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

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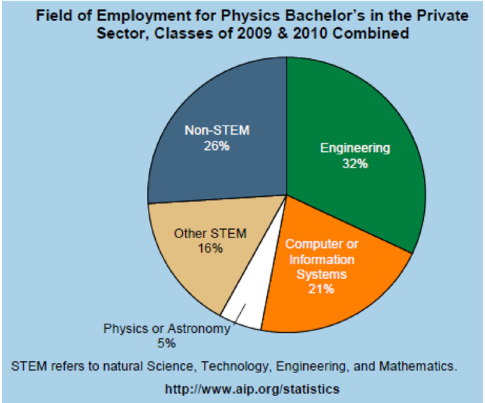
- Paul Fink, Robyn Wangberg, CoAuthors
- Justin Elser, Chris Sullivan (systems)
- Sally Haerer, Saturo S. Kano (consultants, producers)
- Melanie Johnson (Unix Tutorials)
- Hans Kowallik (CP text, sounds, codes, LAPACK, PVM)
- Matthew Ervin Des Voigne (tutorials)
- Bertrand Laubsch (Java sound, decay)
- Jon J Maestri (vizualizations, animations, quantum wave packets)
- Juan Vanegas (OpenDX)
- Al Stetz, David McIntyre (First Course)
- Connelly Barnes (OOP, PtPlot)
- Phil Carter, Donna Hertel (MPI)
- Zlatko Dimcovic (Wavelets, Java I/O)
- Joel Wetzel (figures)
- Pat Cannan, Don Corliss, Corvallis HS (N-D Newton Raphson)
- Brian Schlatter
- Daniel Moore, (REU, Sum 98; Whitman Coll)
- Justin Murray, (REU, Sum 98; Weber State)
- Brandon Smith, (REU, Sum 97; Chico State/SDSC)
- Paul D. Hillard, III (REU, Sum 96; Southern U)
- Kevin Wolver, (REU, Sum 96; St Ambrose)

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, fufillment

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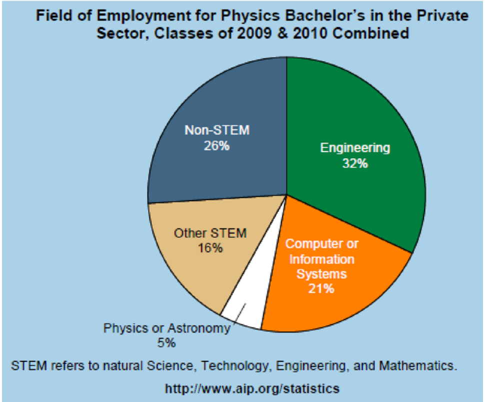

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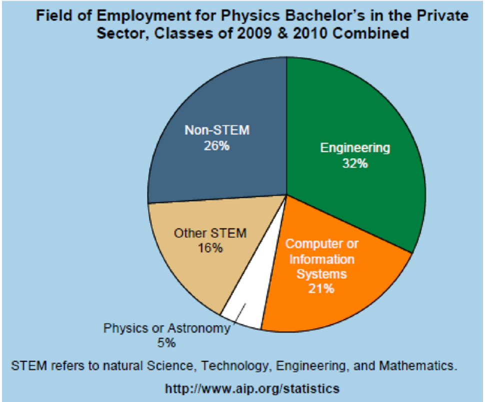

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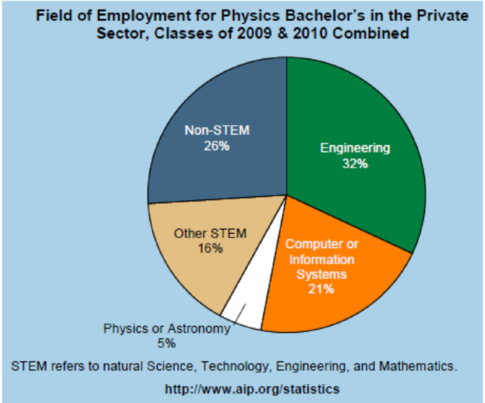

