ECE 595, Section 10
Numerical Simulations
Lecture 1: Introduction to Numerical Simulations

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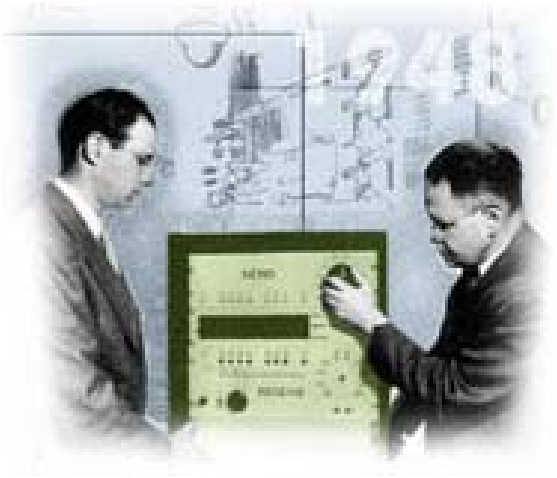
January 7, 2013

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

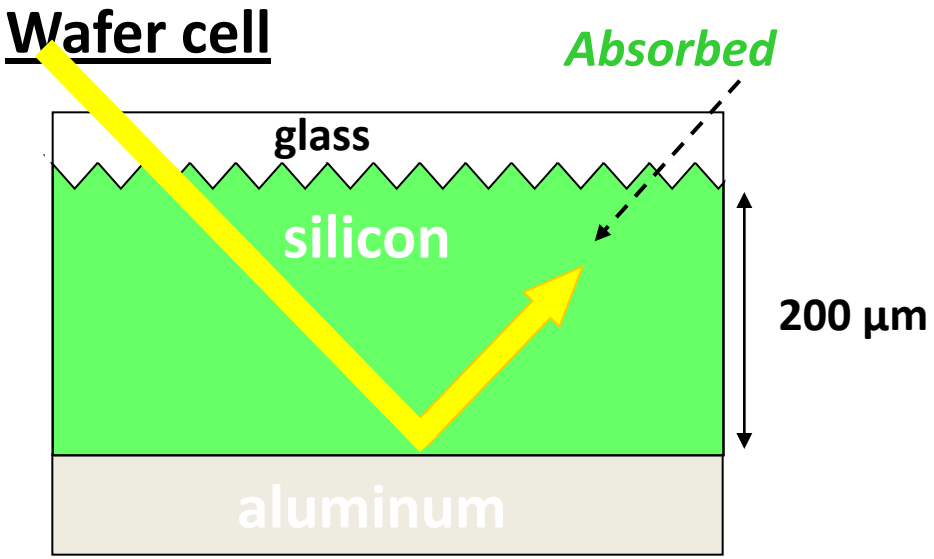
- All degrees in Physics
- Began with Bachelor's at UNC: undergrad research simulating molecular electrostatics
- Continued with Master's at Cambridge University: linear photonic bandstructures
- Completed Ph.D. at MIT on active materials in photonic crystals (Advisor: JD Joannopoulos)
- Continued with postdoc on applications in photovoltaics & thermophotovoltaics (Advisor: M Soljacic)

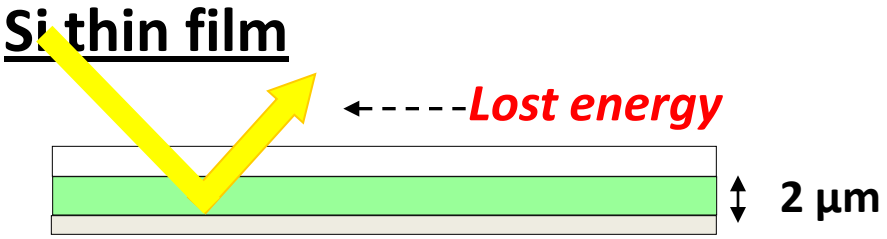
My Research

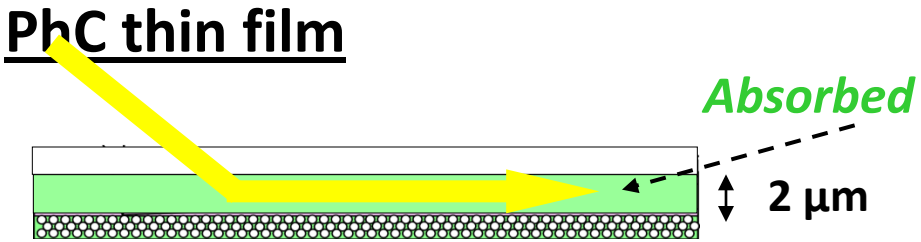
Key areas:

