Advection-Diffusion Equation

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Spring 2024

1 Control volume derivation

Consider a fluid that carries a continuum substance whose density in the fluid is given by $c(x, t)$. For a control volume, we can perform a balance of mass:

$$\frac{\partial}{\partial t} \int_\Omega c d\Omega = - \int_{\partial\Omega} \underline{q} \cdot \hat{n} dS$$

where $\underline{q}$ is the flux of the substance and $\hat{n}$ is an outward facing normal. The minus sign is so that the contribution of outgoing material, where $\underline{q}$ and $\hat{n}$ are parallel, is negative. The quantity c is often called the concentration, which similar to density, measures the amount of the substance at each point. This equation says that the time rate of change of mass is the net loss/gain of material through the boundaries. This assumes no mass source terms. Now, we can write a constitutive law for the flux. We say that gradients in the concentration cause fluxes, which essentially states that things tend to mix toward uniformity. In other words, there is a flow of the substance from high to low concentrations. This analogous to saying that heat flows from high temperature to low temperature, which tends to lead to uniformity of the temperature field in a body. This is called a diffusive effect. Thus we have that

$$\underline{q}_{diff} = -D \frac{\partial c}{\partial \underline{x}}$$

where D is simply a constant of proportionality that measures the resistance of medium to diffusion of concentration. There is another means of mass transport, which is the background fluid moving the substance with the velocity field. This is not a fluid mechanics problem, so we assume that the velocity field is specified and that the concentration has no influence on it. This is called advection. Advective flux is in the direction of the velocity, and depends on the concentration. We can write

$$\underline{q}_{adv} = c(x, t) \underline{u}$$

Plugging this into the balance of mass equation and noting that the control volume is independent of time, we have

$$\frac{\partial}{\partial t}\int_\Omega cd\Omega = \int \frac{\partial c}{\partial t}d\Omega = -\int_{\partial\Omega}(-D\nabla c + c\underline{u})\cdot\hat{n}dS = \int_\Omega \nabla\cdot(D\nabla c - c\underline{u})d\Omega$$

The control volume is arbitrary so this equation must hold pointwise. This leads to the local form of the mass balance law with advection and diffusion:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x_i \partial x_i} - u_i\frac{\partial c}{\partial x_i}$$

Notice we have used the incompressibility of the fluid velocity field $\frac{\partial u_i}{\partial x_i} = 0$, which is often a reasonable assumption that simplifies the governing equation. In one spatial dimension, this equation is

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - u(x)\frac{\partial c}{\partial x}$$

2 Derivation using material derivative

As opposed to using the control volume derivation, which admittedly is pretty natural in this case, it is possible to go about this by applying conservation of mass to a fixed collection of particles. For a set of particles defined by a region in the reference configuration, can say that the rate of change of mass is due to a balance of in and outflow from diffusive flux:

$$\frac{D}{Dt}\int \rho cd\Omega = -\int q\cdot\hat{n}dS = \int D\nabla c\cdot\hat{n}dS = D\int \nabla^2 cd\Omega$$

The Reynold's transport theorem can be used to pass the material derivative inside the integral onto the concentration. Localizing the integral leads to

$$\rho\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + u(x)\frac{\partial c}{\partial x} = D\nabla^2 c$$

where we have assumed that the density of the substance is the constant 1. This is the same equation obtained with the control volume method. The material derivative has the appearance of being a simple application of the chain rule, but it is quite a complex thing when it is further scrutinized. We see from these two methods that we can either look at a fixed region in space and keep track of the in and out flows, or look at a collection of particles but convert (through the material derivative) to the rates of change that particles see with respect to quantities defined in spatial/current configuration. Let's look into the material derivative a bit more carefully with an example. Consider the 1D deformation

$$x(t) = \phi(X,t) = X - X(X-1)\sin(\pi t) = X^2\sin(\pi t) - X(1 + \sin(\pi t))$$

It can be shown that the inverse deformation is

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$$X(t) = \phi^{-1}(x, t) = \frac{1}{2\sin(\pi t)}\left(1 + \sin(\pi t) - \sqrt{(1 + \sin(\pi t))^2 - 4x\sin\pi t}\right)$$

This is a fluid-like deformation because the particles are contained in the same region over all time, which is like fluid flowing in a container. We can specify an Eulerian quantity defined spatially, (not over material points), as $c(x, t)$. This could be the concentration, and it may have explicit time dependence. The rate of change of c that a particle in the reference configuration sees is