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How: Computation too important to leave to CS

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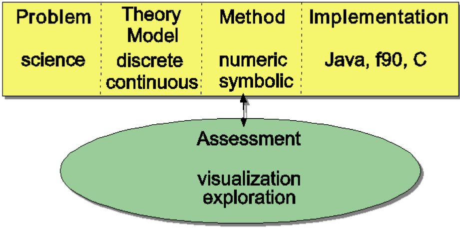

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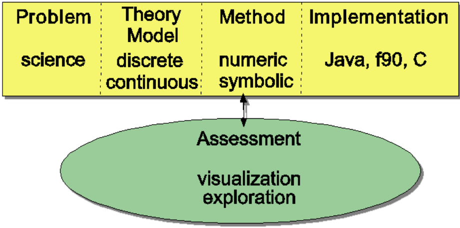

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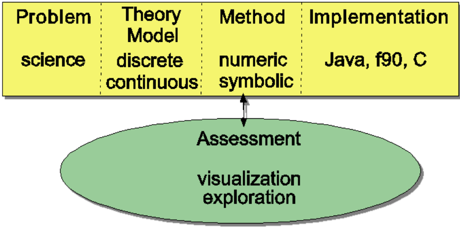

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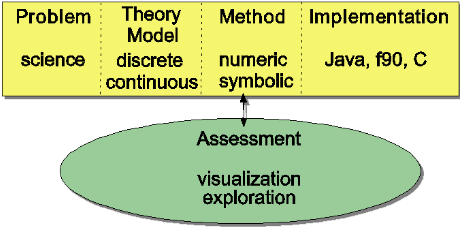

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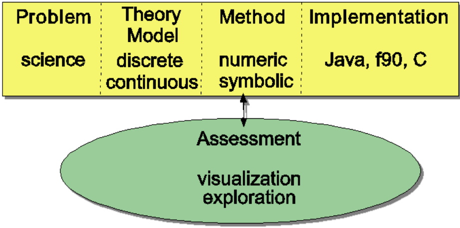

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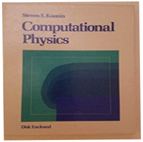

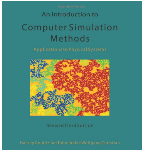

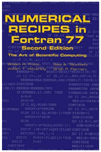

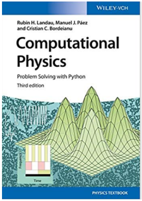

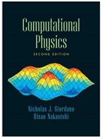

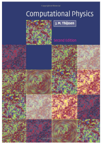

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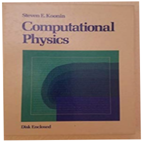

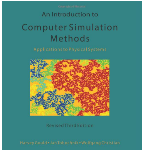

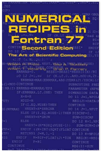

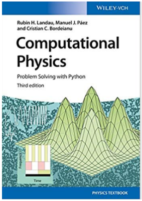

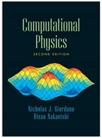

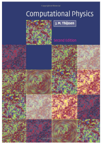

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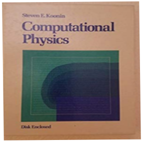

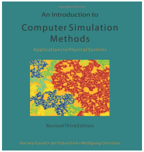

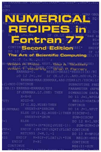

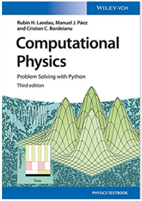

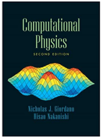

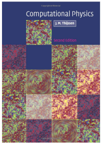

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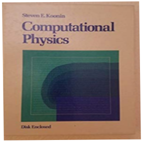

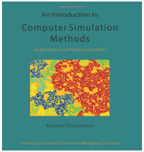

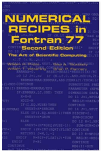

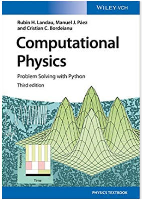

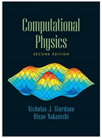

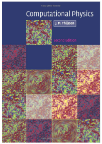

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Computational Competencies by Comp Physicists

