Chapter 1

Methods and Modeling

1.1 Introduction

This course is designed to be a first course in numerical methods that gives you the basic tools (and the *insight* to use them) that allow you to use computers to solve math and science problems that occur regularly but are not solvable with standard closed form analytic techniques. Numerical methods is actually a vast subject spanning much of mathematics and computer science but here we will focus on the nuts and bolts techniques that form the fundamental toolkit that will be expanded on in CM2: Numerical methods for Partial Differential Equations.

Here we will cover seven specific subjects

- Interpolation and Approximation
- Root Finding and optimization of functions of a single variable $f(x)$
- Numerical Integration (quadrature) and differentiation
- Solutions of ODE's for Initial Value problems
- Numerical Linear Algebra
- Solving non-linear systems of equations
- ODE Boundary Value problems and introduction to numerical PDE's

Each of these problems is mathematically interesting in its own right and we will spend considerable time understanding the issues and implementations of each one. However, effective problem solving often requires using many of them to solve real problems. This becomes more apparent when you begin to understand *Mathematical Modeling*, which is the general black-art of taking a narrative from nature or experiment and turning it into a set of mathematical relations that require solution. Much of applied Mathematics is driven by modeling.

This course is not a course in numerical modeling per-se, however, to motivate the course and provide context for many of the methods we will discuss in detail, it is useful to develop some simple models that we will revisit throughout the class. These examples also demonstrate how the needs for many of these numerical methods arise naturally from modeling.

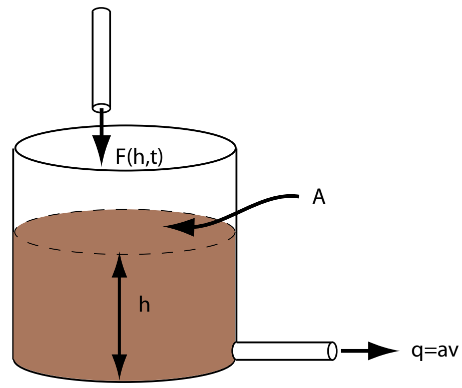

Figure 1.3.1: The Single tank model. For no source term $F = 0$

1.2 The great Boston Molasses Flood of 1919

The motivation for our models is a little known tragedy and red-letter day for zero Reynold's number fluid mechanics: The Great Boston Molasses Flood of 1919. In short, on January 15, 1919, a large tank of molasses 50 feet tall by 90 feet in diameter (holding up to 2.3 Million Gallons) burst sending a tsunami of molasses racing through the north end of boston. The molasses wave was reported to be up to 15 feet high and moved up to 35 mph. The wave had enough force to break girders, move houses. Worse yet, the incident injured ~ 150 people and killed ~ 20 (plus some horses). This is certainly not the common experience with molasses and the question is can we develop a series of mathematical models that would help understand the dynamics of this event (and more usefully demonstrate how to identify the types of methods needed to solve various problems).

1.3 Some models inspired by molasses

Rather, than jump immediately to a complex model of a molasses tsunami, it is worth producing a series of models of increasing sophistication that give insight into different aspects of the process.

1.3.1 The single tank model

Probably the simplest model that can be derived is for a single tank of molasses that drains under its own pressure. A basic question is how fast would we expect the fluid to flow if the tank didn't collapse. Figure 1.3.1 illustrates the problem. Given a cylindrical tank with area A filled to a height h with molasses, it is allowed to drain through a pipe with cross-sectional area a at velocity v. The volumetric flux out of the tank at any time is simply $q = av$.