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{\partial}{\partial t}\phi(X, t)$$

This can be seen with by playing with the time parameter in this plot. The concentration that particle sees as a function of time is due to an explicit time rate of change and moving through concentration gradients via the velocity. This is still a confusing expression though, as it is defined partially in the current configuration and partially in the reference configuration. Remember that the concentration is Eulerian, so if we want all of the quantities defined in terms of a reference particle, we need to write

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t}\Big(\phi(X, t), t\Big) + \frac{\partial c}{\partial x}\Big(\phi(X, t), t\Big)\frac{\partial}{\partial t}\phi(X, t)$$

The particle will occupy different positions in space according to the deformation, so this derivative is not taken at a fixed spatial point. In my opinion, this is the easier version of the material derivative to think about. This quantifies the time rate of change a given particle sees. What if we want to define this derivative at a fixed point in space? This is natural for the concentration which is already defined this way, but strange from the perspective of the deformation. When we want the "particle derivative" at a fixed spatial point, we are no longer tracking a fixed particle, rather just some particle in the reference configuration. Note that it is important to track particles because particles are what respect conservation laws such as those of mass or momentum, rather than regions of space. In our example, we have

$$\frac{\partial \phi}{\partial t} = -\pi\cos(\pi t)X(X - 1)$$

This is the velocity specified in terms of material points. If we want the velocity that some particle sees occupying position x at time t, then we can write

$$\frac{\partial \phi}{\partial t} = -\pi\cos(\pi t)\phi^{-1}(x, t)\Big(\phi^{-1}(x, t) - 1\Big)$$

The expression for the inverse deformation is too long to be worth writing out explicitly. In general, the material derivative evaluated fully in the current configuration is

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t}(x,t) + \frac{\partial c}{\partial x}(x,t)\frac{\partial \phi}{\partial t}\left(\phi^{-1}(x,t),t\right)$$

The second term in this expression says: find the particle corresponding instantaneously to the spatial position x, compute its velocity, then look at the rate of change it experiences as a result of moving through the concentration gradient defined spatially. Of course, the explicit time rate of change is added on to this as well. See this plot, which is a slight variation of the previous one, to help visualize this. Note that if we want to completely avoid keeping track of labeled particles, we can rename the quantity involving the time derivative of the deformation as

$$\frac{\partial \phi}{\partial t}\left(\phi^{-1}(x,t),t\right) := u(x,t)$$

This is simply the velocity of *some* particle at a given spatial point and time. When the velocity is known and does not vary with time, we recover the advection-diffusion equation we derived above.

3   Notes on diffusion

When the velocity is zero, we have a pure diffusion equation. There is a very nice physical interpretation of pure diffusion dynamics. See Figure 1 for the problem setup. We imagine a function f which keeps track of the number of particles of some substance at discrete positions labeled $n-1, n, n+1, \ldots$. This is like measuring the concentration by counting particles. Let's say that over the course of an increment of time Δt, the particles jump around randomly. In one dimension, they have equal probability of staying in place, jumping to the left, or jumping to the right. This is just an assumption, but it seems like a reasonable one. If the particles are moving around randomly, that they would do so with uniform probability seems natural. The central limit theorem states that the variance of the sum of many random quantities is very small. Thus, when the number of particles is large, the variance of the mean of the number of particles of going left, right, and staying in place becomes very small. This means that when the number of particles is very large, then to a good approximation exactly 1/3 of the particles go left, 1/3 stay in place, 1/3 go right. Even without recourse to the central limit theorem, it is intuitive that an averaged response of a system comprising many particles acting independently is a good approximation. What are the odds that every particle goes to the right? Clearly, the likelihood of something "weird" like this happening decreases as the number of particles grows. Note that we are assuming that in a given time increment, a particle cannot jump two positions. We can thus compute the change in the number of particle at position n in the time increment by a simple counting argument:

$$\frac{\Delta f}{\Delta t} = \left(f(n) - \frac{2}{3}f(n) + \frac{1}{3}f(n-1) + \frac{1}{3}f(n+1)\right) - f(n)$$

