ECE 695 – Numerical Simulations of Electro-optic Energy Systems

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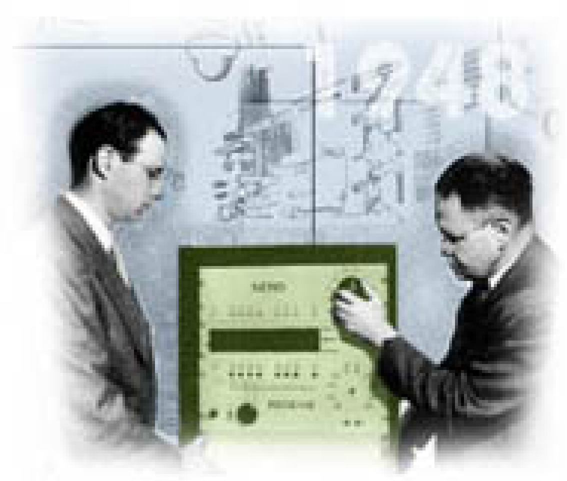
Outline

- Motivation
- My Background and Research
- Topics for This Class
- Goals for This Class
- Assignments
- Grading

Motivation for This Class

- Teach new investigators how to use computers to achieve their research goals
- “The purpose of computing is insight, not numbers!” – Richard W. Hamming

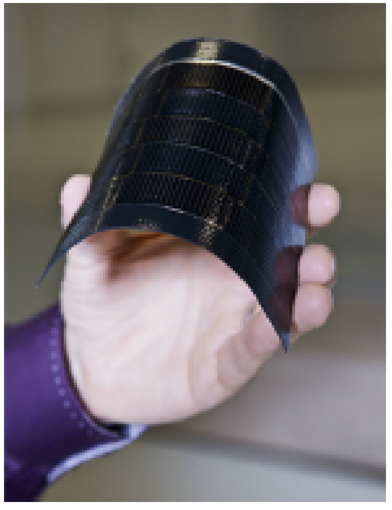


RW Hamming (left), developing error-correcting codes (AT&T)

My Background and Research

- All degrees in Physics
- Master's degree at Cambridge University: linear photonic bandstructures
- Completed Ph.D. at MIT on active materials in photonic crystals (Advisor: JD Joannopoulos)
- Continued with postdoc on applications in photovoltaics & thermophotovoltaics (Advisor: M Soljacic)
- Current work includes PV, TPV, solar thermal, and quantum optics

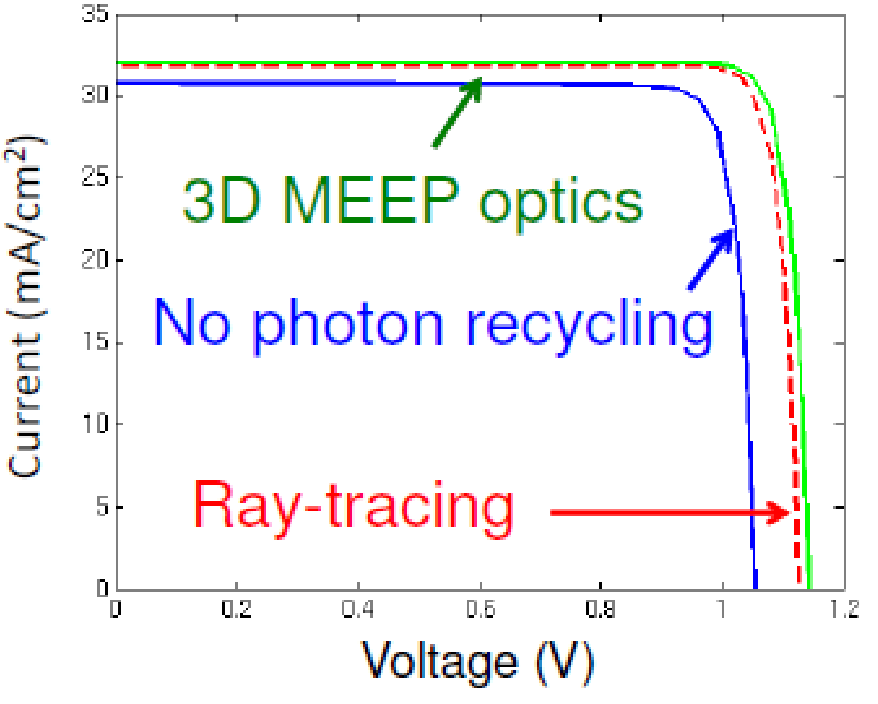
Solar cells approaching theoretical limits: coupling photons and electrons



Alta Devices 28.8%

E. Yablonovitch et al., 38th PVSC (2012)

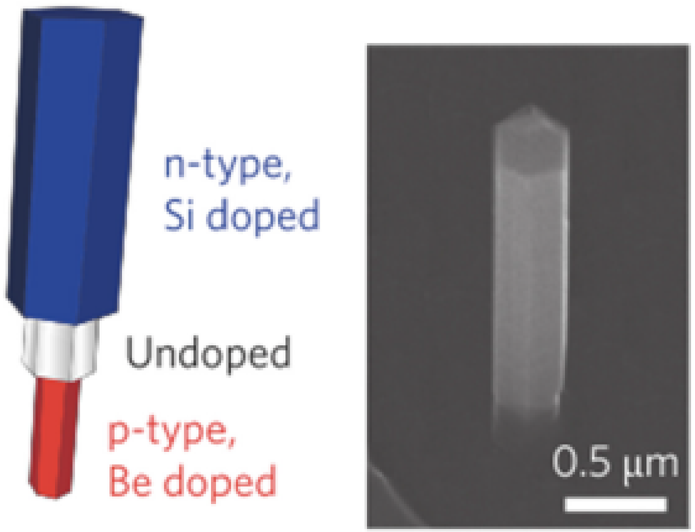
G. Lush and M. Lundstrom, *Solar Cells* **30** 337 (1991).