Most models arise from conservation laws, i.e. fancy statements that "you can't get something for nothing". In this case we need to conserve mass and force balance across the pipe. The basic equation for conservation of mass is

$$\frac{d}{dt}\rho A h = -\rho q \tag{1.3.1}$$

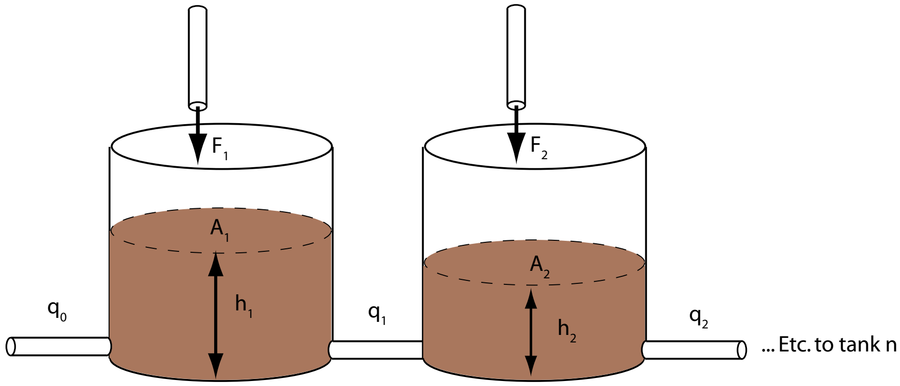

Figure 1.3.2: The two-tank model. By simply adding tanks this is easily extended to a n tank model

where ρ is the density of molasses ($\sim$ 1.2–1.4 times the density of water). Equation (1.3.1) states that the change in the mass of molasses in the tank with time is balanced by the emptying flux (why is the RHS negative?). This equation is a first order ODE but in two variables (h and q). To close the equations we need a relationship between the flux and height of molasses in the tank (clearly if $h = 0$ then $q = 0$). This relationship actually depends on the rate of flow in the pipe, however for *laminar flow*, the pressure drop across a pipe is given by

$$\delta p = \rho C q \tag{1.3.2}$$

where C is a constant of proportionality that depends on things like the pipe diameter, pipe length, and fluid viscosity (for more details see this pipeflow calculator). Now the pressure drop across the pipe should depend only on the weight of molasses in the tank, i.e. $\delta p = \rho g h$ where g is the acceleration due to gravity. Substituting in Eq. (1.3.2) yields

$$q = kh \tag{1.3.3}$$

where $k = g/C$. In this case the flux is *linear* with h. Substituting Eq. (1.3.3) into Eq. (1.3.1) gives

$$\frac{d}{dt}Ah = -kh \tag{1.3.4}$$

Now this problem is a linear first order ODE which you really shouldn't need a computer to solve. For the initial condition $h(t = 0) = h_0$ the solution to Eq. (1.3.4) is $h(t) = h_0 e^{-\alpha t}$ where $\alpha = k/A$. With this model we expect the tank to empty exponentially with e-folding time $1/\alpha$.

Themes and Variations

The simplest 1-Tank model does not require numerical methods, however, it is easy to add minor changes that lead to more complex problems. Here are a few

Turbulent Pipes The model in Eq. (1.3.4) is only valid if the flow in the pipes is laminar, i.e. the Reynolds number $\mathrm{Re} = vd/\nu < 2300$ where d is the pipe diameter and ν

is the dynamic viscosity of molasses (about 100,000–400,000 times more viscous than water, depending on the temperature). For a pipe 1m in diameter moving at a meter per second, molasses should be laminar, however, if the velocity were 16ms^{-1}, comparable to the flood speeds, then $\mathrm{Re} \approx 20,000$ and the flow would be turbulent (alternatively if the material were water rather than molasses, the flow would also be turbulent). In the turbulent regime, there are a number of empirical relationships between pressure drop and flux (see pipeflow calculator) for example $\delta p = \rho C_b q^(7/4)$ in the *Blasius Regime* or more generally $q = k_b h^m$ where m is some exponent other than one. For a single tank problem, this non-linear system can still be solved analytically by seperation. But if there are more than one tank life gets trickier (see below).