- Photovoltaics
- Thermophotovoltaics
- Nonlinear optical combs

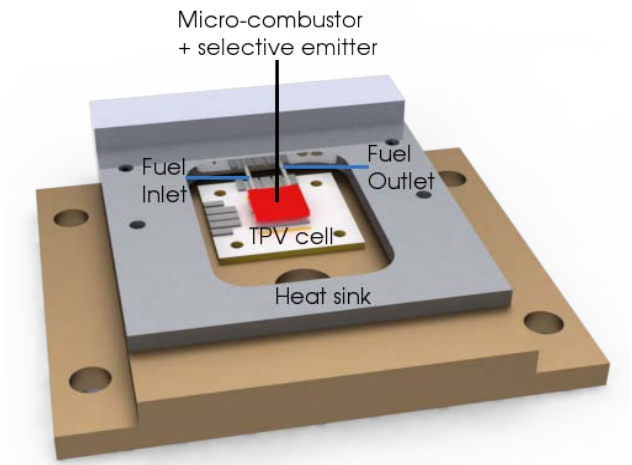
Light Management in Photovoltaics



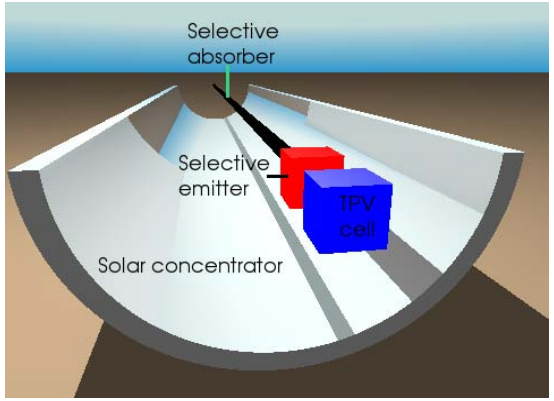




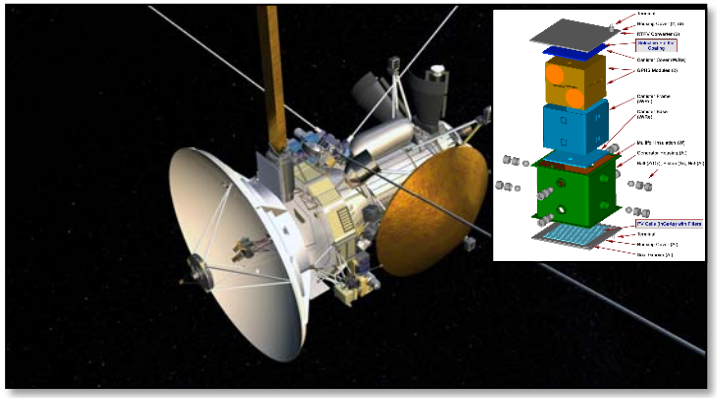
Thermophotovoltaics (TPV) Enables Unique Energy Systems



μTPV portable power generator*



Solar TPV utility scale electricity†



RTPV for long, remote missions‡

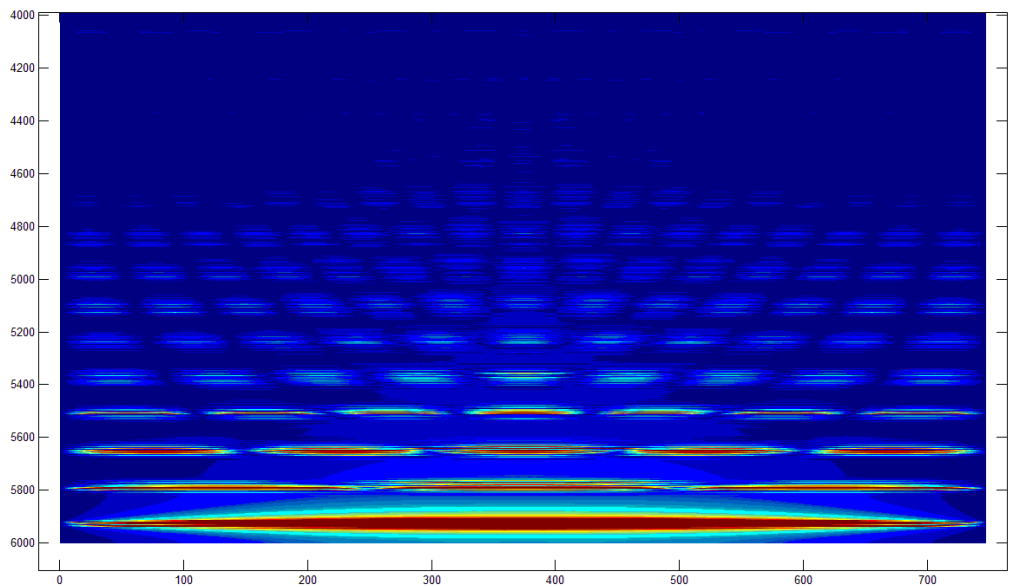
*R. Pilawa-Podgurski *et al.*, *APEC* **25**, 961 (2010); P. Bermel *et al.*, *Opt. Express* **18**, A314 (2010)