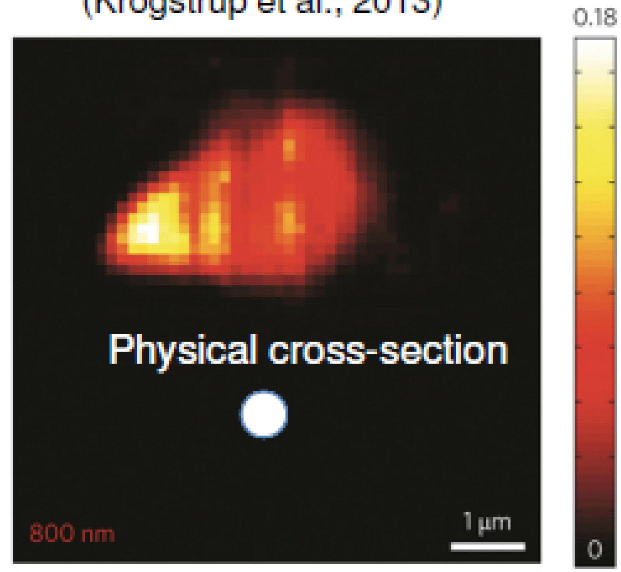
X. Wang *et al. J. Photovolt.* **2** (2013)
P. Bermel, *Opt. Comm.* **10**, 40 (2013)

Nanowire solar cells

(Krogstrup et al., 2013)



Nanowire geometry
(radial junction)

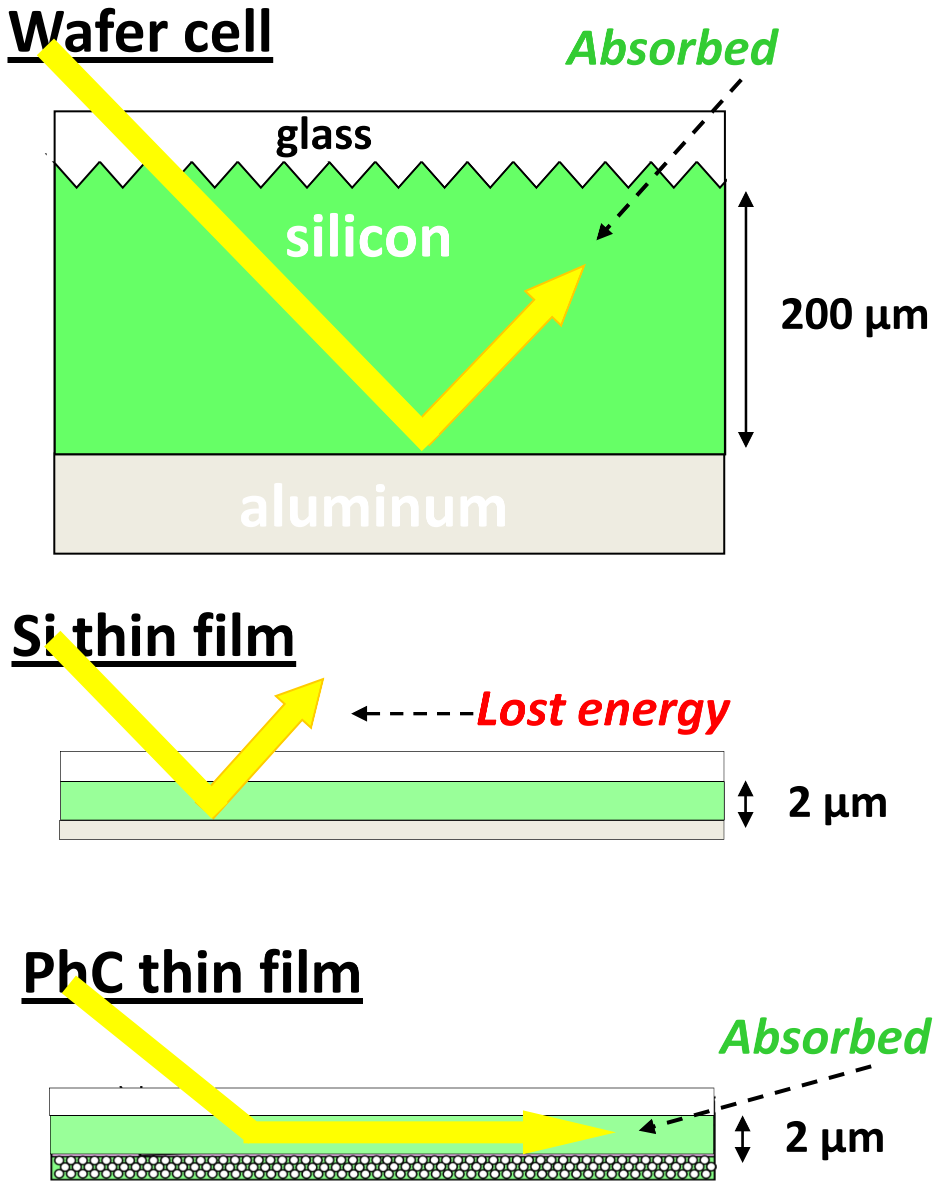


Spatially resolved
light induced current

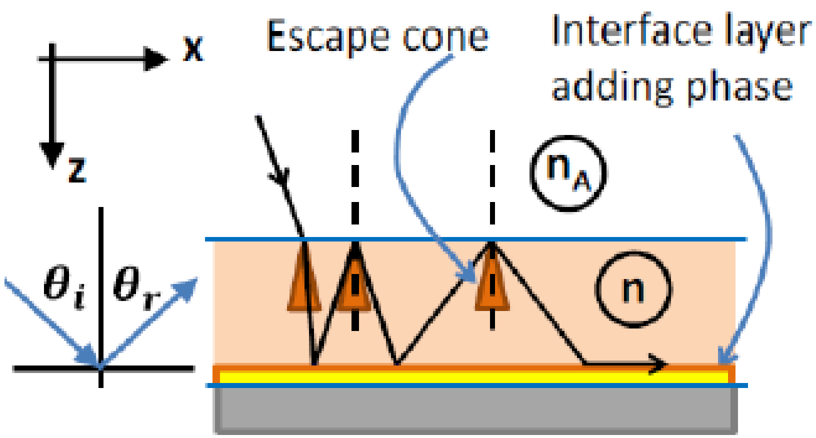
Here, we will investigate:

