Project

• Teams of 2 to 4 students (unless PhD student with own project)
• Computer module provided for your “application”
• You will compare GA, SA, TS and your own improvements in these algorithms
• Later lectures will discuss how to do comparisons
• Written Report
• Short Oral Presentaton
Project Topics Discussed in Lecture

- **Satisfiability Testing for Artificial Intelligence**: Prof. Bart Selman, Computer Science (Sept. 21)
- **Resource Allocation in Cellular Networks**: Prof. Steve Wicker, Electrical Engineering (Sept. 14)
- **Optimal Control of Finite Element Systems with Environmental Applications**: Prof. Christine Shoemaker, Civil and Environ. Engin. (today)
- **Protein Folding**: Molecular and Cell Biology (discussed briefly today)

• None of these topics require prior background beyond what you hear in lecture.
Project on Protein Folding:
Importance of Optimization for Protein Folding

• This is an important scientific problem because understanding the conformation for a protein helps scientists understand the characteristics of the protein and helps predict how the protein will interact with other substances.

• You are using the optimization to determine the angles in the conformations.
Code for Conformations in Protein Folding

• You do not need to have a background in this area for this project since you are given a MATLAB code.

• Once you obtain the best solution using heuristic search for this problem you will get a “picture” of the protein solution (e.g. the minimal energy conformation as defined by the 9 dimensional optimal solution vector)
Protein Folding

- Proteins, you may remember from an undergraduate biology or chemistry class, consist of a sequence of amino acids.
- They have three-dimensional structures (referred to as conformations) that are determined by complex inter-atomic forces.
- Your task is to find the minimal energy conformation of the dipeptide 2-alanine by searching the conformation space defined by nine distinct torsion angles.
ORIE Related Project 1 - Line Balancing

- Manufacturing Line Balancing with Changovers  
  – (Meeting with Dr. Caggiano, 4:30 Monday Sept. 26)

- Send email to me <cas12> by Friday Sept. 23. Project will be cancelled unless enough people respond for at least one team by Sept. 23.

- This project does not require prior background as long as you attend the meeting with Dr. Caggiano or can show you have prior background.

- Description will be posted by this afternoon.
ORIE Related Projects with background required (continued)

- ORIE Project 2: Job Shop Scheduling – requires a team member with a background in job shop scheduling (description posted).

- ORIE Project 3 Financial Engineering—requires team member with background in the area of the project. (description will be posted by Tues. AM)
Similarity of Multiple Projects

• All the projects focus on your application of three heuristic algorithms plus your own variations to a specific problem and to compare the results statistically.

• All of the projects are expected to be equal in difficulty and require a report.

• Each student is free to pick any of the presented projects independent of major or the course number under which you are registered (e.g. a Mech. Engr. Major who registered for ORIE 5340 can do the Satisfiability project)
Purpose of Having Multiple Projects

• The purpose of having multiple projects is:

  – To allow students to work on a problem that is of interest to them

  – To illustrate how flexible these algorithms are to deal with a wide range of problems.
General Project Instructions

• We have posted the general instructions for the projects, which includes all the deadlines.
• We have posted the individual projects for
  – Cellular networks
  – Satisfiability
  – Models of Partial differential equations with environmental example
  – Job Shop Scheduling
  – Protein Folding (computational biochemistry)
• Be sure to attend Prof. Selman’s lecture this Wednesday on heuristic optimization in satisfiability problems arising in artificial intelligence.
Project on Optimization of Partial Differential Equations (PDE)

I will now talk about the course project on heuristics and partial differential equations.

The specific project application is environmental, but the use with PDE’s is general to a wide variety of problems in engineering and science.
Project Topic: Optimization of Systems Described by Partial Differential Equations (PDEs)

• Partial Differential Equations arise in many areas, especially in engineering systems.
• Typically we have a variable \( c(x,y,z,t) \) where \((x,y,z)\) are coordinates in space and \( t \) is time. In many cases \( c \) is itself a vector with many components so the variables are \( c_j(x,y,z,t) \), where \( j=1, \ldots, n \).

handout 9-19-11
Models Involving Partial Differential Equations Arise in Many Areas of Science and Engineering

As a result there are many texts like this.

So descriptions of solid and fluid Mechanics, chemical reactions, Economic systems, ecological systems, medical systems, etc. are often all described by Partial differential equations.
Examples of Systems described by PDE’s for which optimization is important

- **Aerospace**—How do you design an airplane so that you minimize cost (construction and operating cost including fuel and maintenance over the many years of operation).
- **Medical Engineering**—How do you design a joint replacement (e.g. hip joint) that will give satisfactory performance, last a long time, and not be extraordinarily expensive?
- **Structures**—How do you design a structure to minimize the cost for construction (labor and materials) so that it can withstand earthquakes?
Partial Differential Equations in Mathematical Biology

Governing Equations

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \partial((0.5)\frac{\partial u}{\partial x})/\partial x + (1/(1+u^2)) \\
\frac{\partial v}{\partial t} &= \partial((0.5)\frac{\partial v}{\partial x})/\partial x + (1/(1+v^2))
\end{align*}
\]

