School of Earth Sciences and School of Mathematics, Statistics and Computer Science

MATH 322/323, Module on Fluid Flow in Earth Systems

Computer Section--Background Information and Assignment 4

(see last pages) Due 5 PM Friday October 3 2014

In the first three weeks of this module, you examined and determined many analytic solutions for fluid flow of earth materials. As has been noted several times in the text, however, most fluid flow problems cannot be solved with analytic techniques, and so numerical methods are generally employed for present research in fluid dynamics. In this section of the module, to last 3 weeks, we will use several techniques to solve different fluid flow problems. In all problems, analytic solutions exist for the simplest case of isoviscous media. This is very useful, as the programs can be compared to the analytic solutions to be sure that they work properly, before using them for more complicated problems.

As you have no doubt realised, the general problem of fluid flow involves integration of several different differential equations. Numerical methods of integration will therefore be used to solve the problems. The basic concept of using computers to solve calculus problems is conceptually simple. You will recall that derivatives involve taking the limit as small elements get infinitesimally tiny. The basic concept of "brute force" techniques in numerical methods is to treat the differential equations as if they were regular algebraic equations with elements that are small, but still finite. A medium is broken into tiny elements, and the equations are applied on each element. This is called "discretisation". The elements are small enough that the derivatives in the differential equations are converted into ratios of small steps of time, position, etc. In numerical methods, functions tend to be defined over arrays, derivatives become ratios of differences between elements of the arrays and the step size, and integrals become sums over the array. The equations are usually solved iteratively. Complications occur because the elements cannot become truly infinitesimal, and arrays cannot have infinite numbers of elements. There is a huge body of literature and research on the topic of finding the optimum technique for each problem, and we will only touch on a few in the three weeks we have available.

The governing partial differential equation subject to specified boundary (and for transient problems, initial) conditions is transformed into a system of ordinary differential equations (for transient problems) or algebraic equations (for steady-state problems) which are solved to yield an approximate solution for the flow distribution.

The computer section is divided into three weekly assignments. We will start out with calculating integrals and derivatives of functions numerically in a standard fashion, including a problem of 1D fluid flow in a channel. Later weeks will use techniques that use finite difference formulations to solve differential equations.

Notes on methodology:

As stated above, in the finite difference method, equations are changed to algebraic equations involving elements of the array. See Example in Figure 1.