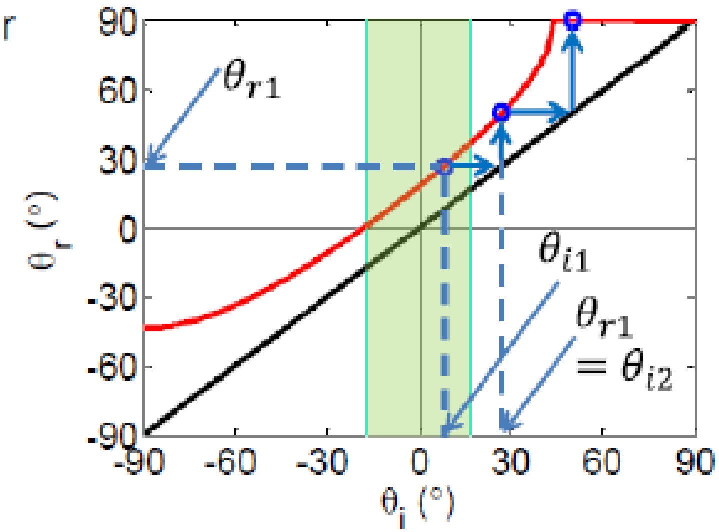
- How the design differs planar solar cells
- Major challenges to higher efficiency
- Maximum obtainable efficiency under realistic assumptions

Light Management in Photovoltaics



Ultrathin Metasurface Absorbers/Emitters

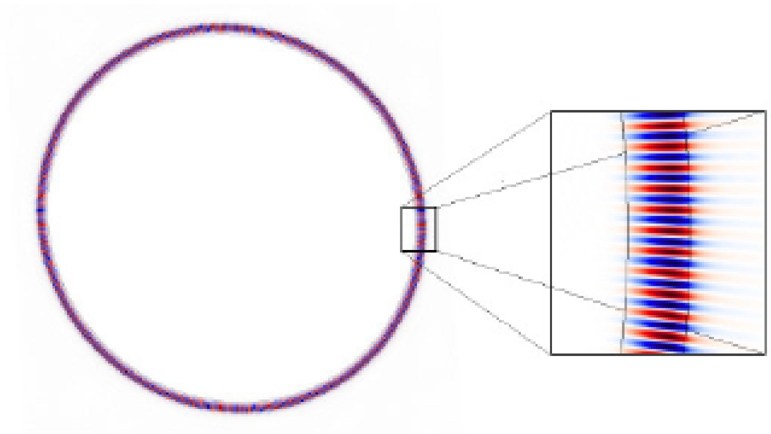




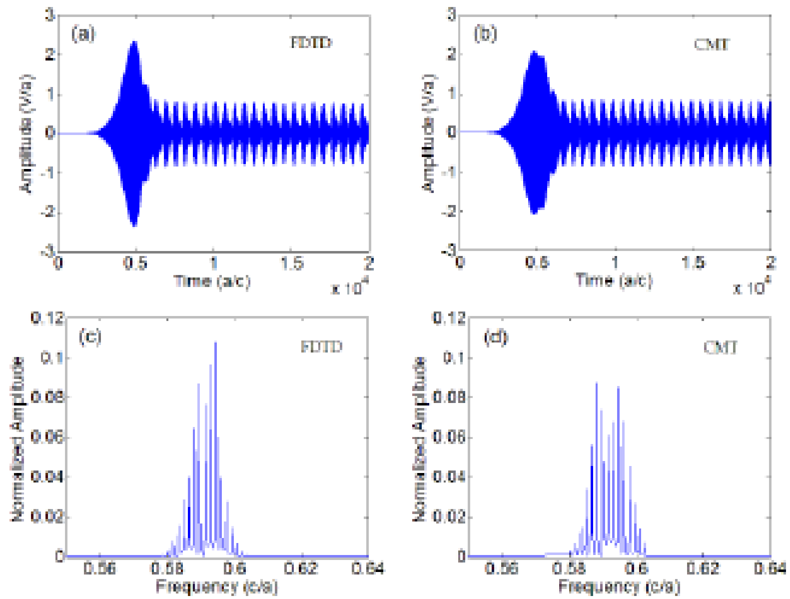
Metasurface bends light at each reflection