Initial Conditions

\[
\begin{align*}
u(0, x) &= 1+0.5*cos(2*pi*x) \\
v(0, x) &= 1-0.5*cos(2*pi*x)
\end{align*}
\]

Boundary Conditions 1 (x = 0)

\[
\begin{align*}
-\frac{\partial u}{\partial x} &= 0 \\
-\frac{\partial v}{\partial x} &= 0
\end{align*}
\]
Examples of Systems described by PDE’s for which optimization is important (continued)

• Chemical Engineering—If you have a biochemical reactor, how should you control its environment to maximize profit that is based on the reactor’s product (which might for example be an expensive drug)

• Environmental Engineering—How do I clean up a contaminated area at the least cost and with the least risk of endangering the public or the ecosystem? (This applies to rivers, lakes, atmospheric pollution as well as to the groundwater problem that we will discuss today.)
PDE’s Arising in Climate Models (that require optimization for parameter estimation)

\[ m\ddot{x} = -\frac{dV}{dx} + f_b(t) + \left[ x(0)\beta C_b(t) - x(t)\beta C_b(0) \right] - \int_0^t \beta C_b(t - t')\dot{x}(t')dt' \]

\[ \frac{\partial f}{\partial t} = -\sum_{i=1}^N \frac{\partial}{\partial x_i} \left[ D_i^1(x_1, \ldots, x_N)f \right] + \sum_{i=1}^N \sum_{j=1}^N \frac{\partial^2}{\partial x_i \partial x_j} \left[ D_{ij}^2(x_1, \ldots, x_N)f \right] \]
Groundwater Optimization

• The project involves optimization of the management of groundwater.

• Groundwater is hard to manage because you cannot see it so we use models to try to predict its behavior.

• Groundwater is a MAJOR source of drinking and irrigation water around the world so its management is very important.
Groundwater Sources and Sinks

- Evaporation
- Condensation
- Precipitation
- Transpiration
- Recharge
- Runoff
- Water table
- Unconfined aquifer
- Confined aquifer
- Impermeable layer

Aquifer - Porous medium that can contain water
Groundwater Aquifers can be large-
This area is 100,000 square miles

The Floridan aquifer system is one of the most productive aquifers in the world. This aquifer system underlies an area of about 100,000 square miles, and it provides water for several large cities, including Savannah and Brunswick in Georgia and Jacksonville, Tallahassee, Orlando, and St. Petersburg in Florida.
Groundwater is Affected by Pumping and by Contamination

Water pumping draws down the water surface and causes flow toward the lower surface.
Groundwater contamination from waste disposal site

Waste disposal site

Recharge area

Water table

Water supply wells

Contaminated groundwater

Pumping things exacerbated by drawing out the contaminated water.

Historically, we did not regulate wastes.
Example Partial Differential Equations (PDE) (groundwater contamination example)

- Flow
  \[
  \nabla \cdot (K \cdot \nabla h) = Q
  \]
  \[
  v = -\frac{K}{\theta} \cdot \nabla h
  \]

- Contaminant
  \[
  \frac{\partial c}{\partial t} - \nabla \cdot (D \cdot \nabla c - v \cdot c) - Q \cdot (c - c_0) = 0
  \]

Q: sink term (pumping well) → how much pumping do I want to do?

h: hydraulic head

K: hydraulic conductivity

v: the pore water velocity

D: the hydrodynamic dispersion

θ: The effective porosity

c₀: concentration of recharge

c(t): contamination concentration

K, D, and θ are model parameters

h, v, and c are dependent variables computed by the PDEs
Solving the PDE as Input to Optimization

• **Understanding the System**
  
  The solutions to the partial differential equations (PDE) can then tell us the value of $c_j(x,y,z,t)$, where $j=1, \ldots,n$.
  
  However, it is usually not possible to solve the complex system of PDEs analytically, so they must be solved numerically using approximation methods.

• **Numerical Solutions**
  
  You are given the mathematical expressions for PDE’s e.g.
  
  You **discretize** your problem (over $x,y,z,$ and $t$). This results a system of **matrix equations**.
Solving PDEs

- **Finite Difference Methods**
- **Finite Element Methods**
- These methods divide space in a grid (next slide)

Implementation of these methods requires complex codes that solve all the matrix equations iteratively (perhaps thousands of times) for each simulation of the model.

- Simulation times require typically minutes to days for one simulation.

