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
My Background

• All degrees in Physics
• Began with Bachelor’s at UNC: undergrad research simulating molecular electrostatics
• Continued with Master’s 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)
My Research

Key areas:

– Photovoltaics
– Thermophotovoltaics
– Nonlinear optical combs
Light Management in Photovoltaics

- **Wafer cell**
  - glass
  - silicon
  - aluminum
  - Absorbed energy
  - 200 μm

- **Si thin film**
  - Absorbed energy
  - 2 μm

- **PhC thin film**
  - Absorbed energy
  - 2 μm
Thermophotovoltaics (TPV) Enables Unique Energy Systems

µTPV portable power generator*

RTPV for long, remote missions‡

Solar TPV utility scale electricity†


Higher-Harmonic Generation (HHG) with Nonlinear Optical Combs

\[
\frac{d a_i}{d t} = -i \omega_i a_i + K_{ijkl} e^{i(\omega_k+\omega_l-\omega_i-\omega_j)t} a_j^\dagger a_k a_l
\]

Here, a high figure of merit for the resonators increase effective coupling for more efficient HHG.
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)
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
Crystal Bandstructures

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

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
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
Finite-Difference Time Domain

- Discretize space and time on a Yee lattice
- “Leapfrog” time evolution of Maxwell’s equations:

\[
\begin{align*}
\frac{d\mathbf{B}}{dt} &= -\nabla \times \mathbf{E} - J_B - \sigma_B B \\
\frac{d\mathbf{D}}{dt} &= -\nabla \times \mathbf{H} - J - \sigma_D D \\
D &= \varepsilon E \\
H &= B / \mu
\end{align*}
\]

- Implemented in MEEP: nanohub.org/topics/MEEP
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)
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
Key Policies

• Textbooks:
  – Salah Obayya, “Computational Photonics”
  – JD Joannopoulos et al., “Photonic Crystals”

• Communication:
  – nanoHUB group: [https://nanohub.org/groups/ece595](https://nanohub.org/groups/ece595)
  – Email: pbermel@purdue.edu

• Full list of policies given on handout; also available under Syllabus on Blackboard
Quizzes

• Will periodically ask questions online about the lecture
• Should be after videos are posted
• No trick questions – just designed to make sure you’re keeping up with the material
Class Participation

• Your attendance is important
• Will be grading your involvement, enthusiasm, and respect for your peers in the class
• **Not** grading your percentage of correct answers during class
Homework

- Homework is essential to learn the material
- 8 total homework assignments this semester, once every other week
  - First one will be available Jan. 11, due Jan. 18
  - Two weeks in a row before Spring Break
- Due at 4:30 pm on the listed dates to pbermel@purdue.edu
Final Project

• Chance for you to teach the rest of the class about a numerical computing topic that interests you!
• OK to pick something related to your research as long as it’s new
• I can suggest topics if you’re not sure what to do
• Can ask peers for general advice but all details and presentations should be done by you
Grading

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<th>Grading Item</th>
<th>Points</th>
<th>Date</th>
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<tbody>
<tr>
<td>Quizzes</td>
<td>100</td>
<td>Various</td>
</tr>
<tr>
<td>Class Participation</td>
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<td>All Semester</td>
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<tr>
<td>Homework</td>
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<td>Every Other Week</td>
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<tr>
<td>Final Project</td>
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<td>End of Semester</td>
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<tr>
<td><strong>TOTAL</strong></td>
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<td></td>
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- Numerical grades of 60% or above will pass
- Roughly speaking: A’s will be 90% +; B’s 80-89%; C’s 70-79%
- Final letter grades will be assigned at my discretion
Next Class

• Discussion of specific goals for numerical computing

• Please read Obayya, Chapter 1