Complete trapping of external radiation in ultrathin layers

Optical Ring Resonators for Frequency Combs

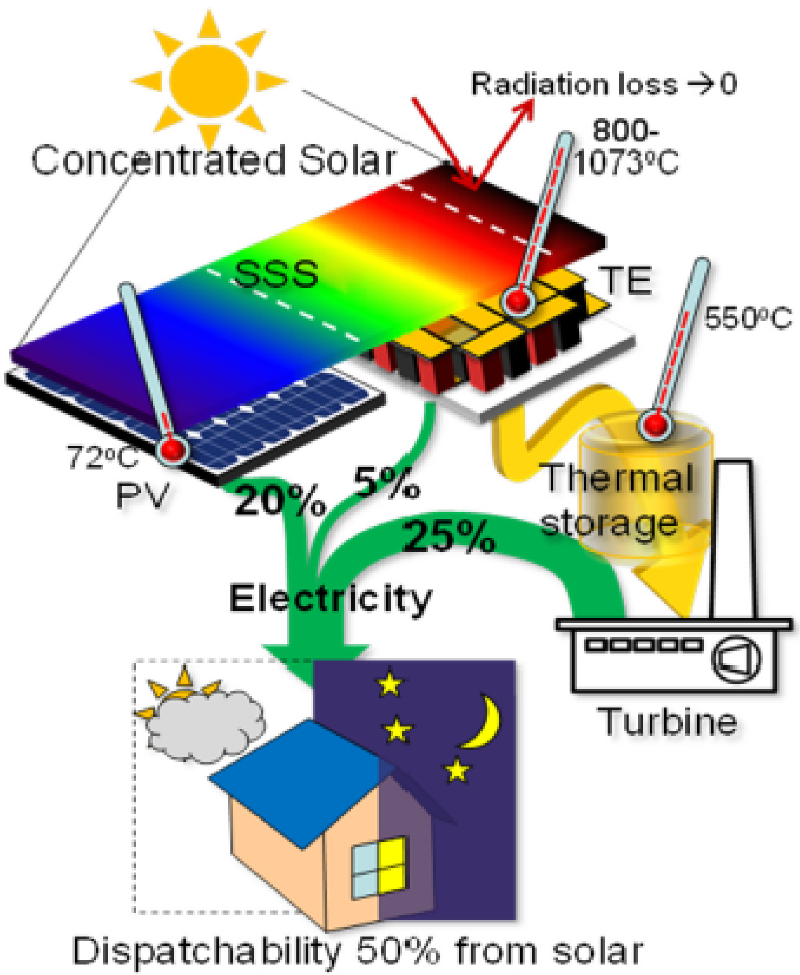


Optical ring resonator, driven by external laser

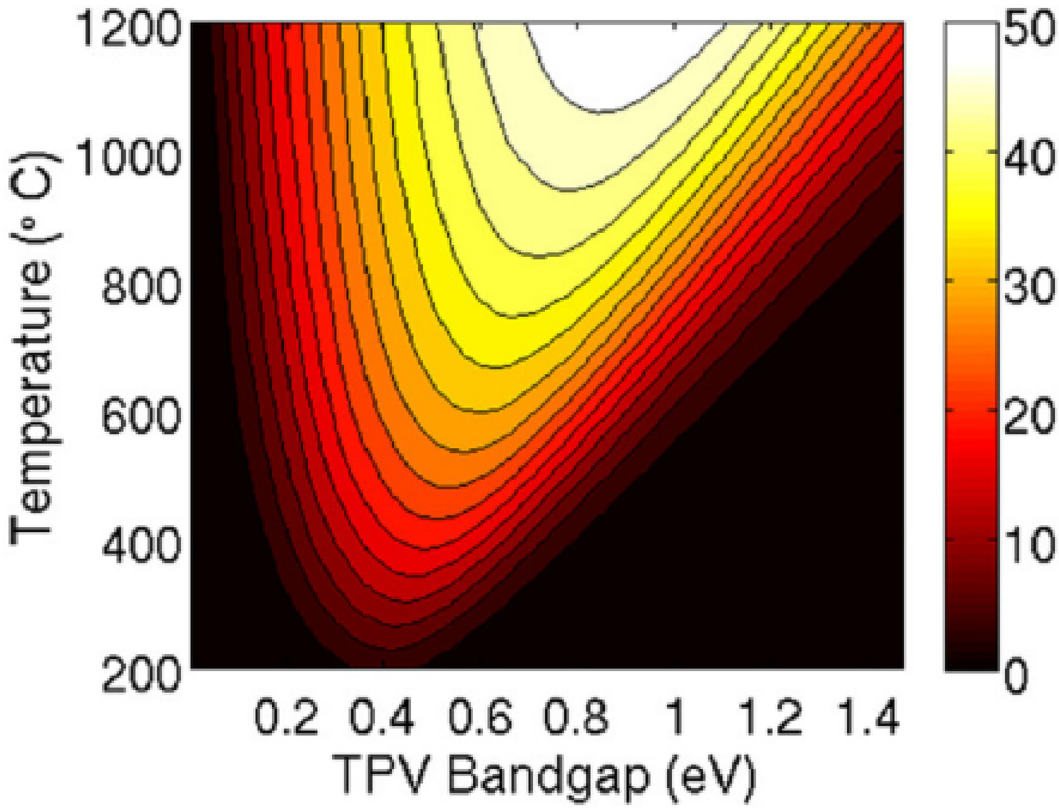


Nonlinear process creates frequency combs for arbitrary optical waveform generation

Efficient Solar PV/Thermal Conversion



TPV Converts 52%* of Heat to Electricity at Reasonable Temperatures†

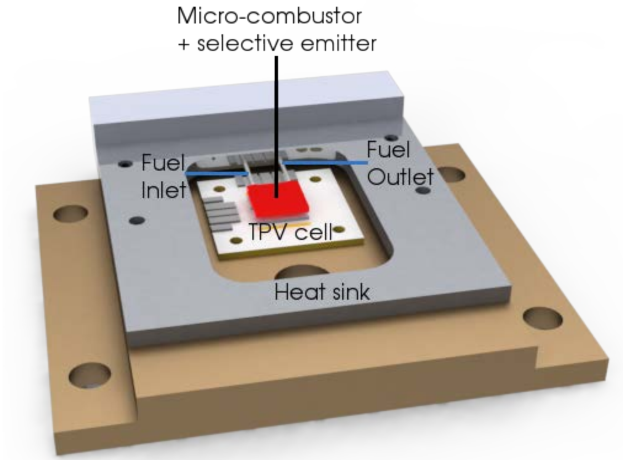


*Using highly selective emitters, with MOVPE-grown GaSb TPV cells

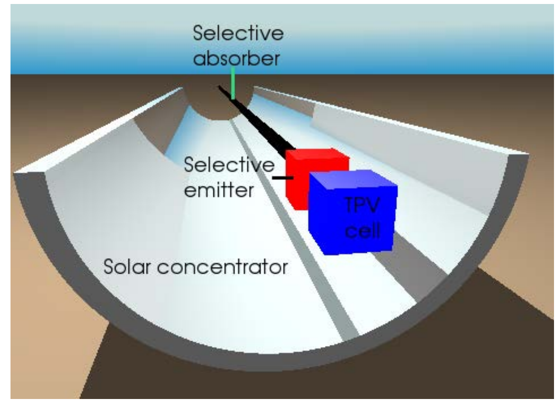
† World record η = 23% at 1050 °C

B. Wernsman *et al.*, *IEEE Trans. Electron Dev.* **51**, 512 (2004)

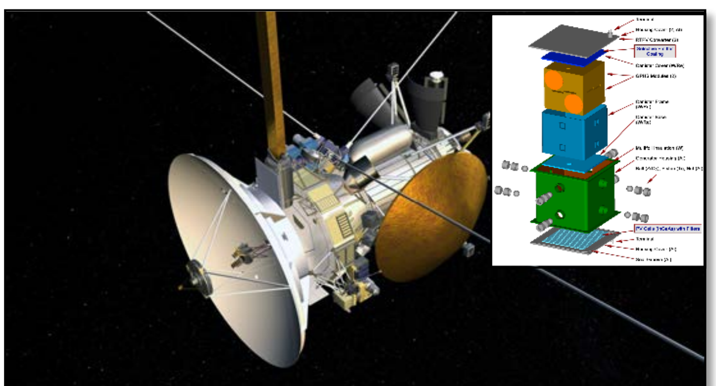
Thermophotovoltaics (TPV) Enables Unique Energy Systems