Steady state with a source term A working tank should stay empty so a simple addition to the problem is to add a source term that automatically adds mollases as the pressure drops. In general the linear problem becomes

$$\frac{d}{dt}Ah = -kh + F(h) \tag{1.3.5}$$

or supposing we want a source that increases as h drops we could try to desing a system such that $F(h) = Be^{-h}$ where B is an adjustable constant. In this case the dynamic problem becomes

$$\frac{d}{dt}Ah = -kh + Be^{-h} \tag{1.3.6}$$

Which is also a non-linear dynamical system. The big question here is whether there exists values of k and B such that this system has a steady state, i.e. such that

$$-kh + Be^{-h} = 0 \tag{1.3.7}$$

. If such a steady state exists, the next question is invariably is it stable. To attack these kinds of problems we first need to solve Eq. (1.3.7) which cannot be done in a closed form. This is a classic non-linear root finding problem and will occupy much of the second section of the course.

1.3.2 Multi-Tank Models

An entire new set of models can be developed assuming if we add tanks to form a coupled system (e.g. a tank farm). This is actually an intermediate step on the way to a full blob model that can be thought of as a very large number of tanks in a row. Figure 1.3.2 shows this new setup and again conservation equations can be formed for each of the tanks. For each tank the change in mass of the tank must be balanced by the *net* fluxes in and out. E.g. for tank 1

$$\frac{d}{dt}A_1h_1 = -(q_1 - q_0) + F_1 \tag{1.3.8}$$

Note: the fluxes are signed quantities...if flux is positive, material moves $\rightarrow$ if the flux is negative materials move $\leftarrow$. Note carefully the signs in Eq. (1.3.8). Likewise the conservation equations for tank 2 become

$$\frac{d}{dt}A_2h_2 = -(q_2 - q_1) + F_2 \tag{1.3.9}$$

or for a generic tank i

$$\frac{d}{dt}A_i h_i = -(q_i - q_{i-1}) + F_i \tag{1.3.10}$$

Again to close the system we need to relate the fluxes to the pressures (heights) in the tank which for the linear model can be written

$$\begin{aligned} q_0 &= -k_0 h_1 \\ q_1 &= k_1(h_1 - h_2) \\ q_2 &= k_2 h_2 \end{aligned} \tag{1.3.11}$$

(1.3.12)

Again. . . be careful about the signs. Substituting these relationships into Eqs. (1.3.8)–(1.3.9) and grouping terms yields

$$\begin{aligned} A_1\frac{dh_1}{dt} &= -(k_0 + k_1)h_1 + k_1 h_2 + F_1 \\ A_2\frac{dh_2}{dt} &= k_1 h_1 - (k_1 + k_2)h_2 + F_2 \end{aligned}$$

(1.3.13)

Now this linear dynamical system can be rewritten using matrix-vector notation as

$$M\frac{d\mathbf{h}}{dt} = K\mathbf{h} + \mathbf{F} \tag{1.3.14}$$

where

$$\mathbf{h} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} \tag{1.3.15}$$

are vectors of tank heights and forcing terms, and

$$M = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \quad K = \begin{bmatrix} -(k_0 + k_1) & k_1 \\ k_1 & -(k_1 + k_2) \end{bmatrix} \tag{1.3.16}$$

are matrices. In particular M is a diagonal matrix that simply scales things and K is a symmetric (negative definite actually) matrix. Thus solutions to this problem require solving the linear dynamical system

$$\frac{d\mathbf{h}}{dt} = A\mathbf{h} + \mathbf{b} \tag{1.3.17}$$

where $A = M^{-1}K$ and $\mathbf{b} = M^{-1}\mathbf{F}$. Without too much work, the two-tank model is easy to solve for both a steady state (which requires solving the linear system $A\mathbf{h} = -\mathbf{b}$) or for the time dependent problem. For example, if there is no forcing ($\mathbf{F} = \mathbf{b} = \mathbf{0}$) and initial condition $\mathbf{h}(t = 0) = \mathbf{h}_0$. The general solution of Eq. (1.3.17) is $h(t) = Se^{\Lambda t}S^{-1}\mathbf{h}_0$ where S is an matrix of eigenvectors and Λ is a diagonal matrix of eigenvalues (assuming these exists). For the two by two case, these are easy to find by hand, but for systems larger than 4 tanks, there are no closed solutions for the eigenvalues.