† 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)

Higher-Harmonic Generation (HHG) with Nonlinear Optical Combs

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



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)

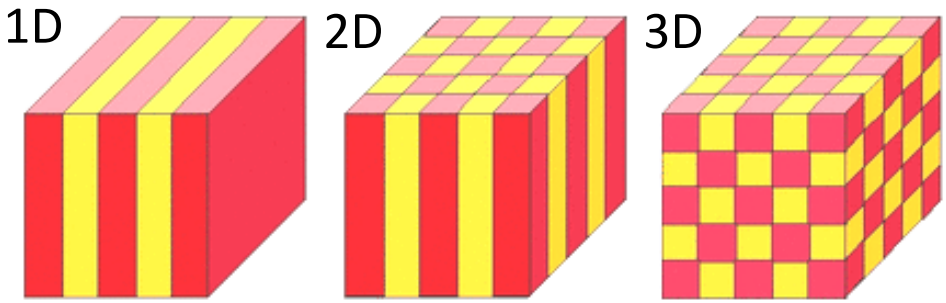
Eigenproblems

- 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

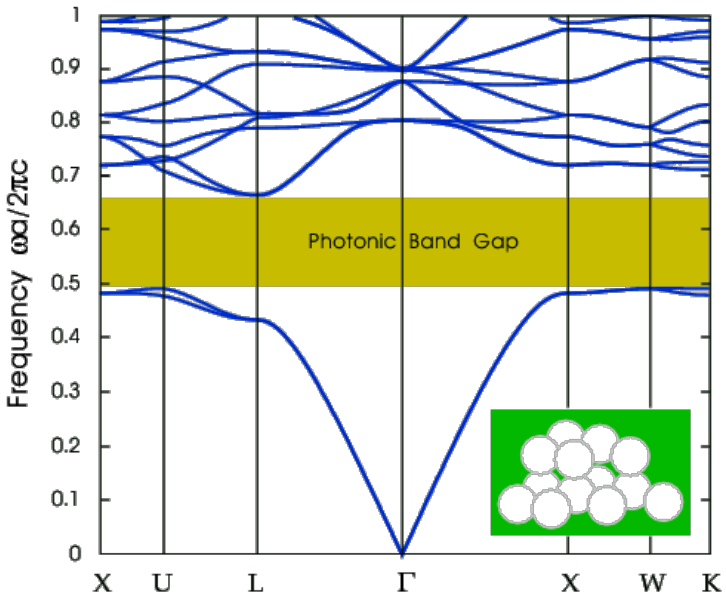
Crystal Bandstructures

- **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)