µTPV portable power generator*



Solar TPV utility scale electricity†



RTPV for long, remote missions‡

*R. Pilawa-Podgurski *et al.*, *APEC* **25**, 961 (2010); P. Bermel *et al.*, *Opt. Express* **18**, A314 (2010)

† M. Castro *et al.*, *Solar Energy Mater. Solar Cells* **92**, 1697 (2008); E. Rephaeli & S. Fan, *Opt. Express* **17**, 15145 (2009)

‡ A. Schock *et al.*, *Acta Astronaut.* **37**, 21 (1995); S.-Y. Lin *et al.*, *Appl. Phys. Lett.* **83**, 380 (2003); D. Wilt *et al.*, *AIP Conf. Proc.* **890**, 335 (2007)

Topics Covered In This Class

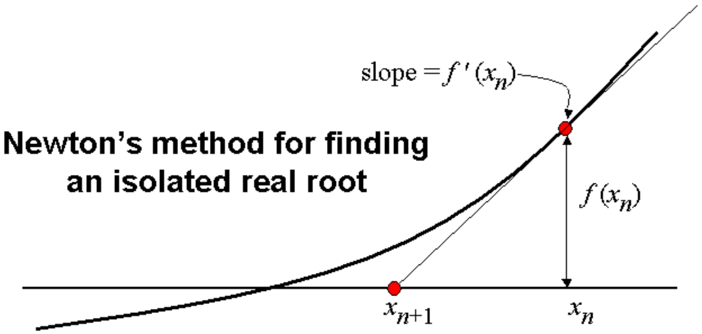
Computational Complexity

- Study of the complexity of algorithms
- Based on Turing machines
- Often, one compares algorithms for best scaling in large problems

Alan Turing (from University of Calgary Centenary event)

Finding Zeros

- Key concept: 1D bracketing
- Bisection – continuously halve intervals
- Brent's method – adds inverse quadratic interpolation
- Newton-Raphson method – uses tangent
- Laguerre's method – assume spacing of roots at a and b:

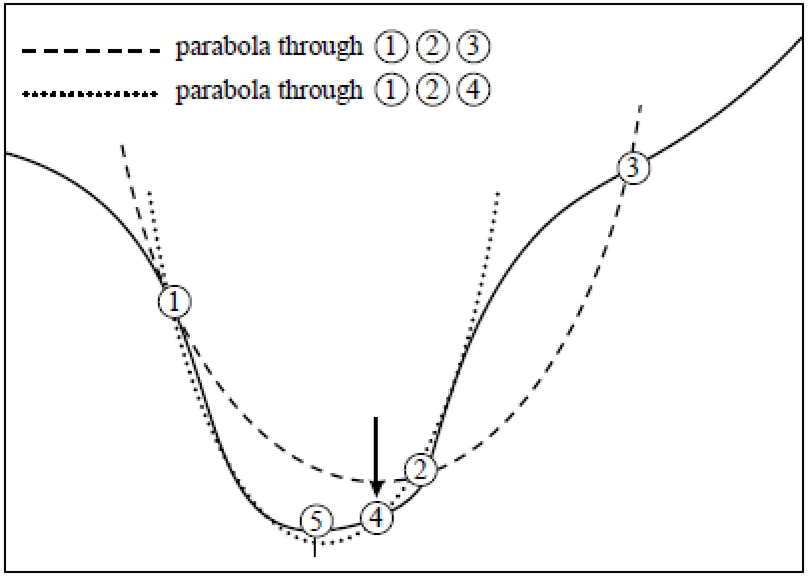


$$x_{n+1} = x_n - \frac{f'(x_n)}{f(x_n)}$$

$$a = \frac{n}{G \pm \sqrt{(n-1)(nH - G^2)}}$$

Finding Minima (or Maxima)

- Golden Section Search: local bisection
- Brent's Method: quadratic fit + fallback
- Downhill Simplex
- Conjugate gradient methods
- Multiple level, single linkage (MLSL): global, derivative



These and further images from "Numerical Recipes," by WH Press *et al*.

Eigenproblems

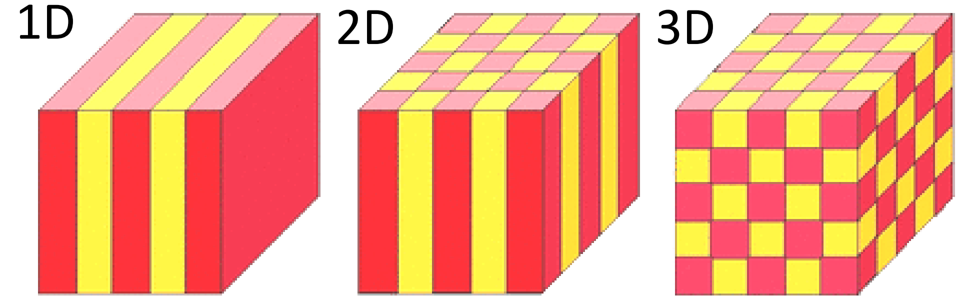
- Generalized eigenproblem: $Ax = \lambda Bx$
- Solution method will depend on properties of A and B
- Techniques have greatly varying computational complexity
- Sometimes, full solution is unnecessary

