G6943y: Myths and Methods in Modeling (M&M's in M)

Instructor Marc Spiegelman, (mspieg@ldeo.columbia.edu, xtn 8425 (LDEO), 212 854 4918 (DAPAM/Columbia))

Teaching Assistant TBA

Dates and Times Spring 2004: Mon., Wed afternoons 1:45-3:00

Location Seismology Seminar Room

Office hours Mon., Wed afternoons 3:00-4:00

Short Description This course is designed to be an introduction to techniques and approaches for formulating and solving quantitative models of earth processes with examples chosen from a wide range of disciplines.

Requirements Linear algebra, vector calculus, ODE's and PDE's to the level of Applied Math I and II (E3101, E3102) plus some programming experience will make your life considerably easier. Assigned programming and examples will primarily be in Matlab (with more advanced topics in Fortran or C), but any language is acceptable for projects.

Rationale The purpose of this course is to develop the numerical and analytical skills required to formulate, execute and *understand* quantitative models of earth (and other) processes. These skills are becoming more and more necessary in quantitative earth science, however, there is, as yet, no formal mechanism for learning these techniques in a context that emphasizes real earth and environmental science problems. In addition to providing hands-on experience in modeling, this course will also attempt to de-mystify (or de-mythify) the general practice of forward modeling and provide enough insight to critically evaluate results of published models. This course is designed to complement G6908x Quantitative methods of data analysis by providing a fundamental set of quantitative tools that would benefit all earth scientists independent of discipline.

Course Description Through a series of lectures and hands-on practical work, this course will provide an introduction to the art of numerical forward modeling. We will develop tools for a wide range of problems from geochemical box models to mantle convection. Most importantly, this class will develop the physical insight required for successful modeling.

The lectures will first teach how to formulate a quantitative model for a range of problems and then introduce a suite of techniques, tools and tricks available for numerical solution of the equations that have been derived. We will illustrate the fundamental behavior of the most commonly occurring equations and demonstrate how to choose effective tools for solution that reflect the physics of the underlying equations. The lectures will also emphasize how to recognize and avoid the many myths, pitfalls and intellectual black holes that abound in modeling.

The lectures will be supported by practical work including homework and a longer term project. As the only real way to gain experience in modeling is to do it, each student will choose a specific problem from their own field of interest and develop, execute and present the results of a quantitative model to describe the process of interest. Ideally, these projects will form the nucleus of Masters or Ph. D. research projects, and will be carried out with reasonable supervision from myself, and the students' own advisors. The final project report will be either in the form of a short GRL paper or a short proposal (depending on whether or not sufficient results are obtained in the given time).

Reading there will be no specified textbook for this course as I will supply copious notes. however, Numerical Recipes in (your favourite language here) , 2nd Edition (Press et al., 1992) is a useful reference. Other useful background texts include:

Schey, H.M., Div, grad, curl, and all that; an informal text on vector calculus, New York, Norton (1973)

Haberman, R, Elementary applied partial differential equations (3rd edition), Prentice-Hall, (1998) (Introductory analytic PDE's)

Strang, G, Introduction to Linear Algebra, Wellesley-Cambridge Press, (2003)

Trefethen, L.N., and D. Bau III, Numerical Linear Algebra, SIAM

Arfken, Mathematical Methods for Physicists

Chapman, S. J., Fortran 90/95 for Scientists and Engineers, McGraw Hill, (1998)

Turcotte, Donald Lawson, and Schubert, G., Geodynamics : applications of continuum physics to geological problems, New York : Wiley, c1982.

I will also supply random papers and suggest various on-line resources.

Syllabus

21 Jan Introduction: Course description, modeling myths and biases, and preview of problems to come; Start "Formulating a model"

26 Jan Formulating a model cont'd: basics of deriving conservation equations, introduction to the basic flavors of equations and *scaling*. **problem set 1**

28 Jan Overview of fundamental earth science problems.

2 Feb (Groundhog Day) Overview cont'd.: Survey of available tools for solution: hardware and software (languages, packages, libraries, visualization, paper and pencil).