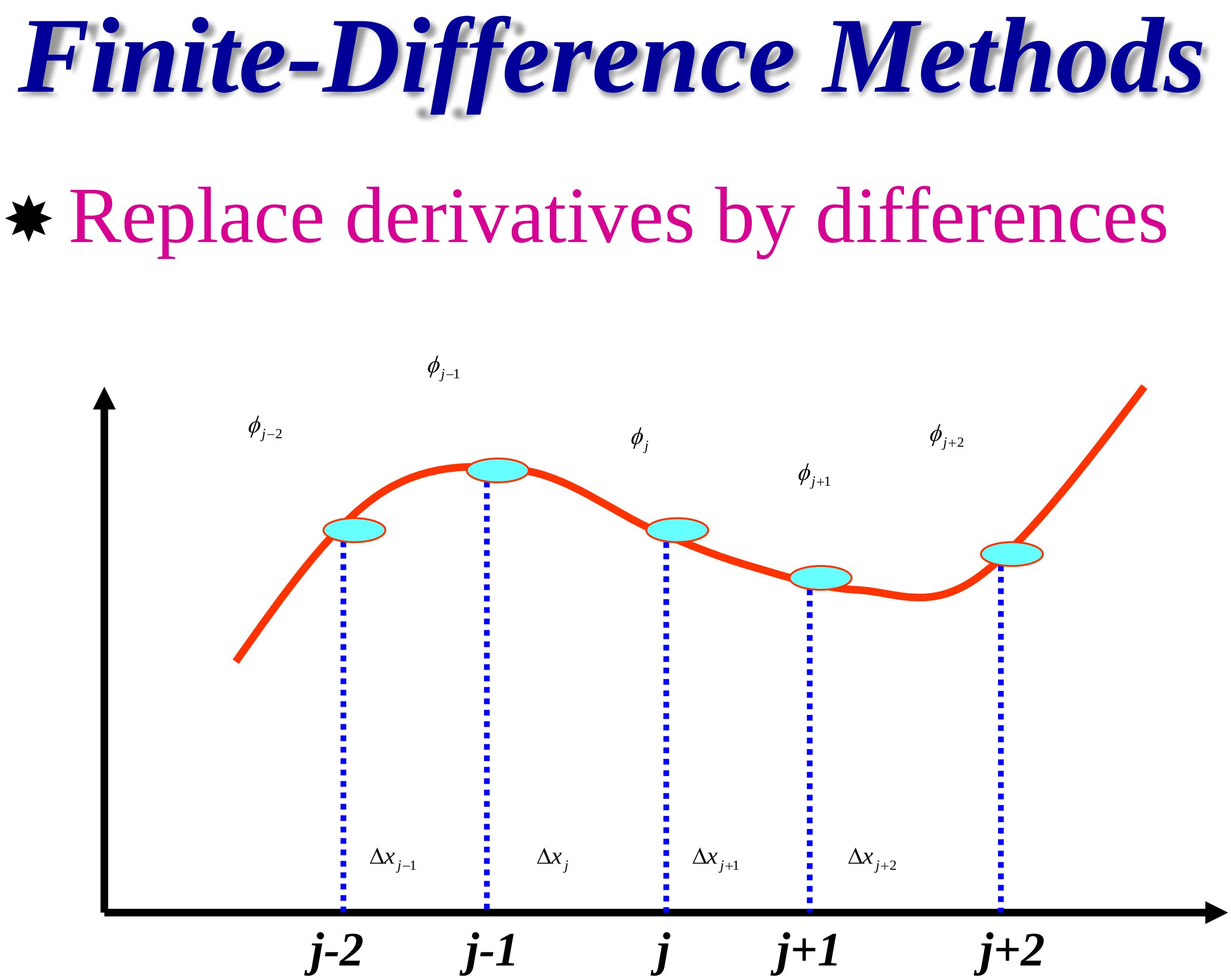

Figure 1. Function $\phi(x)$ discretised.

Steps to Finite Difference Analysis:

1. Choose suitable step size and time increment
2. Replace continuous information by discrete nodal values
3. Construct **discretization (algebraic) equations** with suitable numerical methods
4. Specify appropriate **auxiliary conditions** for discretization equations

Example: Heat Equation

$$\frac{\partial \overline{T}}{\partial t} = \alpha \frac{\partial^2 \overline{T}}{\partial x^2}$$

$$\begin{cases} \overline{T}(0.t) = b, \quad \overline{T}(1,t) = d \\ \overline{T}(x,0) = T_o(x), \qquad 0 \le x \le 1 \end{cases}$$

$$\boxed{\begin{cases} \text{Exact :} & \overline{T}(x,t) \\ \text{Numerical :} & T_j^n = T(x_j, t_n) \end{cases}}$$

One-sided scheme:

$$\boxed{\frac{\partial T}{\partial t} = \frac{T_j^{n+1} - T_j^n}{\Delta t} \quad \text{or} \quad \frac{\partial T}{\partial t} = \frac{T_j^n - T_j^{n-1}}{\Delta t}}$$