$\simeq$ **AAPT Statement** (G, T, L, C, 2011)

$\simeq$ HPC University (Ohio State) Computational Competencies

Tools All Physicists Should Know

- **Basic Numeric Tools**
- Integration $\Rightarrow$ Guassian
- Differentiation
- Floating Point Math [Errors]
- Search Techniques
- Linear Algebra [Libes]
- **Languages, Environments**
- Program compiled (2) ($\neq$ CS)
- Symbolic
- Operating sys (2)
- **ODEs Solutions $\Rightarrow$ 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 $\Rightarrow$ Don't take computation too seriously!

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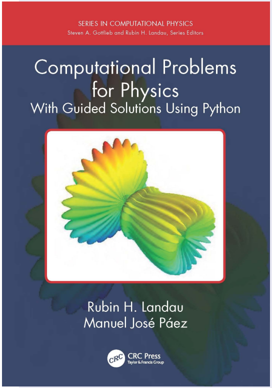
Computational Problems for Physics Courses

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 ($\neq$ 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)
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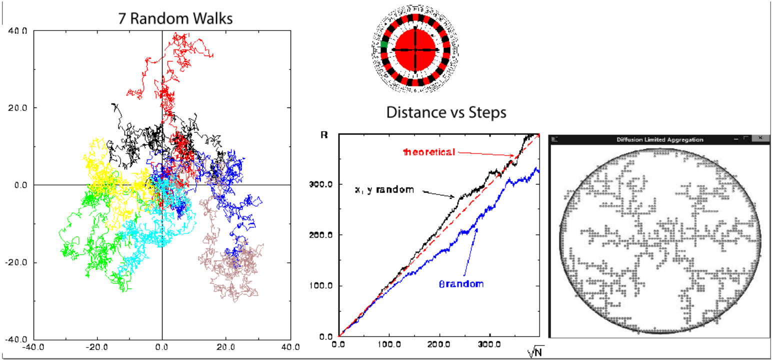
Monte-Carlo Random Walks *Walk3DVis.py*



- $\Delta x_i = r_i, \ \Delta y_i = r_j$
- 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 *DecaySoundVisMod.py*

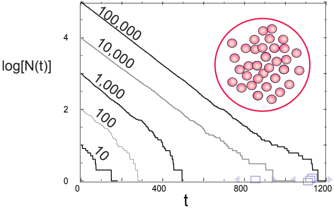
Analytic $= e^{-t/\tau} \simeq$ Simulation (discrete): Closer Nature

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

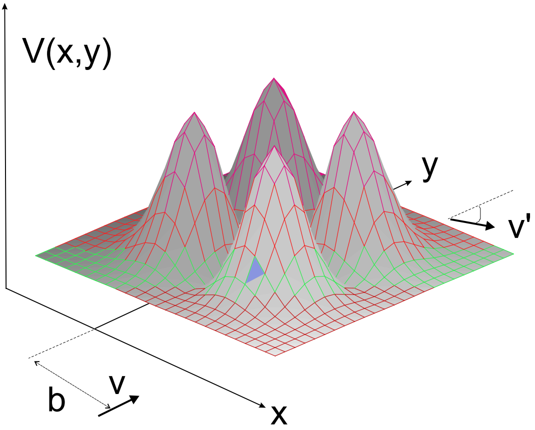
$$\Rightarrow \quad \frac{\Delta N(t)}{\Delta t} = -\lambda N(t) \quad \text{(Real Physics)} \tag{2}$$

$$\not\Rightarrow \quad \frac{dN(t)}{dt} = \frac{dN}{dt}(0)e^{-\lambda t} \quad \text{(Approximate Physics)} \tag{3}$$