Eigenproblems

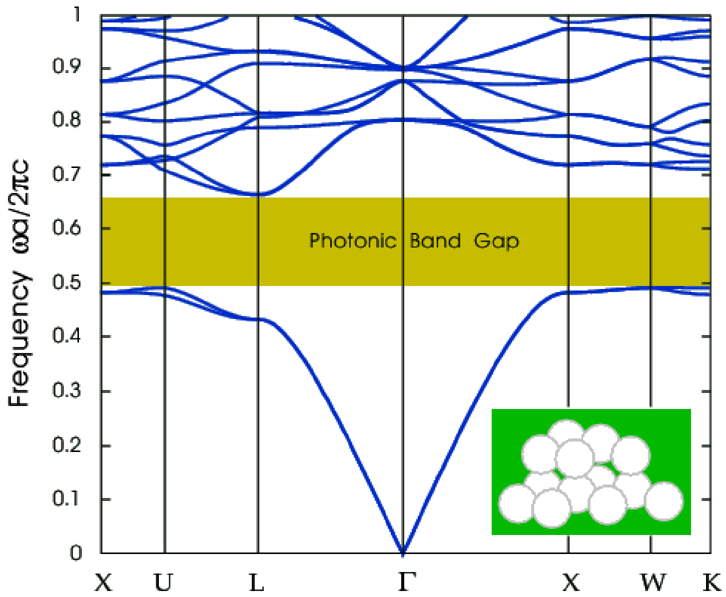
- Direct method: solve det(A-λ1)=0
- Similarity transformations: A→ $Z^{-1}AZ$
  - Atomic transformations: construct each Z explicitly
  - Factorization methods: QR and QL methods

Photonic Crystal Bandstructures

- **Periodic (crystalline) media**
  - **Periodic atoms: semiconductors with electronic bandgaps**
  - **Periodic dielectrics: photonic crystals with photonic bandgaps**
- **Many potential applications for both**



periodic crystalline structures

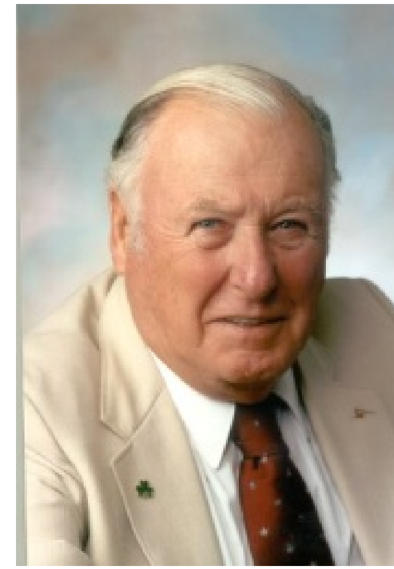


PBG for diamond structure

Joannopoulos *et al.*, *Photonic Crystals* (2008)

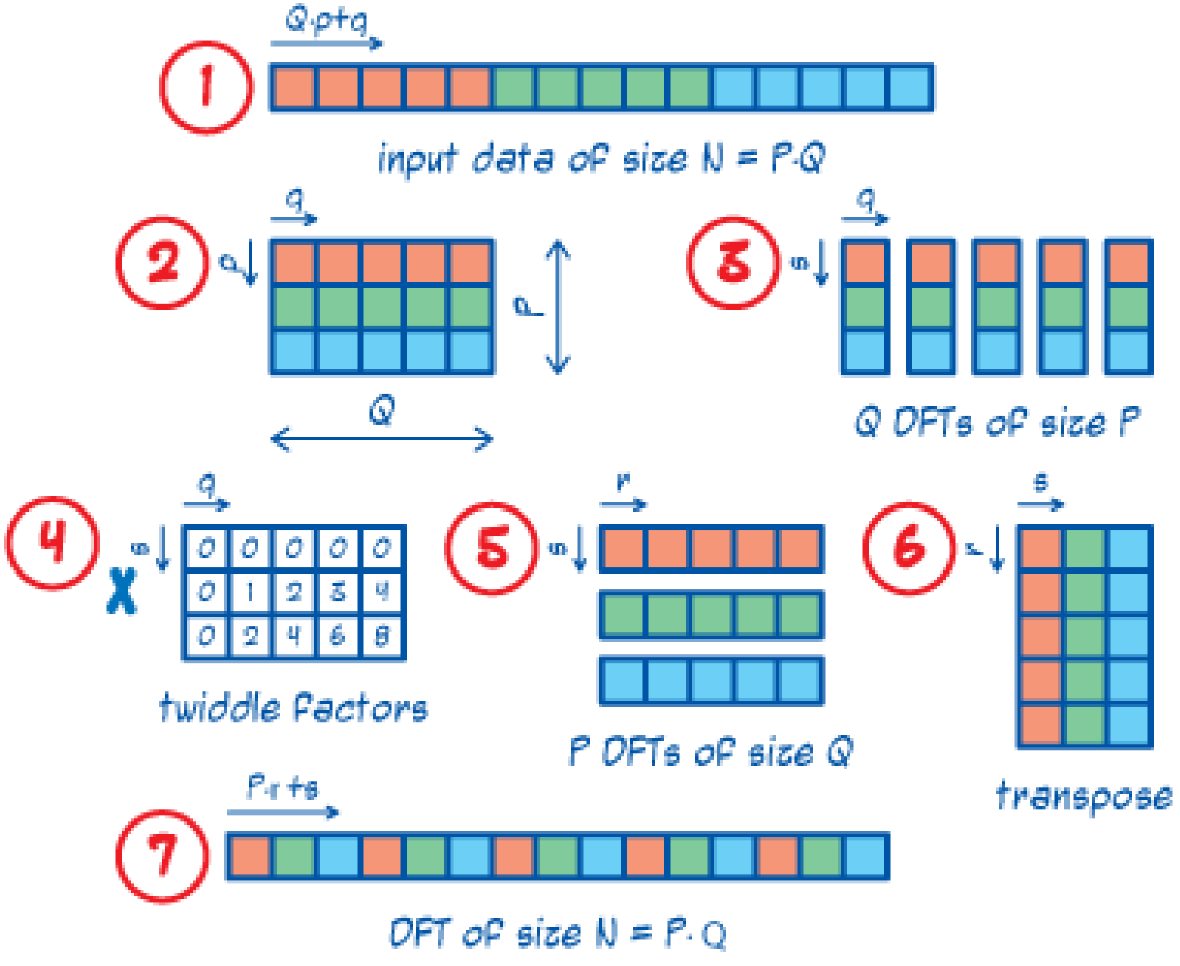
Discrete Fourier Transforms

- DFT defined by:
  $F(n) = \sum_{i=1}^{N} f(x_i) e^{-2\pi j (x_i n / x_N)}$
- Naïve approach treats each frequency individually
- Can combine operations together for significant speed-up (e.g., Cooley-Tukey algorithm)
- Specialized algorithms depending on data type