This is based on the first order Taylor series expansion. Other schemes use higher order expansions, e.g.,

$$\frac{\partial T}{\partial t} = \frac{T^n{}_{j+1} - T^n{}_{j-1}}{2\Delta t}$$

Remember, the Taylor Series Expansion of a function f can be written as follows:

$$\begin{cases} f(x) = a_o + a_1(x - x_o) + a_2(x - x_o)^2 + a_3(x - x_o)^3 + \cdots & \Rightarrow a_o = f(x_o) \\ f'(x) = a_1 + 2a_2(x - x_o) + 3a_3(x - x_o)^2 + \cdots & \Rightarrow a_1 = f'(x_o) \\ f''(x) = 2a_2 + 6a_3(x - x_o) + \cdots & \Rightarrow a_2 = f''(x_o)/2! \\ f'''(x) = 6a_3 + \cdots & \Rightarrow a_3 = f'''(x_o)/3! \\ \qquad \vdots & \\ f^{(m)}(x) = (m!)a_m + (m+1)m(m-1)\cdots 2a_{m+1}(x - x_o) + \cdots & \Rightarrow a_m = f^{(m)}(x_o)/m! \end{cases}$$

$$\therefore f(x) = \sum_{m=0}^{\infty} a_m (x - x_o)^m = \sum_{m=0}^{\infty} \frac{f^{(m)}(x_o)}{m!}(x - x_o)^m$$

Another way of writing it is as follows:

$$f(x) = f(x_o) + (x - x_o) f'(x_o) + \frac{(x - x_o)^2}{2!} f''(x_o) + \frac{(x - x_o)^3}{3!} f'''(x_o)$$

$$+ \cdots + \frac{(x - x_o)^n}{n!} f^{(n)}(x_o) + \cdots \qquad a \le x \le b, \quad a \le x_o \le b$$

Of course, a Taylor's series expansion is infinite, and in the real world, it must be truncated at some value of n, called the order of the expansion.

The second derivative can be written a number of ways as well. Below are some expressions for Finite differences for derivatives with respect to x. The symbol *O(Δx)* means that the errors are of order of Δx, and similarly for the square.

$$\left[\frac{\partial \overline{T}}{\partial x}\right]_j^n = \frac{\overline{T}_{j+1}^n - \overline{T}_j^n}{\Delta x} + O(\Delta x)$$

$$\left[\frac{\partial \overline{T}}{\partial x}\right]_j^n = \frac{\overline{T}_j^n - \overline{T}_{j-1}^n}{\Delta x} + O(\Delta x)$$

$$\left[\frac{\partial \overline{T}}{\partial x}\right]_j^n = \frac{\overline{T}_{j+1}^n - \overline{T}_{j-1}^n}{2\Delta x} + O(\Delta x^2)$$

$$\left[\frac{\partial^2 \overline{T}}{\partial x^2}\right]_j^n = \frac{\overline{T}_{j+1}^n - 2\overline{T}_j^n + \overline{T}_{j-1}^n}{\Delta x^2} + O(\Delta x^2)$$

Truncation Errors

If the Taylor series is truncated at order n, then the truncation error T_E is just all the terms that have been left out. So, if we approximate the Taylor series for x between a and b as below:

$$f(x) = f(x_o) + (x - x_o) f'(x_o) + \frac{(x - x_o)^2}{2!} f''(x_o) + \frac{(x - x_o)^3}{3!} f'''(x_o)$$

$$+ \cdots + \frac{(x - x_o)^n}{n!} f^{(n)}(x_o) + \cdots \qquad a \le x \le b, \quad a \le x_o \le b$$

$$\boxed{T_E = \frac{(x - x_o)^{n+1}}{(n+1)!} f^{(n+1)}(\xi), \qquad a \le \xi \le b}$$

How to reduce truncation errors?

