Numerical Methods II, Courant Institute, Spring 2024
http://www.math.nyu.edu/faculty/goodman/teaching/NumericalMethodsII2024.html
Jonathan Goodman, February, 2024

Assignment 2, Diffusion in steady state,

due March 12, 5:15 pm.

Diffusion is a slow process in which "stuff" (a chemical or heat) re-distributes itself in a background material. A basic model of diffusion involves a density function $u(x)$ and a diffusion coefficient $\mu(x)$. The diffusion coefficient is a property of the material that determines how fast stuff diffuses through it. You can think of a planar sheet of metal with heat flowing through. If the sheet has variable thickness then heat flows faster where the sheet is thicker. The density $u(x)$ says how much "stuff" there is per unit area (or unit volume in 3D).

The Wikipedia article on diffusion is OK, particularly the second half with examples. It might help web searching to look for "diffusive transport" of "heat flow Fourier law", etc. Engineers use "transport" to refer to ways stuff can go from one place to another.

Flux (also called *current*) is what is the basic quantity describing diffusion. It is a vector "field" (which means having a value that can be different at each point) $F(x,y) = (F_x(x,y), F_y(x,y))$. The quantity of stuff inside a "control volume" V (we are doing 2D, so volumes really are areas) is

$$Q_V = \int_V u(x,y)\,dxdy\ .$$

There are two "mechanisms" that can change Q_V, diffusion described by a *diffusive flux* F, and external "forcing" described by a *source term* $f(x,y)$. According to vector calculus, if $B = \partial_V$ is the boundary of V, then the flow rate of stuff across B is

$$\oint_B F\cdot n\,dl\ .$$

Here dl is the element of line length on the curve B and n is the unit outward normal. The divergence theorem is (we write the divergence as $\mathrm{div}(f) = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y}$)

$$\oint_B F\cdot n\,dl = \int_V \mathrm{div}(F)\,dxdy\ .$$

The source term adds or subtracts to Q_V directly "from the outside", f. You can think of u being heat that can be increased by an external heat source ($f > 0$) or radiated away ($f < 0$). The rate of change of Q_v because of external forcing is

$$\int_V f(x,y)\,dxdy\ .$$

In an equilibrium steady state forcing balances diffusion to give zero net rate of change for any control volume. This means

$$\oint_B F \cdot n \, dl = \int_V \mathrm{div}(F) \, dxdy = \int_V f(x,y) \, dxdy \; . \tag{1}$$

This is supposed to hold for every control volume V, so it should hold "pointwise", for every x and y:

$$\mathrm{div}(F)(x,y) = f(x,y) \; . \tag{2}$$

Fick's law[1] is a model of diffusive flow. It says that "stuff" flows from high density (where u is large) toward low density (where u is small) with a flux proportional to the negative gradient:

$$F(x,y) = -\mu(x) \nabla u(x,y) \; . \tag{3}$$

You can combine Fick's law with the flux balance equation (2) to get[2]

$$\mathrm{div} \, (\, \mu(x,y) \nabla u \,) = -f \; . \tag{4}$$

In a homogeneous medium (think of a metal plate of constant thickness), μ will be a constant that can be taken out of the equation, which leaves the Laplace equation

$$\mathrm{div} \nabla u = \frac{\partial}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial}{\partial y} \frac{\partial u}{\partial y} = \triangle u = -f \; .$$

Exercise 1. Show that the Dirichlet integral and variational principle for the Laplace equation generalize to

$$\mathcal{E}(u) = \int_\Omega \mu(x,y) \, |\nabla u(x,y)|^2 \; dxdy = -\int_\Omega u \, \mathrm{div} \, (\, \mu(x,y) \nabla u \,) \; dxdy \; , \tag{5}$$

and

$$u \text{ minimizes } \quad \frac{1}{2} \mathcal{E}(u) - \int_\Omega f(x,y) \, u(x,y) \, dxdy \; . \tag{6}$$

We create a *conservation form* (also called *flux form*) discretization of the PDE (4). There is a grid spacing Δx and $x_j = j \Delta x$ and $y_k = k \Delta x$. The domain for the PDE is the unit square. There are n grid intervals in each direction, so $n \Delta x = 1$.

Unlike before, the discrete variables U_{jk} do not represent *point values* but *cell averages*. The *cell* C_{jk} (also called *control volume*, particularly in 3D or if they are not simple squares) is the square with side length Δx and lower left

[1] The same model is often called the *Fourier law* when it is applied to diffusion of heat. Fourier wrote a book on heat diffusion and showed how Fourier series and Fourier integrals could be used to solve the equations.

[2] You can understand the minus sign with a 1D example. Suppose there is a uniform heat positive source for $0 \le x \le 1$ with boundary conditions $u = 0$ at $x = 0$ and $x = 1$. Then $u(x) = Cx(1-x)$ has $u_{xx} = -2C = f$. The minus sign makes $u > 0$ in the interior when f is positive.