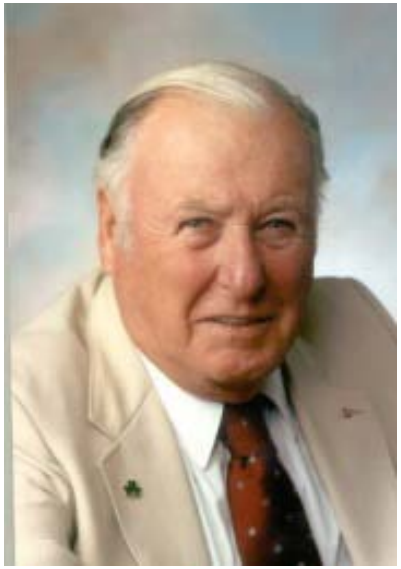
periodic crystalline structures



PBG for diamond structure

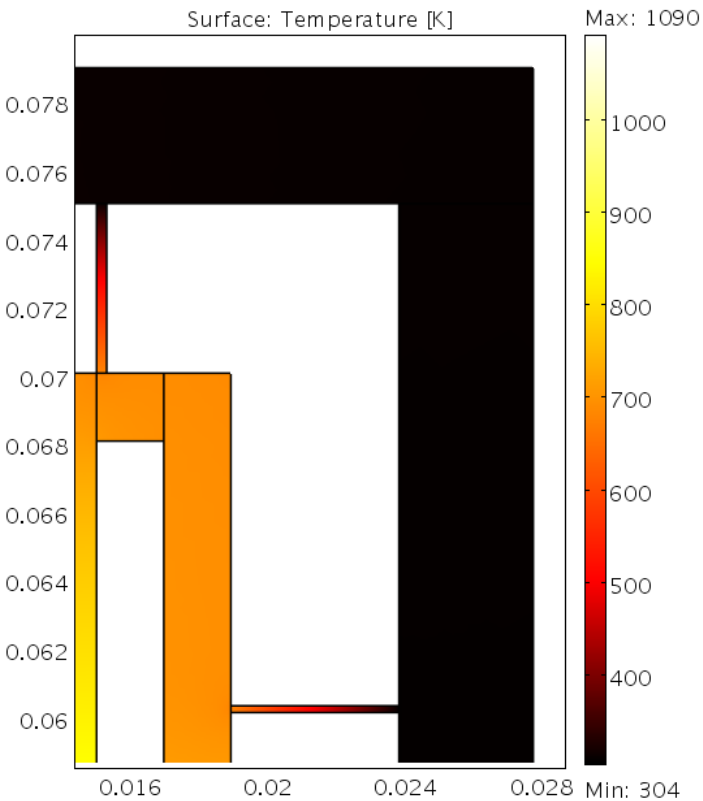
Discrete Fourier Transforms

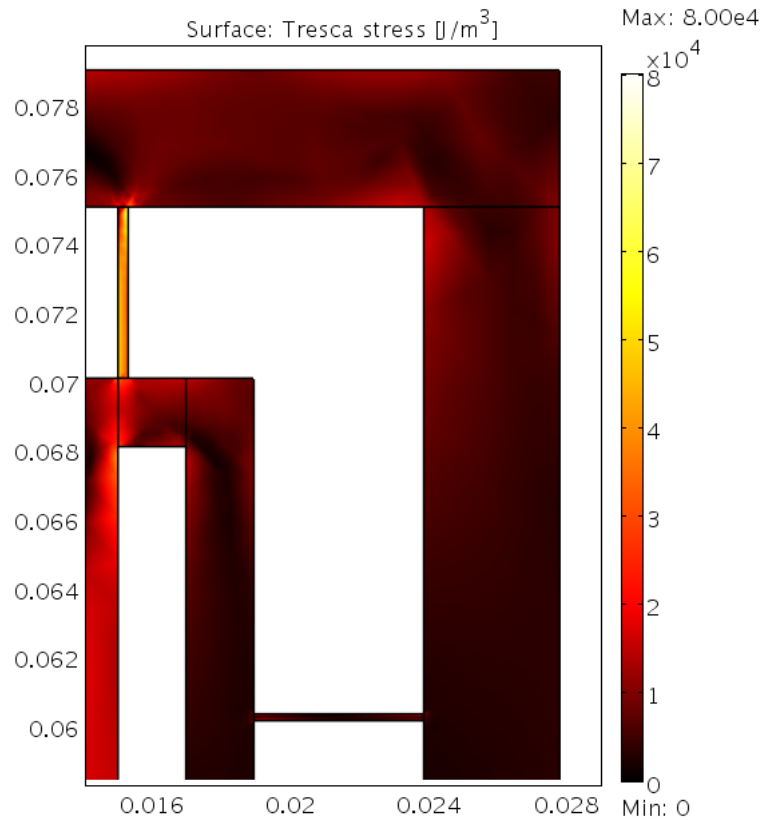
- DFT defined by:
  $F(n) = \sum_{i=1}^{N} f(x_i) e^{-2\pi j (x_i n / x_N)}$
- Naïve approach treats each frequency individually
- Can combine operations together for significant speed-up (e.g., Cooley-Tukey algorithm)
- Specialized algorithms depending on data type



J.W. Cooley (IEEE Global History Network)

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:

