CEE 557
GROUNDWATER MODELING

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Time: MW 1600-1750

Location:

2015 Civil & Envir Eng Bldg

Course Description

In this course, we will learn how to: (a) construct physics-based mathematical models of fluid flow and mass transport in groundwater and surface water systems; (b) develop algorithms to solve the models using a variety of numerical approximation and physics-informed machine learning methods; (c) understand and analyze numerical errors in different methods; and (d) write computer programs to obtain numerical solutions to the mathematical models. Topics will include: Finite Difference and Finite Volume methods; particle-based Lagrangian methods; physics-informed Neural Networks methods, characterization and analysis of numerical errors; models of contaminant transport; introduction to model calibration and uncertainty quantification.

We will mostly focus on subsurface flow and transport applications. However, the numerical methods covered in this course are applicable to a variety of environmental, hydrologic and hydraulic problems since the governing equations in these applications are similar to those for groundwater flow and mass transport. The course will thus be beneficial to students interested in topics such as modeling flow and water quality in rivers, lakes and estuaries, modeling of water and wastewater treatment processes, and air quality modeling.

Prerequisites: Students are expected to know differential equations (e.g., Math 285) and linear algebra (Math 225) and be able to write computer programs for numerical computations in a language of their choice (e.g., C/C+, Matlab, Python).

ILLINOIS CANVAS: https://canvas.illinois.edu/courses/44008
Illinois Canvas will be used to post course materials, homework assignments, etc.

Engineering Workstation Access: All students enrolled in the class should have an account on the College of Engineering Workstation (EWS) Labs. EWS has a wide variety of software (e.g., MATLAB) that you might want to use for computer assignments and the term project.

Course Notes: Course notes will be available on Canvas.

Reference Texts - available in the Engineering Library.

Wang, H.F. and M.P. Anderson, Introduction to Groundwater Modeling, W.H. Freeman and Co., San Francisco, 1982.

Lapidus, L. and G. F. Pinder, Numerical Solution of Partial Differential Equations in Science and Engineering, Wiley, New York, 1982.

These books provide background and enrichment material. Additional background and tutorial material about groundwater modeling and computational methods will be posted on the Canvas Site.

Office Hours

Please email me if you would like to meet.

Teaching Assistant/Grader

To be arranged later.

Grading

Homework Problem Sets (2 or 3 assignments) You can work together but each student submits individually	**30%**
Computer Problems (2) These will be designed to be done in small groups (2 or 3)	**30%**
Term Project	**40%**

Group project (2 students). The project should involve numerical computation but does not need to be related to groundwater. Students select a topic of their choice in consultation with the instructor.

There is no final exam

DETAILED COURSE OUTLINE

(subject to adjustment due to time limits and student interest)

I. Introduction to Modeling Approaches

II. Parabolic, Elliptic PDE's (e.g. groundwater flow, heat conduction, diffusion of dissolved chemicals, …)

A. Derivation (Review)
B. Boundary and Initial Conditions (Review) C. Overview of Analytical Solutions (Review)

D. Numerical Solution by Finite Difference and Finite Volume Techniques

1. basic concepts
2. time-dependent problems
    a. “model” problem formulation for one space dimension
    b. consistency, convergence, stability
    c. Fourier Analysis - amplitude errors
    d. mass conservation; monotonic (non-negative) solutions
    e. 2-D problems
3. solution of the difference equations -- overview of direct and iterative methods for solving systems of linear algebraic equations
4. extensions
    a. variable coefficients
    b. nonuniform grids
    c. flux boundary conditions
    d. source/sink terms
5. nonlinear problems (e.g.,unsaturated flow, unconfined aquifers)
6. steady flow (elliptic) problems
    a. “model” problem formulation in 2D & 3D
    b. solution of sparse linear algebraic system

III. Mixed Parabolic-Hyperbolic PDE's (e.g. pollutant transport in porous media and surface water, flood routing, …)

A. Basic Principles and Governing Equations - nonreactive solutes (Review)
B. Boundary and Initial Conditions (Review)
C. Overview of Analytical Solutions (Review)
D. Numerical Solution by Finite Difference and Finite Volume Techniques
    1. sample problem formulation in 1D
    2. consistency, convergence, stability
    3. Fourier Analysis - amplitude and phase errors
    4. numerical diffusion, phase errors, numerical oscillations
    5. mass conservation; monotonic (non-negative) solutions
    6. 2D problems