(a) Reduce grid spacing, use smaller Δ*x* = *x-xo*

(b) Increase order of accuracy, use larger *n*

Example: The second derivative of velocity in the y direction can be approximated using the following finite difference scheme:

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{dy^2}$$

Numerical Integration

One simple way to integrate an equation is through use of the trapezoidal rule. Basically, it uses the idea that the integral is the area under the curve made by the function. It approximates this area by a trapezoid. Therefore, to integrate a function f(z) over a very small interval z_2-z_1, we can write the function as follows:

$$\int_{z_1}^{z_2} f(z)dz = \frac{1}{2}(z_2 - z_1)(f(z_2) + f(z_1))$$

Integrating over a larger interval then becomes a sum over N such small intervals:

$$\int_A^B f(z)dz = \frac{1}{2}\sum_{i=0}^{N}(z_{i+1} - z_i)(f(z_{i+1}) + f(z_{i1}))\,.$$

If we use equally spaced intervals, then z_{i+1}-z_i = Δz = constant and the equation becomes:

$$\int_A^B f(z)dz = \frac{1}{2}\sum_{i=0}^{N}(f(z_{i+1}) + f(z_i))\Delta z$$

Another way to think about it is that you are approximating the function over a small interval by the average of the function at the two endpoints of the interval.

More resources (mainly for later parts of the module):
Web pages on numerical modeling:
http://www.ldeo.columbia.edu/~mspieg/mmm/
(especially http://www.ldeo.columbia.edu/~mspieg/mmm/Diffusion.pdf (Chapter 6)
This is the best overall resource I've found on numerical modeling of Geophysics problems. Mark Spiegelman is one of the leading Geophysical modellers.

Some of the notes above were excerpted from the following web page
http://ceprofs.tamu.edu/hchen/cven688/chap03a.ppt

Assignment 4 Maths 323 Fluid Flow module 2013: Numerical differentiation and integration

The final goal of this week and the start of next is to solve the problem of fluid flow in 1D. The analytic solution was solved in Chapter 6-2 of Turcotte & Schubert for the case of a constant viscosity fluid, and you checked some aspects of it in your problem set. Next week we will be extending the problem to allow for an arbitrary viscosity structure, and will solve the problem numerically. To get you used to numerical methods, however, we will start with a couple of simpler problems.

Part I: Numerical Differentiation

I have created a very simple Excel spreadsheet, which I will give to you, that integrates and differentiates the function $f(z) = az^n$. The "analytical solutions" are the ones you have learned in high school calculus classes—$f'(z) = anz^{n-1}$ etc. The "numerical solutions" are the ones made using differences or sums of parts of the array. Note that the spreadsheet has been implemented so that the values don't update automatically when you change them—On a PC, you need to hold down the "Control" key and hit the "+" button to update it. (On Apple, is also Control + or Apple +, but only for the + sign that is near the letters of the keyboard (not on the number pad). Answer the following questions, being sure to label and explain your graphs as discussed below. **Your mark will depend on the writeup—spreadsheets can help as an aid to help me understand where you've gone wrong and a check to be sure they work, but spreadsheets with no explanation are not acceptable.**

1. Try the spreadsheet, and modify it to use different values for a, n and dz, for integration to z=5. You may need to press the "ctrl +" keys to get the computer to respond to any changes you make. Be sure to look at least at n=1,2, and a higher value, and at dz=0.01, 0.1, 1. Note that you may need to change the number of rows you use in each case. If you know another language, e.g., Matlab, C or fortran, and want to use it instead, you may do so. Explain how the spreadsheet or program implements the numerical differentiation and integration discussed above. (For example, you could pick a particular set of cells and explain how the formulas in the cells relate to the definitions of the integrals and derivatives.) Explain why there are or are not differences between the analytic and numerical solutions for the different cases. Graph your solutions (including graphs of the differences between the numerical and analytical results) and explain your graphs. (15 marks) **Your mark will depend on the writeup—spreadsheets can help as an aid to help me understand where you've gone wrong and a check to be sure they work, but spreadsheets with no explanation are not acceptable.**

2. Which differentiation form have I used? Try one other form of differentiation and explain why it yields better or worse solutions for the higher order values (i.e, for n equal to 3 or greater). Show

examples through graphs of differences between the analytic and numerical solutions to the functions. (10 marks)