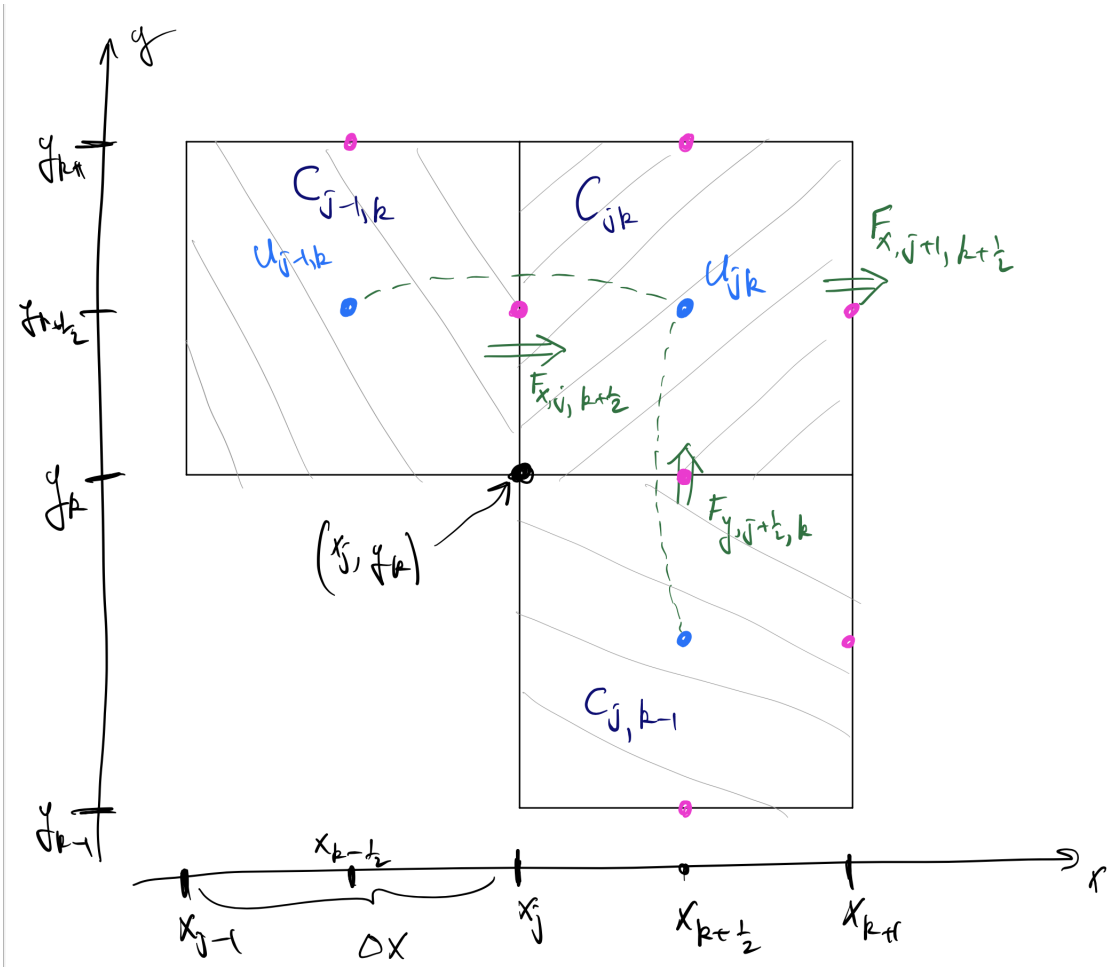

Figure 1: Cells (control volumes): black squares with gray shading. Cell centers: blue dots. Cell edge centers: magenta dots. Fluxes: green arrows based on differences connected by green dashed lines. Cell $C_{j,k}$ has (x_j, y_k) as its lower left vertex.

vertex at (x_j, y_k) (see Figure 1). The area of each cell is Δx^2. The discrete variables U_{jk} are meant to approximate the cell averages

$$U_{jk} \approx \overline{u}_{jk} = \frac{1}{\Delta x^2} \int_{C_{jk}} u(x,y)\, dxdy \ .$$

There are n^2 cells, with j and k running from 0 to $n-1$.

We say that the value U_{jk} is *cell centered* because it is a second order accurate estimate of the solution at the center of the cell, which is $u(x_{j+\frac{1}{2}}, y_{k+\frac{1}{2}})$. If the scheme is second order accurate, then

$$U_{jk} = \overline{u}_{jk} + O(\Delta x^2) = u(x_{j+\frac{1}{2}}, y_{k+\frac{1}{2}}) + \Delta x^2 \ . \tag{7}$$

In particular, U_{jk} is only first order accurate as an estimate of vertex value $u(x_j, y_k)$.

