Numerical modeling : tutorial #3

Frédéric Hourdin
hourdin@lmd.ens.fr

5 décembre 2012

1 Numerical computation of diffusion

We study here the diffusion of a trace species

$$\frac{\partial q}{\partial t} = K \frac{\partial^2 q}{\partial x^2} \tag{1}$$

whose concentration $q(x,t)$, in kg/kg of air, depends on x and time only, over a domain $[0, L]$ in x and $[0, T]$ in time.

For the coding, one can start from the program developed for tutorial #2, conserving a copy of it.

1. Let us assume that at initial time, the tracer is the superposition of two sin modes, and of a "numerical oscillation" at the grid scale :
   $q_{i,1} = \sin(4\pi x_i/x_{\max}) + \sin(17\pi x_i/x_{\max}) + OSC(i)/2$
   where $OSC(i) = 1$ for even and -1 for odd values of i, soit, en fortran

   ```
   pi=2.*asin(1.)
   xxx(i)=i*deltax
   qinitial(i)=sin(4*pi*xxx(i)/xmax)+sin(17*pi*xxx(i)/xmax)+0.5*(-1.+2.*mod(i,2))
   ```

   Plot the initial tracer concentration.
2. Code a numerical scheme for diffusion with a diffusion coefficient K given by $\beta = K\delta t/\delta x^2 = 0,1$ The flux $-K\partial q/\partial x$ will be computed at the interface between two meshes or control volumes. An explicit time scheme is retained here for the time integration.

   Only the computation of the initial concentration and the numerical scheme have to be modified with respect to tutorial #2. One can assume $q_{1,n} = q_{2,n}$ and $q_{im,n} = q_{im-1,n}$ (zero flux boundary condition) or $q_{1,n} = 0$ and $q_{im,n} = 0$, or adopt a periodic domain in x.

   It is desirable to introduce explicitely in the code a specific variable for the flux, computed as the gradient of the tracer, and then take the divergence of this flux.
3. Which scales dissipate first ? Comment with respect to the time evolution of the amplitude $A(t)$ of a sin mode $A(T)\sin(kx)$ solution of Eq 1.
4. Rerun the computation of didssipation over 10 time steps, saving results at each individual time step, but with β=0.3 and 0.6. Analyse the results obtained considering a sollution of the discretized scheme of the form $q_{i,n} = A_n OSC(i)$, where n is the time step (a link can be established with the results of tutorial #1).

5. Starting from the same initial concentration, compute advection with an upstream scheme $q_{i,n+1} = \alpha q_{i-1,n} + (1-\alpha)q_{i,n}$ avec $\alpha = U\delta t/\delta x$ (cf. TD2 and take the corresponding lines from the code). Compute 100 iteration with $\alpha = 0,2$. How can the results be interpreted ? Show that the scheme can be rewritten in the form $q_{i,n+1} = q_{i,n} + \alpha/2(q_{i+1,n} - q_{i-1,n}) + \xi(q_{i-1,n} - 2q_{i,n} + q_{i+1,n})$. From the above results, discuss the difference between the upstream and centered advection schemes observed in tutorial #2.

Remark :

as for tutorial 2, fields can be written in ascii format each 10 time step usingii par exemple tous les 10 pas de temps en utilisant, comme pour le TD2 :

```
character*4 file
do it=1,nt
....
    if (mod(it,10)==1) then
       file="q..."
       write(file(2:4),'(i3.3)') it
       open (10,file=file,form='formatted')
       do i=1,imax
          write(10,*) xxx(i),qqq(i)
       enddo
       close(10)
    endif
```

Then curves can be plotted on the screen with the following command :

```
xmgrace q*
```

You can also send the image in a file directly with the line command

```
xmgrace -hardcopy -hdevice JPEG -printfile out.jpg q*
```

('q*' means that the command is applied for all the files starting by letter 'q' in your current directory, ie here : q001, q011, q021 ... But you can use any other mean to plot the curves.