IV. Transport Models and Solution Techniques for Chemically Reacting Solutes (interaction between reaction and transport)

V. Introduction to Finite Element Techniques

A. Interpolation and approximation concepts
B. Solution of the Parabolic/Elliptic Problems (e.g., Groundwater Flow)
    1. sample problem formulation for a 1D steady problem (Galerkin FEM)
    2. sample problem formulation for a transient problem

3. convergence & stability
4. two-dimensional problems
5. local coordinates and numerical quadrature
6. two-dimensional elements
7. extensions
    a. variable coefficients
    b. sources/sinks
    c. nonlinear problems
8. comparison of Finite Element and Finite Difference Methods
9. mixed methods (pressure-velocity) and calculation of velocity

C. Solution of Mixed Hyperbolic-Parabolic Problems (e.g., Solute Transport)
    1. sample problem formulation in 1D
    2. Fourier Analysis - numerical diffusion, phase errors, numerical oscillations
    3. Special methods related to the Method of Weighted Residuals (e.g., PetrovGalerkin FEM, optimal test function; stabilized FEM)

VI. Overview of Other Special Numerical Techniques for the Solute Transport Problem (time permitting)

A. Physics-Informed Machine Learning Methods (physics-informed neural network (PINN) method, etc)
B. Smoothed Particle Hydrodynamics Method
C. Mixed Eulerian-Lagrangian Methods
B. Locally Adaptive Mesh Refinement
C. Random Walk Method
D. Streamline Based Methods
E. High-Order Finite Volume Methods & Flux Limiters

VII. Recent Research Results and Special Topics (time permitting)

A. Model Calibration and Verification
    1. overview of the inverse problem
    2. sensitivity coefficients
    3. automatic (regression-based) inverse methods
    4. case studies of model applications to field problems
B. Spatial Variability -- geostatistical and stochastic concepts

USEFUL TEXTS AND REFERENCE BOOKS

AGU E-Book Numerical Methods in the Hydrological Sciences, George Hornberger and Patricia Wiberg. 2006. http://onlinelibrary.wiley.com/book/10.1002/9781118709528

General Groundwater

Bear, Jacob, Hydraulics of Groundwater, McGraw-Hill, New York, 1979.

Domenico, P.A. and F.W. Schwartz, Physical and Chemical Hydrogeology, 2nd Edition, John Wiley & Sons, New York, 1998.

Fetter, C.W., Applied Hydrogeology, 4th ed., Prentice Hall, 2001.

Fetter, C.W., Contaminant Hydrogeology, Prentice Hall, 1993.

Freeze, R.A. and J.A. Cherry, Groundwater, Prentice-Hall, Englewood Cliffs, New Jersey, 1979.

Hunt, B., Mathematical Analysis of Groundwater Resources, Butterworth, London, 1983.

de Marsily, G., Quantitative Hydrogeology, Academic Press, London, 1986.

Pinder, G. and M. Celia, Subsurface Hydrology, Wiley Interscience, 2006.

Strack, O.D.L., Groundwater Mechanics, Prentice-Hall, 1989.

Finite Difference and Finite Volume Methods

Abbott, M.B., Computational Hydraulics, Pitman Publishing Ltd., London, 1979.

Anderson, Tannehill, and Fletcher, Computational Fluid Mechanics and Heat Transfer, Hemisphere Publishing Corp., New York, 1984.

LeVeque, R. Finite Volume Methods for Conservation Laws. Cambridge University Press, Cambridge, UK, 2002.

Peaceman, D.W., Fundamentals of Numerical Reservoir Simulation, Elsevier, New York, 1977.

Richtmyer, R.D. and K.W. Morton, Difference Methods for Initial-Value Problems, 2nd ed.,Wiley, New York, 1967.

Roache, P.J., Computational Fluid Dynamics, Hermosa Publishers, Albuqerque, N.M., 1976.

Smith, G.D., Numerical Solution of Partial Differential Equations:Finite Difference Methods, 2nd ed., Clarendon Press, Oxford, 1978.

Toro, E. Riemann solvers and numerical methods for Fluid Dynamics. Springer, 1997.

Finite Element (and related) Methods

Donea, J. and A. Huerta, Finite Element for Flow Problems, Wiley, 2004.

Huebner, K.H., The Finite Element Method for Engineers, Wiley, New York, 1975.

Huyakorn, P. and G.F. Pinder, Computational Methods in Subsurface Flow, Academic Press, 1983.

