3 Problem set #3: Non-diffusive transport

All the example codes shown in class can be found in on the webpage. Just download and unpack `probset3.tar.gz`. (i.e. `gzcat -v probset3.tar.gz |tar -xvf -`. Good luck and may the force be with you.

Radioactive Tracer transport in an aquifer

This problem addresses the more general problem of advection with non-diffusive source terms or variable velocities. One geologically relevant problem that demonstrates all of these issues is the transport of a radioactive trace element in chemical equilibrium in a porous flow system of fluid and solid. The general dimensional 1-D equation for conservation of mass of the element can be written

$$\frac{\partial}{\partial t}\left[(\rho_f\phi + \rho_s(1-\phi)D)c^f\right] + \frac{\partial}{\partial x}\left[\rho_f\phi w c^f\right] = -\lambda[\rho_f\phi + \rho_s(1-\phi)D]c^f \tag{3.1}$$

where ρ_f, ρ_s are the densities of the fluid and solid respectively, ϕ is the porosity, D is the equilibrium partition coefficient of the tracer[1], c^f is the fluid concentration and w is the fluid velocity (we will assume that we are in the frame of the solid such that $W = 0$)

1. **Show that** that by defining the *total tracer density* $\rho = (\rho_f\phi + \rho_s(1-\phi)D)c^f$, Eq. (3.1) can be rewritten as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho w_{eff}}{\partial x} = -\lambda\rho \tag{3.2}$$

   where

$$w_{eff} = \frac{w}{1 + D'(x)} \tag{3.3}$$

   is the *effective tracer velocity* and

$$D'(x) = \frac{\rho_s(1-\phi)D}{\rho_f\phi} \tag{3.4}$$

   is the *effective partition coefficient*. Note if $D' = 0$ the tracer moves at the fluid velocity and as $D' \to \infty$, $w_{eff} \to 0$ as the tracer spends all its time in the solid. Note that even for constant porosity and constant w, if the partition coefficient varies along the path, then the tracer velocity will vary.

2. **non-dimensionalize (3.2)** using the time it takes an element that moves at the fluid velocity w to move a distance d. Assume that we can scale the tracer density by some characteristic value ρ_0. From here on out we will assume w, ρ_s, ρ_f and ϕ are constant. How many adjustable dimensionless parameters remain and what do they mean physically? You can drop the primes in all the dimensionless equations as long as you are clear about it.

[1] In chemical equilibrium the concentration of a tracer in the solid is related to the concentration in the liquid by $c^s = Dc^f$.

3. **Write down the following algorithms** to solve the dimensionless equations
   (a) control-volume staggered leap-frog scheme
   (b) semi-Lagrangian scheme with source terms (do not assume that w'_{eff} is constant)
   (c) 2nd-order iterative Runge-Kutta Pseudo-spectral scheme. (for simplicity you can use the notation PSdx$[\rho^n]$ to denote the pseudo-spectral approximation to the first partial spatial derivative of ρ at time step n. Just know how to calculate PSdx...).

4. Now **choose one** of the following variants to solve
   (a) **Constant velocity and radioactive decay:** Assume a constant dimensionless effective velocity $w'_{eff} = 1$.
      i. What is the appropriate rescaling of distance such that the dimensionless equations can be written

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x} = -\rho \tag{3.5}$$

      What does a dimensionless distance $x = 1$ correspond to physically? How about a dimensionless time $t = 1$?
      ii. Solve the following artificial problem. We have a section of aquifer that is 1000m long. Wedumpit Corp. has magically placed into this aquifer, a Gaussian peak of Spiegelmonium 211 with the convenient dimensions

$$\rho' = \exp\left[-\left(\frac{x - x_{max}}{\sigma}\right)^2\right] \tag{3.6}$$

      where the peak is located at $x_{max} = 200$ m and the peak width is $\sigma = 50$m. ^{211}Sp has a decay constant of 10^{-4} per day (i.e. a half-life of ~ 19 years) and an effective transport velocity of $w_{eff} = 1$ cm/day in this aquifer. Your mission, if you choose to accept it, is to figure out the position and concentration of ^{211}Sp in 109.59 years (which should be $t' = 4$). After this time the number of practicing hydrologists will have expanded exponentially to match the number of lawyers.
      - Solve Eq. (3.5) analytically by the method of characteristics and give me the position and the peak at $t' = 4$ to 6 significant digits.
      - Now solve it numerically using any (or all) of the algorithms in Question 3. You can use the example matlab codes in `probset3/matlab/pure_advection` as templates. Play with grid spacing and time steps until you can get the fractional error of the peak concentration

to less than 5×10^{-3} and let me know what it takes. **Hint:** be careful about how you difference the decay term for the staggered-leapfrog scheme. For certain choices you can get some rather amusing and bizarre behavior.

Non-constant velocity and no decay Okay, this one's a bit harder. Assume the decay rate is zero but that the effective partition coefficient looks like

$$D'(x) = D_0 \left(1 - \exp\left[-\left(\frac{x - x_0^D}{\sigma_D}\right)^2\right]\right) \tag{3.7}$$

i. Pick one or more algorithms from question 3 and write a matlab code to to solve for advection with non-constant w_{eff}. If you get stuck, you can find fully worked example codes in `probset3/matlab/non_constant_velocity`. This problem simply reproduces the results from class.

ii. As a first problem try solving a problem with parameters $x_{max} = 40$, $D_0 = 1$, $x_0^D = 15$, $\sigma_D = 2$, $t_{max} = 40$. Play with various numerical parameters. Present your best and worst solution and argue why you think they're right/wrong. What additional information would you need to plot c_f?

iii. **Extra credit:** Solve the equations analytically using the method of characteristics and compare the true solution with the calculated solutions.

(b) **Da Works** Assume that you have both variable velocity and radioactive decay. Solve the Spiegelmonium problem (Question 4.a.ii), with the partition coefficient structure in Eq. (3.7) with $D_0 = 1$, $x_0^D = 400m$, $\sigma_D = 200m$. Show me figures for your favorite solution and argue why you think it is accurate.