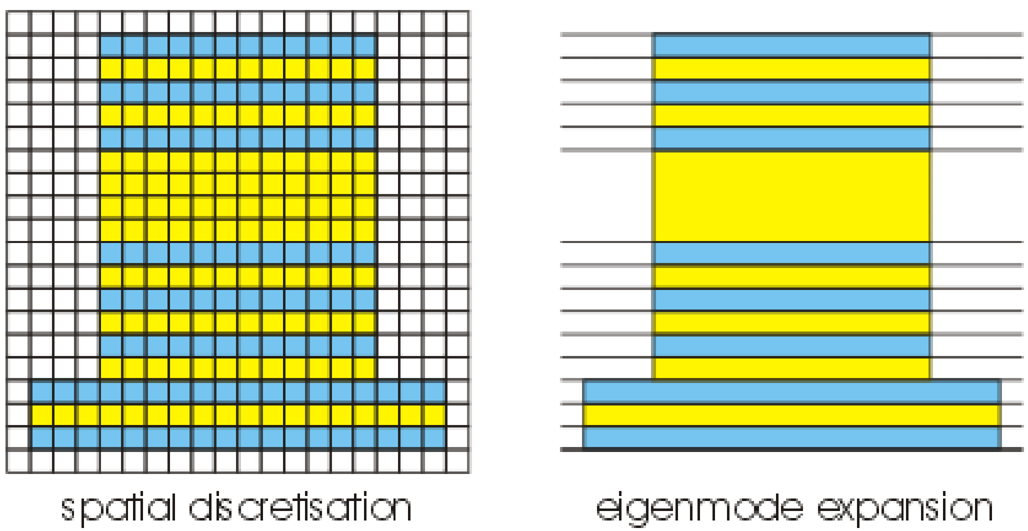
J.W. Cooley (IEEE Global History Network)

Cooley-Tukey Algorithm



Transfer Matrices and Rigorous Coupled Wave Analysis

- Divide space into layers for efficiency
- For uniform layers – transfer matrix approach
- For periodic gratings or similar in certain layers – RCWA



From the CAvity Modeling FRamework (CAMFR)

Finite-Difference Time Domain

- Discretize space and time on a Yee lattice
- "Leapfrog" time evolution of Maxwell's equations:

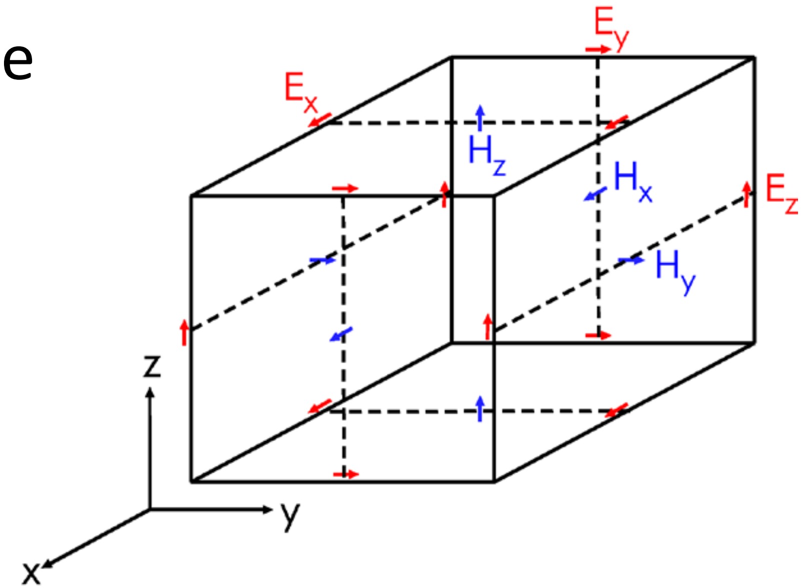
$$\frac{dB}{dt} = -\vec{\nabla} \times \vec{E} - J_B - \sigma_B B$$

