental statistics \( \leq \) taught
Monte-Carlo Decay Simulation

Analytic $= e^{-t/\tau} \simeq$ Simulation (discrete): Closer Nature

$$P = \frac{\Delta N(t)/N(t)}{\Delta t} = -\lambda \quad \text{(Law of Nature)} \quad (1)$$

$$\Rightarrow \quad \frac{\Delta N(t)}{\Delta t} = -\lambda N(t) \quad \text{(Real Physics)} \quad (2)$$

$$\Rightarrow \quad \frac{dN(t)}{dt} = \frac{dN}{dt}(0)e^{-\lambda t} \quad \text{(Approximate Physics)} \quad (3)$$

One line algorithm: if $r_i < \lambda$, $\Delta N = \Delta N + 1$
Classical Chaotic Scattering, 3-Body Problems

- Just Coupled ODEs
  \[ F = ma \]

\[ F = - \nabla \left( x^2 y^2 e^{-x^2 - y^2} \right) \]

- Chaotic Scattering
- 3 Body Applet
Classical & Quantum Chaos

Solve Same Problem Classically & Quantum Mechanically

- Billiards in enclosed figure can be chaotic (BC)
- Quantum Chaos hard to “see”
- Look for signature of classical chaos in QM
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**Linear Algebra Packages, HS Problem ⇒ HPC**

*NewtonNDAnimate.py*  
<Ex: 3 masses>

- $T_i, \theta_i = ?$
- 9 nonlinear equations

\[
L_1 \cos \theta_1 + L_2 \cos \theta_2 + L_3 \cos \theta_3 = L, \]
\[
L_1 \sin \theta_1 + L_2 \sin \theta_2 - L_3 \sin \theta_3 = 0, \]
\[
\sin^2 \theta_1 + \cos^2 \theta_1 = 1 \]
\[
\sin^2 \theta_2 + \cos^2 \theta_2 = 1 \]
\[
\sin^2 \theta_3 + \cos^2 \theta_3 = 1
\]

- Newton-Raphson search
- Use matrix libes

\[
T_1 \sin \theta_1 - T_2 \sin \theta_2 - W_1 = 0
\]
\[
T_1 \cos \theta_1 - T_2 \cos \theta_2 = 0
\]
\[
T_2 \sin \theta_2 + T_3 \sin \theta_3 - W_2 = 0
\]
\[
T_2 \cos \theta_2 - T_3 \cos \theta_3 = 0
\]
Realistic Waves: Catenary + Friction

PDE with Time Stepping

\[ c^2 \frac{\partial^2 y}{\partial x^2} - \frac{2\kappa}{\rho} \frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial t^2} \quad \text{(with Friction)} \quad (1) \]

\[ \frac{\partial T(x)}{\partial x} \frac{\partial y(x, t)}{\partial x} + T(x) \frac{\partial^2 y(x, t)}{\partial x^2} = \rho(x) \frac{\partial^2 y(x, t)}{\partial t^2} \quad \text{(Variable } \rho \text{ & } T) \quad (2) \]
### Time-Dependent Schrödinger Eqn

#### Wavepacket – Wavepacket Interactions

\[
i \frac{\partial \psi(x, t)}{\partial t} = -\frac{1}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x)\psi(x, t) \quad \text{(1 particle)}
\]

\[
i \frac{\partial \psi(x_1, x_2, t)}{\partial t} = -\frac{1}{2m_1} \frac{\partial^2 \psi(x_1, x_2, t)}{\partial x_1^2} - \frac{1}{2m_2} \frac{\partial^2 \psi(x_2, x_2, t)}{\partial x_2^2} + V(x_1, x_2)\psi(x_1, x_2, t) \quad \text{(2 particles)}
\]

- Often ignored in QM
- 1 packet, 2 Slits
- Packet\((x_1)\)-Packet\((x_2)\)
Shock Wave Physics

Singularity $\Rightarrow$ Better Algorithm (Lax)  

Singularity Nature?

\[
\frac{\partial \rho(x, t)}{\partial t} + c \frac{\partial \rho(x, t)}{\partial x} = 0 \quad \text{(Advection/Continuity)} \quad (1)
\]

\[
\frac{\partial \rho(x, t)}{\partial t} + \epsilon \rho(x, t) \frac{\partial \rho(x, t)}{\partial x} = 0 \quad \text{(Burgers’ Eqn $\Rightarrow$ Shock)} \quad (2)
\]
(Shock Waves) Dispersion, Solitons

**KdV Equation**: Dispersion Balances Shock

\[ \frac{\partial \rho(x, t)}{\partial t} + \epsilon \rho(x, t) \frac{\partial \rho(x, t)}{\partial x} = 0 \]  

Burgers’ Equation \hspace{1cm} (1)

\[ \frac{\partial \rho(x, t)}{\partial t} + \epsilon \rho(x, t) \frac{\partial \rho(x, t)}{\partial x} + \mu \frac{\partial^3 \rho(x, t)}{\partial x^3} = 0 \]  

Shock + Dispersion \hspace{1cm} (2)
Molecular Dynamics

Straightforward, Obvious, Ridiculously Effective

- > Chem 101: walls $\Rightarrow PV = nRT$
- Just $F_{QM} = ma_i$; $10^8$ times
- Deterministic $\neq$ statistics ($kT$)
Split Space-Time Steps

Problem: waveguide

\[ \tilde{E}_{x}^{k,n+1/2} = \tilde{E}_{x}^{k,n-1/2} + \beta \left( H_{y}^{k-1/2,n} - H_{y}^{k+1/2,n} \right) \]  

\[ H_{y}^{k+1/2,n+1} = H_{y}^{k+1/2,n} + \beta \left( \tilde{E}_{x}^{k,n+1/2} - \tilde{E}_{x}^{k+1,n+1/2} \right) \]  

Coupled \( E_{x}, H_{y} \) drive other

Easy: even Excell
Computations Part of Real-World Physics

- Include Research-like & Computation problems
- Within physics course
- Computation Problems Book may help
- Agree: faulty math $\Rightarrow$ bad science?
- So uncertain computation $\Rightarrow$ bad physics?
- Computation too important to leave to CS