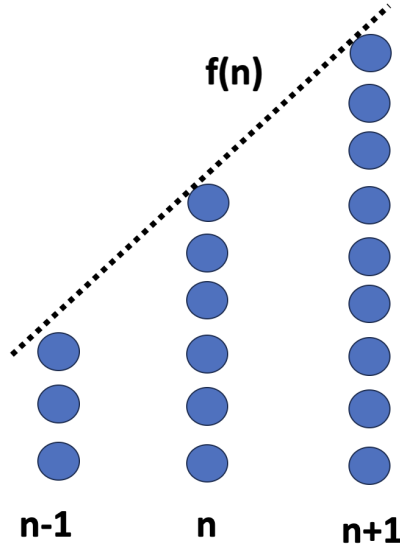$$= \frac{1}{3}\Big(f(n-1) - 2f(n) + f(n+1)\Big)$$

Figure 1: Counting the number of particles at different position in a 1D medium.

Note that if each labeled point is separated by a small distance Δn, the second derivative of f can be approximated with

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{1}{\Delta n^2}\Big(f(n-1) - 2f(n) + f(n+1)\Big)$$

Thus we see that the rate of influx from the random jumping of particles is proportional to the second spatial derivative of the function f, which counts the number of particles. This also states that when $f(n)$ is linear, the same number of particles exit and enter on average. Calling the empirical constant of proportionality D, and taking the limit as the time step becomes small, we obtain the governing PDE for 1D diffusion:

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}$$

This argument is a bit hand-wavey, but it appears to get at the essential dynamics of a diffusive process. Explicitly counting the number of particles of some substance is obviously impractical, so the counting function f is replace with the concentration c, which measures something more like a relative density of particles. It is interesting to see that the dynamics of a diffusive process arise from a probabilistic argument about some quantity (it could be number of particles, energy, momentum, etc.) spreading out due to random motion.

4 Numerical Solution

We can solve this PDE with a space-time weak form. Integrate against a basis for the solution approximation defined in terms of space-time shape functions $f_i(x,t)$. The weak form is

$$\int_0^T \int_0^L \frac{\partial c}{\partial t} f_i(x,t)dxdt = \int_0^T \int_0^L D\frac{\partial^2 c}{\partial x^2} f_i(x,t) - u(x)\frac{\partial c}{\partial x} f_i(x,t)dxdt$$

We assume zero concentration boundary conditions at $x = 0, L$ which ensures that $f_i(0,t) = f_i(L,t) = 0$. The problem is driven by an initial condition on the concentration $c(x,0) = c_0(x)$. The velocity $u(x)$ is prescribed. The first thing we will do is integrate by parts the second spatial derivative. The weak form becomes

$$\int_0^T \int_0^L \frac{\partial c}{\partial t} f_i(x,t)dxdt = -\int_0^T \int_0^L D\frac{\partial c}{\partial x}\frac{\partial f_i}{\partial x} - u(x)\frac{\partial c}{\partial x} f_i(x,t)dxdt$$

Now we discretize the solution field. We build in the initial condition so that it is automatically satisfied. The solution can be written as

$$c(x,t) = c_0(x)g(p,t) + \sum_i c_i f_i(x,t)$$

where the first term enforces the initial condition and the hyperparameter p controls how quickly the initial concentration stops contributing to the solution approximation.

$$\int_0^T \int_0^L \left(c_0\frac{\partial g}{\partial t} + \sum_j c_j\frac{\partial f_j}{\partial t}\right) f_i(x,t)dxdt = -\int_0^T \int_0^L D\left(\frac{\partial c_0}{\partial x}g(t) + \sum_j c_j\frac{\partial f_j}{\partial x}\right)\frac{\partial f_i}{\partial x}dxdt$$

$$-\int_0^T \int_0^L u(x)\left(\frac{\partial c_0}{\partial x}g(t) + \sum_j c_j\frac{\partial f_j}{\partial x}\right) f_i(x,t)dxdt$$

$$\sum_j c_j\left(\int_0^T \int_0^L \frac{\partial f_j}{\partial t} f_i dxdt + D\frac{\partial f_j}{\partial x}\frac{\partial f_i}{\partial x} + u(x)\frac{\partial f_j}{\partial x} f_i dxdt\right)$$

$$= -\int_0^T \int_0^L u(x)\frac{\partial c_0}{\partial x}g(t)f_i - c_0\frac{\partial g}{\partial t}f_i - D\frac{\partial c_0}{\partial x}g(t)\frac{\partial f_i}{\partial x}dxdt$$