Themes and variations

As usual, it's easy to take a problem that is solved easily by hand and turn it into one that requires numerical methods. Here are a few examples

Multi-tank linear model Increasing the number of tanks doesn't change the symbolic form for the linear problem Eq. (1.3.14). However it does change the length of the vectors and the structure of the matrices. In particular M remains a diagonal matrix but K becomes a symmetric *tri-diagonal* matrix (i.e. the only non-zero elements are on the diagonal and on the adjacent upper and lower diagonals). These matrices have special properties and can be solved efficiently numerically. Finding eigenvalues for matrices larger than 3×3 however, cannot be done in closed form and require iterative methods which we will introduce later in the course.

Multi-tank non-linear model Finally, by simply changing the fluxes from being linear combinations of the heights to a turbulent model, the system becomes an non-linear dynamical system. For example, if we use the blasius model, the two tank system becomes

$$\begin{aligned} \frac{d}{dt}A_1h_1 &= -k_0h_1^m - k_1(h_1-h_2)^m + F_1 \\ \frac{d}{dt}A_2h_2 &= k_1(h_1-h_2)^m - k_2h_2^m + F_2 \qquad (1.3.18) \\ & \qquad (1.3.19) \end{aligned}$$

This problem is much more difficult to solve analytically however, the basic questions remain. For a given F_1, F_2, does this problem have a steady state? If it exists is it unique? is it stable? Moreover, from a practical point of view, how does one find the steady state which can be recast as finding the solutions to $\mathbf{F}(\mathbf{h}) = 0$ (where **F** is now a vector valued non-linear function of **h**. Efficient solution of non-linear systems is a complicated but important realm of scientific computation and we will investigate this problem in some detail.

1.3.3 The Blob

From one tank to two tanks to n tanks, we build up a more complex system until we're close to solving the problem of a spreading blob. In truth this problem is in the realm of partial differential equations, however, we will show that the discrete version of this problem is closely related to the multi-tank problem. The continuous model of a thin spreading blob that is collapsing under is own weight can be written as a non-linear diffusion problem

$$\frac{\partial h}{\partial t} = \frac{g}{12\nu}\frac{\partial}{\partial x}h^3\frac{\partial h}{\partial x} \qquad (1.3.20)$$

where $h(x)$ is the profile of the blob height (Figure 1.3.3), g is gravity and ν is the blob viscosity as before (see [2, 3, 1]) . There are many numerical methods required to solve Eq. (1.3.20) and many different approaches, all with pros and cons. Strictly speaking this is the realm of numerical PDE's but by the end of this course you should be well prepared to begin tackling these problems.

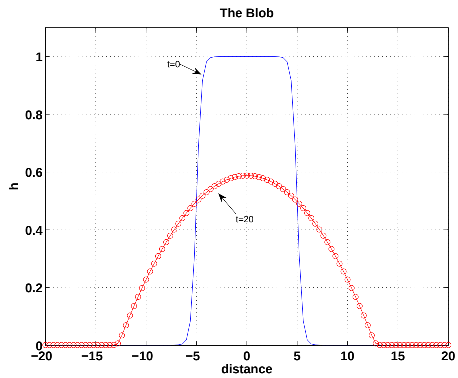

Figure 1.3.3: The blob: a discrete control volume, method-of-lines solution to Eq. (1.3.20) for an initial condition shown in blue at $t = 0$ which spreads under its own weight to the profile shown at $t = 20$. This particular model discretizes the continous space operators as piece-wise linear functions and integrates in time with a 5th order embedded runge-kutta scheme.

The big key to handling all of these problems is to develop the fluency in both math and computation that allows you to move smoothly between the discrete and continous approximations of models and keep your heads straight about all the underlying errors that arise from models, discretization errors and the fundamental issues of pretending to handle real numbers on finite-precision computers. This is our next step to understand the sources of error.

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