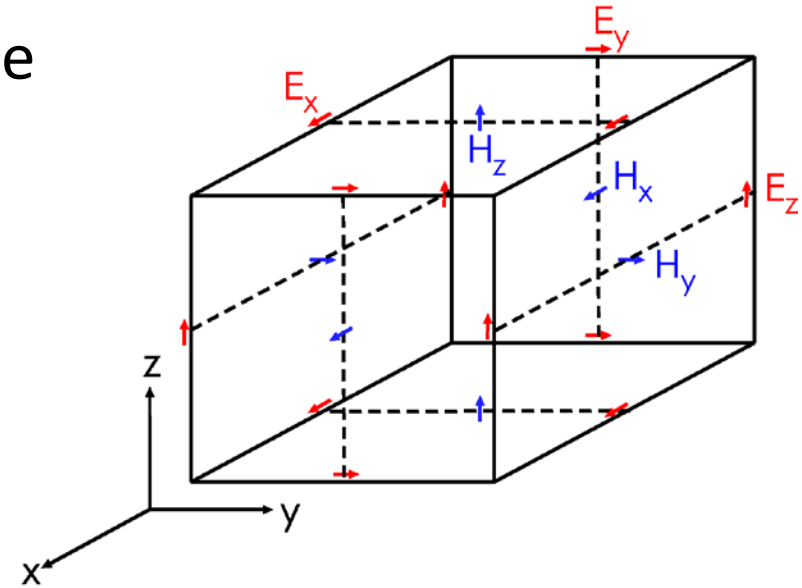
$$\frac{dB}{dt} = -\vec{\nabla} \times \vec{E} - J_B - \sigma_B B$$

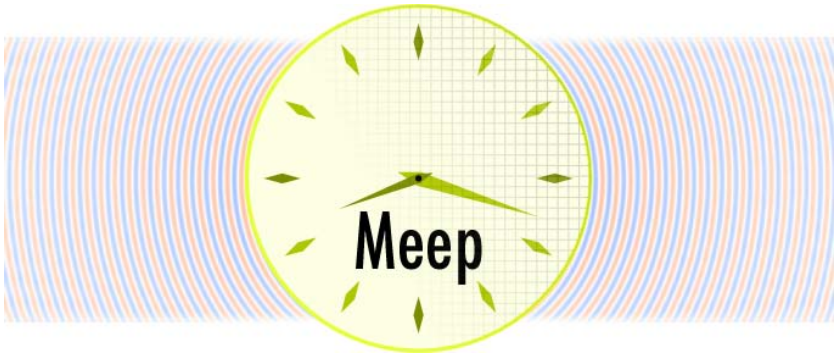
$$\frac{dD}{dt} = \vec{\nabla} \times \vec{H} - \vec{J} - \sigma_D D$$

$$D = \varepsilon E$$

$$H = B / \mu$$

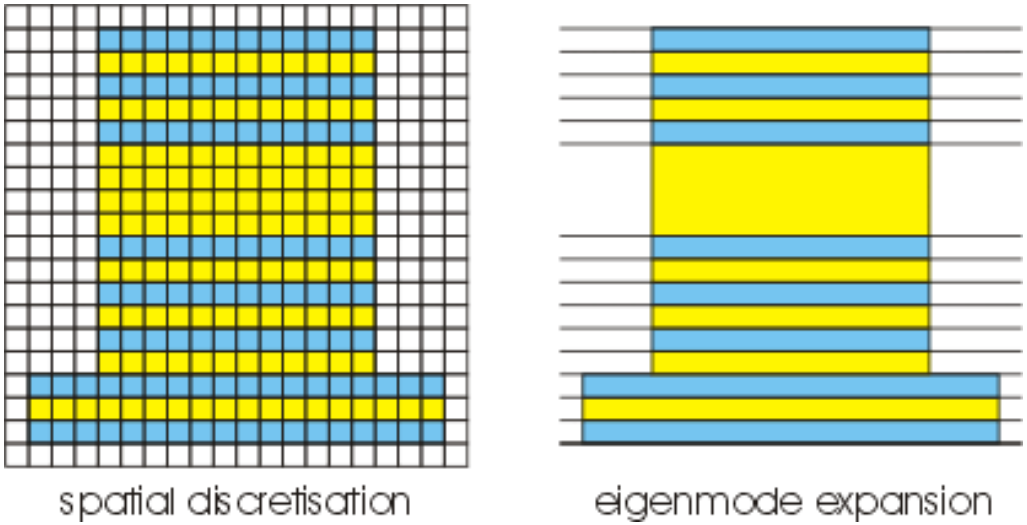
- Implemented in MEEP: `nanohub.org/topics/MEEP`





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:
  - Course website: http://web.ics.purdue.edu/~pbermel/ece595/
  - nanoHUB group: 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 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

Grading Item	Points	Date
Quizzes	100	Various
Class Participation	100	All Semester
Homework	100	Every Other Week
Final Project	200	End of Semester
TOTAL	500	

- 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