3. Use one of the forms given above to calculate the 2nd derivative numerically, and verify how well it matches the analytic solution, for at n=3 and n=5, and two different values of dz. (10 marks)

Part II: Numerical Integration

4. Create your own spreadsheet or program to calculate the error function discussed in Chapter 4 of Turcotte and Schubert. This is an example of a function that has no analytic solution. Again try different values of the increment dz and see how well you match the values in Table 4-5 on p. 155. (Ed. 2) Explain any differences. (10 marks)

Part III 1-d fluid flow in a channel

We will now calculate 1-dimensional fluid flow in a channel that can have arbitrary viscosity as a function of depth.

5. a) If the viscosity is a function of depth, and the pressure gradient *dp/dx* is a constant *P*, then show that Turcotte and Schubert (2nd Edition) equations 6-1 and 6-8 lead to a modification of equation 6-10 of that becomes:

$$\frac{d(\mu(y)\frac{du}{dy})}{dy} = \frac{dp}{dx} = P \quad \text{(Eq. FF1)}$$

Where as usual, u is the velocity in the x direction, y is depth, and μ is viscosity.

b) Given boundary conditions of $u(0) = u_0$ and $u(h) = 0$ (for example, as in asthenospheric flow driven by a rigid plate moving above it), show that the equation FF1 above can be rewritten as follows:

$$u(y) = u_0 + s\int_{y'=0}^{y} \frac{1}{\mu(y')}dy' + P\int_{y'=0}^{y} \frac{y'}{\mu(y')}dy' \quad \text{(FF2)}$$

Where the constant of integration $s = du/dy$ evaluated at $y = 0$, is given by:

$$s = -\frac{u_0 + P\int_0^h \frac{y'}{\mu(y')}dy'}{\int_0^h \frac{1}{\mu(y')}dy'} .$$

Hint: y' is a dummy variable of integration. Try setting w(y') = μ(y')(du/dy') and integrating the expression. (10 marks total for parts a and b)

6. Make an excel spreadsheet (or other type of program if you like) to allow you to calculate the integral numerically for an arbitrary viscosity structure. Next week you will use the spreadsheet to carry out the calculations for arbitrary structures. This week, however, please use a constant viscosity to show that it gives the expected response for the two simplified flow conditions (Couette flow and when dP/dx=constant but u=0). (20 marks)

Hint 1: You should have one column of depths and one column that is the viscosity at that depth. Even though the viscosity you will use this week is constant, this form will allow it to be varied arbitrarily next week. You should be able to carry out the integration with two separate calculations for the two integrals, and add them together in a final column. The constant *s* will depend on the values of the last row in the integrals.

Hint 2: If you use a viscosity that is close to the real viscosity of the mantle, you could run into numerical problems because computers are not all set up to deal with such large values. Instead, use a viscosity of 1 during the main calculations and later on when you are asked about real earth problems--multiply the answers by the appropriate value to get an answer for the real earth.

Email your spreadsheet to me to back up the plots and discussion. Save your spreadsheet for the next assignment, as you will use it for further calculations. **Your mark will depend on the writeup though—spreadsheets with no explanation are not acceptable.**

Guidelines for writing reports on spreadsheet results:

1) Graphs are better than tables to explain most points.
2) Graphs must be labelled so that somebody else can understand them. If there are two types of lines or symbols, they need to be explained in a key or a caption. If you print your graphs in black and white, be sure that something besides colour distinguishes them--e.g., symbol shape.
3) Font size should be large enough for me to read--e.g, 12 point, both in the text and on figures.
4) Give your graphs figure numbers so that when you discuss them, you can refer to them.
5) You don't need to plot every single graph you've generated--showing a few that explain the points you are trying to make will be sufficient.
6) Be sure that you *do* explain your graphs so that it's clear you understand what you've done. And be sure that when you make points, you *do* include the graphs that illustrate those points.