One line algorithm: if $r_i < \lambda, \quad \Delta N = \Delta N + 1$



Classical Chaotic Scattering, 3-Body Problems



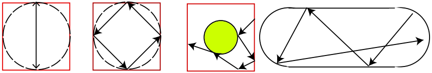
- Just Coupled ODEs

$$\mathbf{F} = m\mathbf{a}$$

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

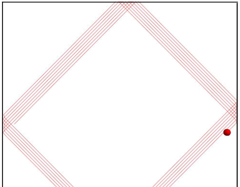
- **Chaotic Scattering**
- **3 Body Applet**

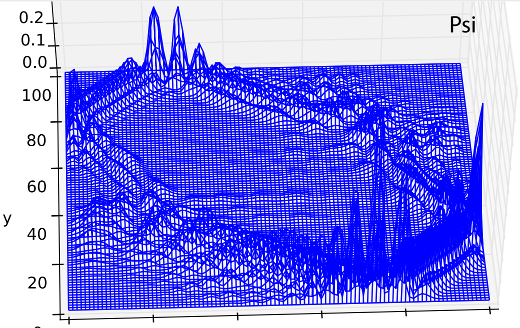
Classical & Quantum Chaos



Solve Same Problem Classically & Quantum Mechanically

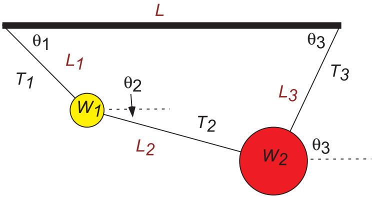
- Billiards in enclosed figure can be chaotic (BC)
- Quantum Chaos hard to “see”
- Look for signature of classical chaos in QM





Linear Algebra Packages, HS Problem $\Rightarrow$ HPC

NewtonNDanimate.py <Ex: 3 masses>



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

$$
\begin{aligned}
L_1 \cos\theta_1 + L_2 \cos\theta_2 + L_3 \cos\theta_3 &= L, \\
L_1 \sin\theta_1 + L_2 \sin\theta_2 - L_3 \sin\theta_3 &= 0, \\
\sin^2\theta_1 + \cos^2\theta_1 &= 1 \\
\sin^2\theta_2 + \cos^2\theta_2 &= 1 \\
\sin^2\theta_3 + \cos^2\theta_3 &= 1
\end{aligned}
$$

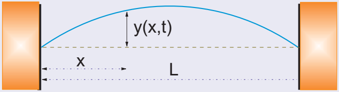
- Newton-Raphson search
- Use matrix libes

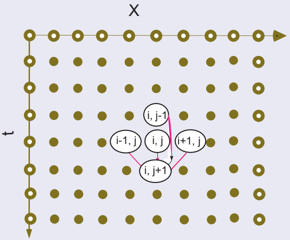
$$
\begin{aligned}
T_1 \sin\theta_1 - T_2 \sin\theta_2 - W_1 &= 0 \\
T_1 \cos\theta_1 - T_2 \cos\theta_2 &= 0 \\
T_2 \sin\theta_2 + T_3 \sin\theta_3 - W_2 &= 0 \\
T_2 \cos\theta_2 - T_3 \cos\theta_3 &= 0
\end{aligned}
$$

Realistic Waves: Catenary + Friction

EqStringAnimate.py

PDE with Time Stepping





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

$$\frac{\partial T(x)}{\partial x}\frac{\partial y(x,t)}{\partial x} + T(x)\frac{\partial^2 y(x,t)}{\partial x^2} = \rho(x)\frac{\partial^2 y(x,t)}{\partial t^2} \qquad (\text{Variable } \rho \;\&\; T) \qquad (2)$$

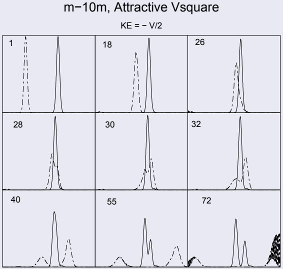
Time-Dependent Schrödinger Eqn

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)

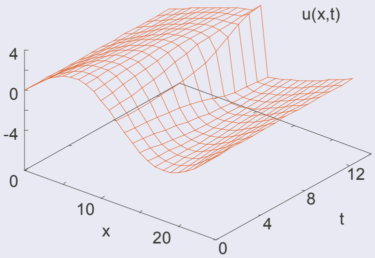


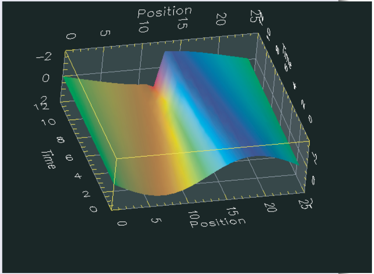
Shock Wave Physics

Singularity ⇒ Better Algorithm (Lax) Singular Nature?