$$\frac{dD}{dt} = \vec{\nabla} \times \vec{H} - \vec{J} - \sigma_D D$$

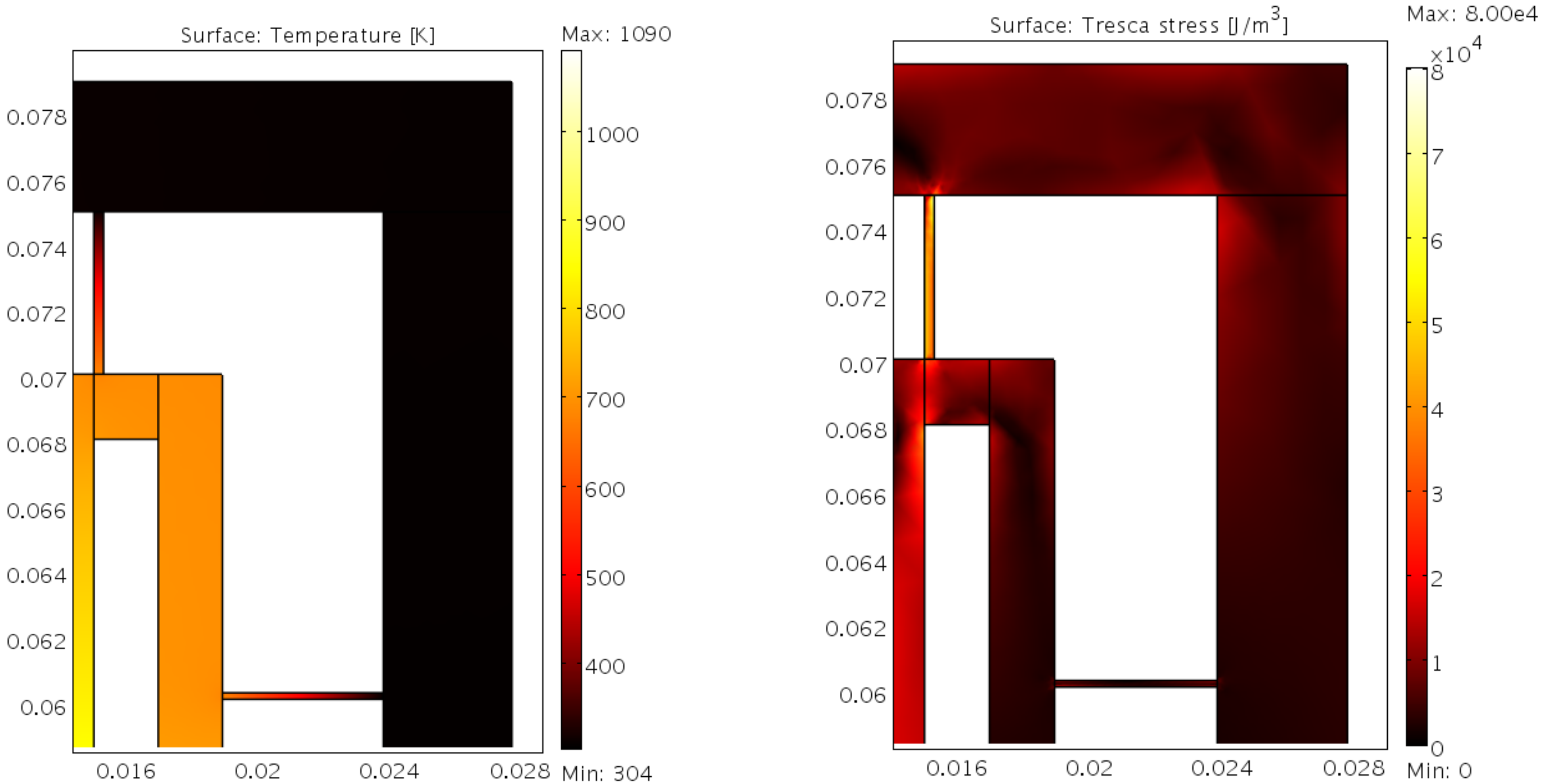
$$D = \varepsilon E$$

$$H = B / \mu$$

- Implemented in MEEP: `nanohub.org/topics/MEEP`



Finite-Element Methods

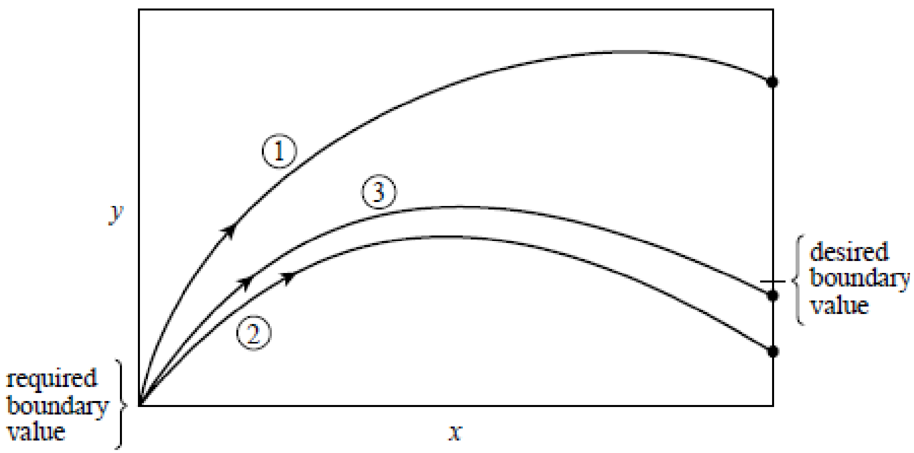


- For 2D or 3D problems, divide space into a mesh
- Solve a wide array of partial differential equations – well suited for multiphysics problems

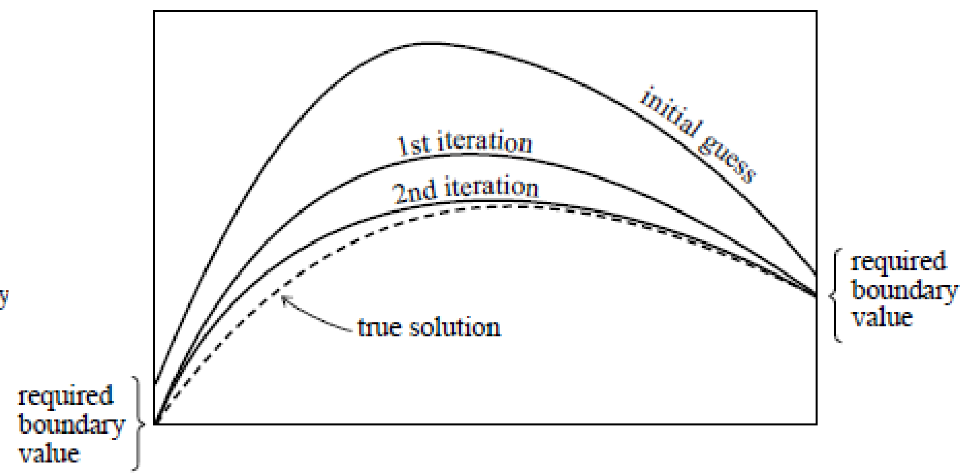
Ordinary Differential Equations

- Euler method – naïve rearrangement of ODE
- Runge-Kutta methods – match multiple Euler steps to a higher-order Taylor expansion
- Richardson extrapolation – extrapolate computed value to 0 step size
- Predictor-corrector methods – store solution to extrapolate next point, and then correct it

ODE Boundary Value Problems



Shooting Method



Boundary Value Method

Partial Differential Equations

- Classes: parabolic, hyperbolic, and elliptic

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) \qquad \frac{\partial^2 u}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2} \qquad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)$$

- Initial value vs. boundary value problems
- Finite difference
- Finite element methods
- Monte-Carlo
- Spectral
- Variational methods

Goals for This Class

- Learn/review key mathematics
- Learn widely-used numerical techniques just discussed
- Become a capable user of software utilizing these techniques
- Appreciate strengths and weaknesses of competing algorithms; learn how to evaluate the results
- Convey your research results to an audience of your new colleagues

Textbooks

– Salah Obayya, “Computational Photonics”
– JD Joannopoulos et al., “Photonic Crystals”
– WH Press *et al*., “Numerical Recipes in C”

Next Class

- Introduction to computational complexity
- Please read Chapter 1 of "Computational Complexity: A Modern Approach" by Arora & Barak