The conservation form discretization of the PDE (4) may be regarded as an approximation of the conservation law (1) for each control volume C_{jk}. There are *numerical fluxes* that are *centered* at the centers of the cell edges (see Figure 1).

$$F_{x,j,k+\frac{1}{2}} \approx F_x(x_j, y_{k+\frac{1}{2}}) = \frac{1}{\Delta x} \int_{y_k}^{y_{k+1}} F_x(x_j, y)\, dy + O(\Delta x^2) \tag{8}$$

$$F_{y,j+\frac{1}{2},k} \approx F_y(x_{j+\frac{1}{2}}, y_k) = \frac{1}{\Delta x} \int_{x_j}^{x_{j+1}} F_y(x, y_k)\, dx + O(\Delta x^2) \ . \tag{9}$$

The numerical fluxes are estimated using Fick's law and finite difference approximations of the derivatives, all centered at the midpoints of the appropriate cell edges (see where μ is evaluated in each case):

$$F_{x,j,k+\frac{1}{2}} = \mu(x_j, y_{k+\frac{1}{2}}) \, \frac{U_{jk} - U_{j-1,k}}{\Delta x} \tag{10}$$

$$F_{y,j+\frac{1}{2},k} = \mu(x_{j+\frac{1}{2}}, y_k) \, \frac{U_{jk} - U_{j,k-1}}{\Delta x} \ . \tag{11}$$

The discretization consists of an approximation to the divergence condition (2) at each cell center

$$\frac{1}{\Delta x} \left[F_{x,j+1,k+\frac{1}{2}} - F_{x,j,k+\frac{1}{2}} \right] + \frac{1}{\Delta x} \left[F_{y,j+\frac{1}{2},k+1} - F_{y,j+\frac{1}{2},k} \right] = f(x_{j+\frac{1}{2}}, y_{k+\frac{1}{2}}) \ . \tag{12}$$

Exercise 2. Verify the second order accuracy of cell and edge averages. These are the second inequalities in (7), (8), and (9). Verify the second order accuracy of the fluxes. That is, if you use $\overline{u}_{jk}$ instead of U_{jk} in (8), the result is a flux approximation that agrees with the true flux at the midpoint of the cell edge to second order:

$$\overline{F}_{x,j,k+\frac{1}{2}} = F_x(x_j, y_{k+\frac{1}{2}}) + O(\Delta x^2) \ .$$

Warning. You might think differences of second order accurate approximations yield only first order approximations. Suppose you have $G_j = g(x_j) + O(\Delta x^2)$. The centered derivative approximation might be only first order:

$$g'(x_{j+\frac{1}{2}}) \approx \frac{G_{j+1} - G_j}{\Delta x} + O(\Delta x) \ .$$

However, it is second order if the error in G is, at least to leading order, a smooth function of x, as in

$$G_j = g(x_j) + \Delta x^2 h(x_j) + O(\Delta x^3) \ .$$

We want to apply Dirichlet boundary conditions $u = 0$ when $x = 0$ or $x = 1$ or $y = 0$ of $y = 1$. This may be implemented using a version of the ghost cell trick. Create ghost cell values outside the domain whose values are the "reflections" of values just inside the domain. This is $U_{-1,k} = -U_{0,k}$, $U_{n,k} = -U_{n-1,k}$, etc. With this, the equations (12) form a system of n^2 equations for the n^2 unknowns U_{jk} for $j = 0, \cdots, n-1$ and $k = 0, \cdots, n-1$.

Exercise 3. Assume that the diffusion coefficient μ is strictly positive and smooth. Show that these equations may be formulated in matrix form as $AU = f$ where A is a symmetric and positive definite matrix. Find a formula for the discrete Dirichlet functional that is a second order accurate approximation to the continuous Dirichlet integral (5). Find a variational formulation of the discrete equations and derive a Gauss Seidel algorithm that is guaranteed to converge to the solution. *Extra credit.* Formulate and prove continuous and discrete Poincaré inequalities.

Computing exercise

Write a code to implement the finite volume discretization and solve the equations using Gauss Seidel. Please produce the following "deliverables", do some experiments on your own, and comment on the results.

1. Take $\mu(x, y) = 1 + Ae^{-\frac{(x-\frac{1}{2})^2}{2r^2}}$ with $A > -1$.

2. Take $u = xy(1-x)(1-y)$ and compute f so that the PDE (4) is satisfied. Show that your method produces a second order accurate approximation to this u. [It is a common trick to do code validation using a made-up problem you know the answer to.]

3. Make contour plots of the solution and plots of the size of the update as a function of Gauss Seidel iteration number.

4. Apply your code to model a heat conducting plate with a vertical strip of high conducting material in the middle, with uniform heat forcing $f = 1$ for all x and y. Numerically, this means taking A large and r small,

in a way you will determine by numerical experiments. Intuitively, this should be similar to setting $u = 0$ when $x = \frac{1}{2}$. Can you verify this computationally?

Suggestions for more experiments Do not to all of these, or possibly even any of them. Feel free to ask other questions – interesting configurations to try, etc.

- Is the code second order when f or μ is discontinuous?
- Is the convergence rate of Gauss Seidel proportional to Δx^2?
- If you write in a compiled language it will run far faster. You can notice a big difference between the run times with you put j or k in the inner loop.