4 Feb Survey cont'd: Computer refresher Unix, Matlab, Compiled (and other) Languages… *1-page preliminary Project proposal due. (individual conferences to be set up)*

Basic Methods The next few weeks will provide specific examples of simple model problems with emphasis on the physical meaning of the equations and how to choose an appropriate technique for solution. We'll begin with time dependent initial value problems and progress to steady state boundary value problems.

9 Feb Ordinary differential equations: geochemical box models to the Lorenz equations. Mid-point, Runge-Kutta, and adaptive stepping. ODE solvers in Matlab **problem set 2**

11 Feb I'll be at a meeting at Lawrence Berkeley Labs but can schedule a review session if interested

16 Feb Ordinary differential equations cont'd: the relationship between ODE's and PDE's.

18 Feb Flux conservative problems and advection I: transport to non-linear waves: Basic Finite differencing and stability **problem set 3**

23 Feb Flux conservative problems and advection II: Semi-lagrangian and Pseudo-spectral techniques

25 Feb Diffusive initial value problems : heat flow. Explicit methods (FTCS) and Implicit methods (Crank Nicholson) schemes. Living with boundary conditions**problem set 4**

1 March Putting it together: Combined advection-diffusion (reaction?): geochemical transport. Operator splitting and hybrid schemes.

3–8 March Initial value problems in multiple dimensions **problem set 5**

10 March Boundary value problems I: Stress and creeping flow, steady state heat flow: Direct methods for Poisson problems, using netlib and the Web **problem set 6**

15–19 March Spring-Equinox Romps

22–24 March Boundary value problems II: Simple relaxation methods and SOR. Krylov schemes (GMRES and CG).

29 March Boundary value problems III: Krylov Schemes continued: Preconditioners, non-linear problems and Newton Krylov methods.

31 March Boundary value problems IV. Introduction to Multigrid techniques.

5 April advanced Multi-Grid and other techniques

7–12 April Finite Element and Spectral Element techniques. (Enrique Curchitser)

14–19 April High-performance computing and parallel programming Introduction to PETSc (Rich Katz/David Keyes)

Show and tell: real examples The remainder of the course will be spent discussing specific real earth-science problems to demonstrate solution of systems of PDE's. Each section will be presented by a practitioner with in depth knowledge of the tweaks, fudges and peculiarities of each problem. Each lecture will describe the model equations and assumptions, basic physical behaviour of the model, preferred method of solution, results and implications. (Tentative schedule)

21 Apr Atmospheric Models (Adam Sobel/Gavin Schmidt)

26 Apr Ocean Models (Enrique Curchitser)

28 Apr Earthquake Models (Bruce Shaw)

3 May Magma/Mantle dynamics (your's truly) **Projects due**

Modeling Myths

- Modeling is Difficult
- Numerical models can do everything
- Numerical models will solve your problems

Modeling Facts

- Modeling is simple book-keeping (plus a bit of magic)
- There are no black boxes!
- Numerical models have a life of their own and make their own problems

Used carefully, numerical solutions are a very powerful tool for gaining insight into possible physical processes. Used indiscriminately, they become an intellectual black-hole. We need to emphasize the two end-member approaches to modeling

1. **The Kitchen Sink Approach**: Throw everything into it and hope something useful comes out (BAD IDEA)
2. **The Model Problem Approach**: Gain insight by developing simple model problems that balance interesting behaviour with comprehensibility (GOOD IDEA – but takes finesse).

This course will stress the 2nd approach and will emphasize the following axioms

- Be problem driven
- Understand your problem
- Keep it simple
- Never model more than you can understand (or observe)
- Avoid the ‘reality trap’ (models $\neq$ ‘reality’)
- Choose your techniques to mimic the underlying physics.
- The only successful model is an insightful model.