- As a result the value of the optimization method is measured by its ability to find a good solution (perhaps not truly OPTIMAL) with a limited number of simulations since you cannot afford to do a very large number of simulations.
Example of Grid for Finite Difference Solution of PDEs for Groundwater Contamination Problem


Numbers are initial contaminant concentration
Derivative versus Non-Derivative methods for PDE systems

- PDE’s contain derivatives, but the derivatives you want for optimization are derivatives of the objective function with respect to the decision variables, which are not given directly by the basic PDE equations.
- It is hard or impossible to compute the derivatives for optimization for complex simulation model for nonlinear PDE’s.
- Hence, there is a big advantage for using derivative-free optimization methods like heuristics.
- The disadvantage of many heuristic methods is that they require many simulations.
Optimization for Calibration

• The Partial Differential Equations contain parameters.
• Typically you have some data on your system that the PED’s are trying to solve.
• You usually want to estimate parameter values (that can’t be measured directly) by adjusting (calibrating) the parameters so that the error between model prediction and data is minimized.
• Optimization can be used for minimization.
• This is process is called “calibration” or “parameter estimation” or “solving the inverse problem”.
Optimization for Obtaining the Best Design

- Another way PDE models are used is to evaluate the effect of changes in the way a “system” is designed (e.g. length of an airplane’s wings) or operated (e.g. how do I operate groundwater pumps to clean up toxic groundwater).

- Given a COST(S) function that describes how one alternative is better than another (e.g. in terms of cost or income), then optimization can be used to search among various alternatives to find the one that minimizes the COST(S) function.
Environmental Engineering Problem

- So now to illustrate the PDE problem I will discuss several of my research project on applications of optimization methods to groundwater remediation.
- Carbon Sequestration Plume Estimation (calibration)
- Groundwater Model for Beijing Water Supply (calibration)
- Groundwater Remediation (detoxification) (optimal design problem)
Carbon sequestration example

- Carbon sequestration: storage of super critical carbon dioxide in geological formations
CO2 Sequestration Plume Estimation Calibration Example

• Carbon can be captured from coal plants and injected into the deep subsurface, where it is expected to remain.

• To make sure the system is working properly and Carbon is not leaking from deep subsurface, we want to predict the location of the CO2 “plume” and its pressure.

• Serious environmental and economic issues will arise if the system is not working properly so plume estimation is very important.
CO2 Sequestration Plume Estimation

• Because it is so deep in the surface, monitoring wells are expensive so there is little data.
• We can model the fluid mechanics of injected CO2 with partial differential equations.
• Then we use the optimization to pick the model parameters that minimize the error between model predictions and the data (e.g. model calibration)
Results from our research (with Espinet).

The figure on the left is the “true” CO2 Plume. The figure on the right is the plume predicted by the PDE equations, with model parameters selected by optimization to calibrate.

In the real world there is no way to know the true plume. We have only the calibrated one!
Optimization Applications to PDE Systems Related to Water

Many Applications of fluid mechanics PDEs for Surface Water including contamination
PDEs also important for subsurface Problems: Application to Groundwater Aquifer around Beijing

Elements are triangular. Color for different rock material.
Cross section of depth underneath Groundwater Repeated Slide
Optimization Algorithm Comparison on Groundwater Model

DDS is best Algorithm
Importance of Beijing Aquifer Study

- This groundwater aquifer is a major supply of drinking water for millions of people in Beijing.
- There is currently a water shortage so water pumping must be carefully done.
- The calibrated model can be used to understand the spatial relationship between water pumping, water table height, and available water supply under different weather and climate conditions.
Introduction to Groundwater Remediation
(Application in your project)

• Groundwater Remediation (= cleaning contaminated groundwater) is a very expensive problem in US.

• Optimization can provide a valuable tool to help identify cost effective solutions to groundwater contamination problem.

• Detoxifying Contaminated Groundwater will cost hundreds of billions dollars.

• Current estimate is $250 Billion to $1000 Billion to decontaminate existing sites.

• The clean up will continue for decades.
Pump and Treat Groundwater Decontamination

- The engineer can decide where to locate wells and time varying pumping rates
- The computational difficulty of finding an optimal policy is much greater if the pumping rates are time-varying than for time-invariant pumping optimization.
- A less expensive clean up policy can be identified if pumping rates are allowed to change over time.
Example Partial Differential Equations (groundwater contamination example)

• Flow

\[ \nabla \cdot (K \cdot \nabla h) = Q \]

\[ v = -\frac{K}{\theta} \cdot \nabla h \]

• Contaminant

\[ \frac{\partial c}{\partial t} - \nabla \cdot (D \cdot \nabla c - v \cdot c) - Q \cdot (c - c_0) = 0 \]

Q: sink term (pumping well)
K: hydraulic conductivity
D: the hydrodynamic dispersion
\( c_0 \): concentration of recharge

h: hydraulic head
v: the pore water velocity
\( \theta \): The effective porosity
The optimization goal is to figure out how much water to pump from each well in each time period to minimize the total cost of getting the contamination below an EPA standard.

The pictures show you the movement of the contamination plume give the optimal pumping rates.

a.
• Pumping reduces the pressure (called “hydraulic head” at the pumping point.
• Water flows from a high hydraulic head area to a low hydraulic head area.
• The movement of contaminant is computed by substituting the optimal pumping policy into the system of PDE’s that describe “hydraulic head” and the contaminant movement in response to pumping.
Summary Optimization of PDE’s

• Optimization of PDE’s is a very important area of both research and engineering practice.
• Heuristic optimization is most helpful if the equations are nonlinear
• Computationally feasibility is an issue for PDE’s since each evaluation of the cost function can take a long time.