Liggett, J.A. and P. Liu, Boundary Integral Equation Method for Porous Media Flow, George Allen & Unwin, London, 1982.

Istok, J., “Groundwater Modeling by the Finite Element Method,” Water Resources Monograph 13, American Geophysical Union, 1989.

Pinder, G. and W. Gray, Finite Element Simulation in Surface and Subsurface Hydrology, Academic Press, New York, 1977.

Strang, G. and G. Fix, An Analysis of the Finite Element Method, Prentice-Hall, Englewood Cliffs, New Jersey, 1973.

Vichnevetsky, R., Computer Methods for Partial Differential Eqns. Vol. I, Prentice-Hall, 1981.

General Groundwater Modeling and Computational Methods

Allen, M.B., I. Herrera, and G.F. Pinder, Numerical Modeling in Science and Engineering, Wiley - Interscience, New York, 1988.

Anderson, M.P., W.W. Woessner, and R. Hunt., Applied Groundwater Modeling: Simulation of Flow and Advective Transport, 2nd ed. Elsevier, 2015.

Celia, M.A., and W.G. Gray, Numerical Methods for Differential Equations, Prentice Hall, 1992.

Chen, Z., G. Huan, and Y. Mia, Computational Methods for Multiphase Flows in Porous Media, Society for Industrial and Applied Mathematics, Philadelphia, 2006.

Huyakorn, P. and G.E. Pinder, Computational Methods in Subsurface Flow, Academic Press, New York, 1983.

Javandel, I.,C. Doughty, and C.F. Tsang, Groundwater Transport: Handbook of Mathematical Models, AGU, WR Monograph 10, 1984.

Wang, H.F. and M.P. Anderson, Introduction to Groundwater Modeling, W.H. Freeman, San Francisco, 1982.

Zheng, C. and G.D. Bennett, Applied Contaminant Transport Modeling, 2nd ed. J. Wiley & Sons., New York, 2002.

Stochastic/Geostatistical Analysis and Inverse Problems

Dagan, G., Flow and Transport in Porous Formations, Springer Verlag, 1989.

Gelhar, L.W., Stochastic Subsurface Hydrology, Prentice Hall, 1993.

Hill, M. C. (1998), Methods and Guidelines for Effective Model Calibration, U.S. Geological Survey Water-Resources Investigations Report 98-4005, Denver, Colorado.

Hill, M. and Tiedeman, C. (2006), Effective Groundwater Model Calibration with Analysis of Sensitivities, Predictions, and Uncertainty, Wiley, New York

Kitanidis, P.K., Introduction to Geostatistics: Applications to Hydrogeology, Cambridge University Press, New York, 1997.

Rubin, Y., Applied Stochastic Hydrogeology, Oxford University Press, 2003.

Sun, N.-Z. (1995), Inverse Problems in Groundwater Modeling, Kluwer Academic Publishers, the Netherlands.

Zhang D. 2002. Stochastic Methods for Flow in Porous Media: Coping with Uncertainties. San Diego CA: Academic Press.

JOURNALS

(very incomplete list)

Advances in Water Resources
Computational Methods in Applied Mechanics and Engineering
International Journal for Numerical Methods in Engineering
International Journal for Numerical Methods in Fluids
Journal of Computational Physics
Journal of Contaminant Hydrology

Journal of Hydraulic Engineering, ASCE
Journal of Hydrology
Transport in Porous Media
Water Resources Research
SIAM Journal on Numerical Analysis
Society of Petroleum Engineers, Journal

WORLD WIDE WEB: Software & Related Information

http://numericalmethods.eng.usf.edu/about.htm
Instructional site for teaching undergraduates about numerical methods; includes tutorial documents, YouTube videos, etc.

http://cee.illinois.edu/transport/
Interactive analytical models for flow and transport developed by Professors Valocchi & Werth. (Used in CEE 457)

water.usgs.gov/software/ground_water.html
Free groundwater related software developed & supported by the USGS, including MODFLOW

https://water.usgs.gov/software/lists/surface_water
Free surface water related software developed & supported by the USGS, including MODFLOW

http://www.groundwatermodels.com/
ESI Environmental Simulations International; GW Vistas is a user-friendly interface for MODFLOW

http://inside.mines.edu/~epoeter/583/index.shtml
On-line Groundwater Modeling Course, Prof. Eileen Poeter, Colorado School of Mines