

Advection-diffusion of a scalar

YBS

August 4, 2017

1 Governing equations

The time evolution of the concentration $c(\mathbf{r}, t)$ of a chemical which undergoes simultaneous diffusion (with diffusion constant η) and advection by a velocity field $\mathbf{v}(\mathbf{r}, t)$ is given by

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \eta \nabla^2 c \quad (1)$$

The left-hand-side is the material time derivative (aka advective derivative). The right-hand-side is diffusion. Physically, \mathbf{v} should also satisfy an evolution equation of its own, but for our purposes we'll just assume it's constant in time. However, we will add the (physically valid) constraint that \mathbf{v} is divergence-free, i.e. $\nabla \cdot \mathbf{v} = \sum_i \partial_i v_i = 0$. In 2D, a divergence-free vector field over a periodic domain $[0, 2\pi] \times [0, 2\pi]$ can be decomposed to Fourier components of the form

$$v_x = \sum_i A_i m_i \cos(m_i y + \beta_i) \cos(n_i x + \alpha_i) , \quad v_y = \sum_i A_i n_i \sin(m_i y + \beta_i) \sin(n_i x + \alpha_i) , \quad (2)$$

where A_i is the amplitude, m_i, n_i are integers ((m_i, n_i) is the wave-vector), and α_i, β_i are phases. For the simulation I simply draw all these parameters from a uniform distribution, using 5 terms for each simulation.

2 Numerical implementation

First, we write the time derivative explicitly as

$$\frac{\partial c}{\partial t} = \eta \nabla^2 c - \mathbf{v} \cdot \nabla c = \eta \nabla^2 c - \nabla \cdot (c \mathbf{v}) . \quad (3)$$

The last transition is valid because $\nabla \cdot \mathbf{v} = 0$.

The equations are solved on a square grid, using a staggered grid for v . That is, c is calculated on the points $(2\pi \frac{i}{N}, 2\pi \frac{j}{N})$ where N is the number of grid points in each dimension (currently 200) and i, j are integers between 0 and $N-1$. v is (pre-)computed on the points $(2\pi \frac{i-\frac{1}{2}}{N}, 2\pi \frac{j-\frac{1}{2}}{N})$. This allows implementing the right-hand-side of Eq. (3) in a conservative way, i.e. the spatial integral the right-hand-side vanishes (or alternatively, the spatial integral of c remains constant in time, as it should).

The generation of the velocity field (and the shifted spatial mesh) is done by `generate_v_field`. The script `run_collect_save` runs many simulations and collects them in a `hdf5` file. The file produced by `run_collect_save` have this format:

- The name of the file is the value of η .
- `t` is the list of times for which the solutions are calculated (uniformly spaced).
- `x` and `y` are matrices of shape $N \times N$ with the `x` and `y` coordinates of the finite-differences grid for `c`.

- Each file contains 50 realizations, which are at groups /001, /002, ..., /050:
- /XXX/c is an ndarray of shape [n,n,len(t)] that contains the concentration field. $c[i,j,k]$ is the value of the concentration field at position $x[i,j]$ and $y[i,j]$ at time $t[k]$. In other words, $c[\dots,i]$ is the snapshot of the concentration field at time $t[i]$.
- The group /XXX also contains /XXX/u,/XXX/v, which are the x and y components of the velocity field. Note that u and v are not evaluated at the same grid points as c since we use a staggered scheme to ensure conservation. The functional form of u and v is given in both MATLAB and Mathematica syntax in the attributes of /XXX.