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

$$\frac{\partial \rho(x,t)}{\partial t} + \epsilon\, \rho(x,t)\frac{\partial \rho(x,t)}{\partial x} = 0 \qquad \text{(Burgers' Eqn} \Rightarrow \text{Shock)} \qquad (2)$$

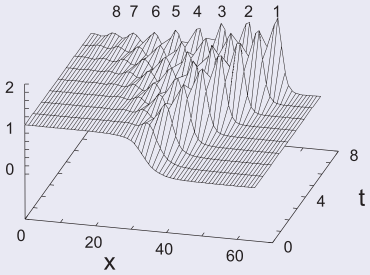


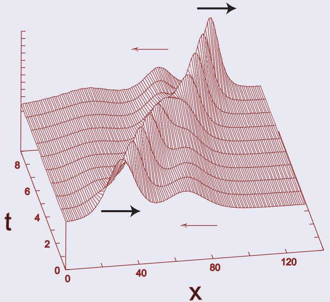


(Shock Waves) Dispersion, Solitons

SolitonAnimateVis.py

KdeV Equation:Dispersion Balances Shock





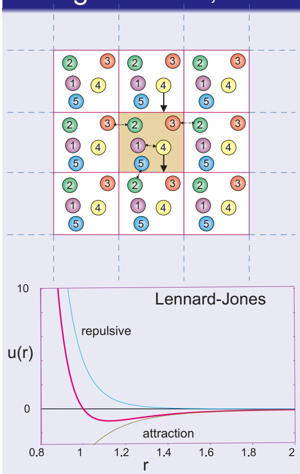
$$\frac{\partial \rho(x,t)}{\partial t} + \epsilon\, \rho(x,t) \frac{\partial \rho(x,t)}{\partial x} = 0 \qquad \text{Burgers' Equation} \qquad (1)$$

$$\frac{\partial \rho(x,t)}{\partial t} + \epsilon\, \rho(x,t) \frac{\partial \rho}{\partial x} + \mu \frac{\partial^3 \rho(x,t)}{\partial x^3} = 0 \qquad \text{Shock + Dispersion} \qquad (2)$$

Molecular Dynamics

Applet *MD1D.py* *MD2D.py*

Straightforward, Obvious, Ridiculously Effective



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

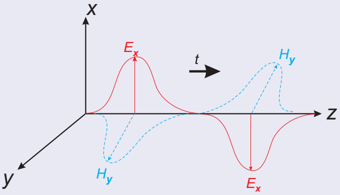
Maxwell: Finite Difference Time Domain

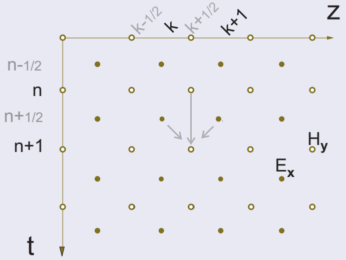
FDTD.py

Split Space-Time Steps — Problem: waveguide

$$\tilde{E}_x^{k,n+1/2} = \tilde{E}_x^{k,n-1/2} + \beta\left(H_y^{k-1/2,n} - H_y^{k+1/2,n}\right) \quad (1)$$

$$H_y^{k+1/2,n+1} = H_y^{k+1/2,n} + \beta\left(\tilde{E}_x^{k,n+1/2} - \tilde{E}_x^{k+1,n+1/2}\right) \quad (2)$$





- Coupled E_x, H_y drive other
- Easy: even Excell

Take Home Lessons: Rejuvenate Physics Ed

Computations Part of Real-World Physics

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