Syllabus for ESS 524
Numerical Heat and Mass Flow Modeling in the Earth Sciences
Spring 2010

Course overview and curriculum content

Many heat and mass-transport processes in the Earth Sciences are represented by advective-diffusion equations. With increased availability of fast computers, many ESS graduate students now need to carry out numerical simulations of Earth processes in their thesis research, often without formal training in numerical analysis.

This course introduces students to ways to set up systems of equations representing advective-diffusive earth processes, and to solve them numerically using the Finite-Volume method and MATLAB programming language, to obtain reliable, accurate and stable solutions. Processes for which solutions are obtained include

- steady and transient diffusion,
- steady and transient diffusion with a specified flow field,
- steady and transient diffusion coupled with simplified flow calculations.

Students will be introduced to concepts behind Finite-Volume solutions of the Navier-Stokes equations of motion with the SIMPLE algorithm or with co-located velocity and pressure grids, although this introductory course stops short of full numerical solutions of those equations.

Some MATLAB finite-volume solvers for rectangular grids are provided, and students gain hands-on experience by adapting and extending those codes to solve their own specialized applications, as term projects.

The course consists of lectures, student reading and discussion of concepts, homework assignments, and student term projects. The course helps students to develop numerical skills for their thesis research, and contributes to their professional development in Earth and Space Sciences through technical writing and oral presentation of their work. Through exposure to other student projects, students learn to recognize common threads in a multidisciplinary field such as Earth Sciences.

Learning Goals/Objectives

- Students will be able to formulate conservation laws for mass, momentum, and energy for advective-diffusive flow systems in Earth Sciences.
- Students will be able to design and solve stable and accurate numerical representations of slow non-turbulent heat and mass flows, using the Finite-Volume method.
- Students will gain practical experience with issues of convergence, with reduction in residuals, and with various schemes of over-and-under relaxation when solving nonlinear problems.
- Students will be able to critically assess the merits and weaknesses of Finite-Element methods, Finite-Difference methods, and Finite-Volume methods for a range of numerical Earth Science problems, and explain why the chosen procedures are effective.
- Students will understand the importance of verification of numerical codes, and validation of model physics, and will be able to verify their own codes.

This course will cover fundamentals of steady and transient flow modeling, applied to slow (non-turbulent) flows. These fundamentals also apply to any advective-diffusive system, not just heat and mass flow. Procedures to treat nonlinearities in the governing equations will be described and implemented.

The course will start with conservation laws, and develop numerical solutions using finite volume (or control-volume) methods. We will explore the relationship of Finite-Volume methods to Finite-Difference and Finite-Element methods.

The course will develop and use some 1-D and 2-D MATLAB steady and transient codes for diffusion with advection as we progress through the Quarter.

Required Texts, readings, films, websites, etc

- Versteeg, H.K. and W. Malalasekera. *An Introduction to Computational Fluid Dynamics: the Finite Volume Method*. (second ed.) Longman 2007.

Supplementary text –

- Patankar, S.V. *Numerical Heat Transfer and Fluid Flow*. CRC 1980.

- Other reading materials on specialized topics.

Evaluation and grading, assignments, projects

Students attend and participate in discussions in lectures, and maintain a journal in which they note new concepts that they have learned, and progress on a term project.

Homework assignments (every second week) ask students to formulate approaches and to write MatLab code to solve particular problems arising in the current topics in lectures. These exercises provide deeper understanding of numerical methods, and provide a learning opportunity for students to develop their computer programming skills

The term project requires formulation and numerical solution of a heat and/or mass flow problem relevant to a student's thesis research project. Students deliver an oral presentation of their results, in a format typical of earth science meetings such as American Geophysical Union or Geological Society of America, and will write a paper describing their project in a format typical of journals that publish short papers of broad interest to Earth Scientists, such as *Geology* or *Geophysical Research Letters*.

Students are evaluated based on written journals, homework, projects, and participation in class.

- Weekly assessment of journals 20%
- Homework 20%
- Attendance/participation 20%
- Project presentation 20%
- Written project report 20%

Course Schedule

Week 01

- Conservation Laws
- What are numerical methods?
- Discretization approaches

- One-way and two-way coordinates

Week 02
- Definition of participant projects.
- Introduction to MATLAB.
- Steady heat flow in 1-D.
- Boundary conditions.

Week 03
- Unsteady heat flow in 1-D.
- Explicit and implicit solution methods, numerical instability.
- Numerical accuracy, time stepping.
- Steady heat flow in 2-D.

Week 04
- Unsteady heat flow in 2-D.
- Advection and diffusion in 1-D, specified flow field.
- Upwinding (1-D space coordinates).
- Kinematic waves.

Week 05
- Advection and diffusion in 2-D, with a specified flow field.
- Advective-diffusive systems in Earth Sciences.

Week 06
- Nonlinearities in governing equations.
- Iterations and convergence.
- Relaxation.

Week 07
- Solving for flow field in 2-D with simplified stress equations.

Week 08
- Solving for flow field in 2-D (Navier Stokes).
- SIMPLE algorithm, staggered grids for velocity and pressure.
- collocated grids.

Week 09
- Finite volumes in curvilinear coordinates.
- Finite volumes in unstructured grids.
- 3-D considerations.

Week 10
- Verification and validation of computational results.
- Oral presentations of student projects.

Exam Week
- Written Project reports due.