Numerical Techniques Practicum 2

Solving the advection equation

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1 Introduction

The advection equation describes transport at a constant speed c:

$$\frac{\partial \psi}{\partial t} + c\frac{\partial \psi}{\partial x} = 0 \tag{1}$$

The exact solution is given by

$$\psi(x,t) = \psi(x - ct, 0) \tag{2}$$

For this exercise, runs will be done on the HPC of UGent, while visualization will be done in a Jupyter notebook. Check the practicum on Linux and Fortran if something is unclear about this.

Preparations:

1. From the command line, create a directory for this practicum and enter it with

```
$   mkdir -p ${HOME}/numtech/adveq
$   cd ${HOME}/numtech/adveq
```

2. Copy the Jupyter notebook for visualization with

```
$   cp /user/gent/407/vsc40744/ugent/numtech/practica/practicum2-adveq/adveq.ipynb .
```

2 The upstream scheme

The upstream scheme discretizes the advection equation as

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$

or

$$\phi_j^{n+1} = (1-\mu)\phi_j^n + \mu\phi_{j-1}^n$$

where $\mu = \frac{c\Delta t}{\Delta x}$ is the Courant-number.

Exercises:

1. Copy the directory containing the upstream scheme model to your own directory

   ```
   $   cd ${HOME}/numtech/adveq/
   $   cp -r /user/gent/407/vsc40744/ugent/numtech/practica/practicum2-adveq/src/upstream/ .
   ```

2. Go to this directory with

   ```
   $   cd upstream
   ```

3. Compile and run the code with

   ```
   $   ./run.sh
   ```

4. Launch a Jupyter notebook from `https://login/hpc.ugent.be`. Go to the directory `numtech/adveq/` and open the file `adveq.ipynb`.

   The first two cells are just for loading packages and defining a plotting routine; execute them with `shirt+enter`

   The next cell allows to animate the results of the upstream scheme. Execute it with `shift+enter` (this takes some time!).

5. The stability condition for the upstream scheme is $0 \leq \mu \leq 1$. Find 3 ways to make the model unstable by changing parameters in `setup.F90` (open the file in Geany). Rerun after each modification.

6. Check the wavelength-dependency of the damping when $\mu = 0.5$. This is done by modifying the wavenumber `KX` in the file `exact_solution.F90`.

   Note: the amplification factor for $\mu = 0.5$ is $A = \frac{1+\cos k\Delta x}{2}$ where k is the wavenumber varying between 0 and $\pi/\Delta x$.

7. Why are the shortest waves often the most unstable?

3 Forward scheme, centered spatial finite differences

This scheme discretizes the advection equation like

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + c\frac{\phi^n_{j+1} - \phi^n_{j-1}}{2\Delta x} = 0$$

or

$$\phi^{n+1} = \phi^n - \frac{c\Delta t}{\Delta x}\frac{\phi^n_{j+1} - \phi^n_{j-1}}{2}$$

Exercises:

1. Start from a copy of the upstream scheme:

   ```
   $   cd ${HOME}/numtech/adveq/
   $   cp -r upstream/ forward_centered
   $   cd forward_centered
   ```

2. Change the name of this scheme in `setup.F90`:

   ```
   WRITE (77,*) '"exact" "forward_centered"'      ! experiment names
   ```

3. Change the spatial discretization into centered finite differences by modifying the file `timestep.F90`:

   ```
   IF ( IX>1 .AND. IX<NX ) THEN
     PHI1(IX)=PHI0(IX)-C*DT/DX*(PHI0(IX+1)-PHI0(IX-1))/2.
   ELSEIF ( IX==1 ) THEN
     ! periodic boundary conditions at left boundary
     PHI1(1)=PHI0(1)-C*DT/DX*(PHI0(2)-PHI0(NX))/2.
   ELSE
     ! periodic boundary conditions at right boundary
     PHI1(NX)=PHI0(NX)-C*DT/DX*(PHI0(1)-PHI0(NX-1))/2.
   ENDIF
   ```

4. Run with

   ```
   $   ./run.sh
   ```

5. The scheme is unstable, especially for short waves. Try to make it stable by reducing the timestep in `setup.F90`.

6. The scheme is unconditionally unstable! Centered finite differences are 2nd order accurate, while the upstream scheme is only 1st order accurate. How is it possible that going to a more accurate scheme leads to worse results?

4 Leapfrog time stepping, centered spatial finite differences

The discretization of this scheme is

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} + c\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

or

$$\phi_j^{n+1} = \phi_j^{n-1} - \frac{c\Delta t}{\Delta x}\left(\phi_{j+1}^n - \phi_{j-1}^n\right)$$

Exercises:

1. Calculate the dispersion relation on paper. What is the stability condition?

2. Start from a copy of the forward-centered scheme:

   ```
   $   cd ${HOME}/numtech/adveq
   $   cp -r forward_centered/ leapfrog/
   $   cd leapfrog
   ```

3. During the first timestep, the leapfrog scheme cannot be used. So a forward scheme will be taken during the first timestep. Separate subroutines for the forward and leapfrog schemes will be created:

   Rename the file `timestep.F90` to `timestep_forward.F90`:

   ```
   $   mv timestep.F90 timestep_forward.F90
   ```

   Change the subroutine name in this file to `TIMESTEP_FORWARD`.

4. Implement the leapfrog scheme starting from a copy of the forward scheme:

   ```
   $   cp timestep_forward.F90 timestep_leapfrog.F90
   ```

   Change the subroutine name in this file to `TIMESTEP_LEAPFROG`.

   Modify this file so that it implements the leapfrog scheme. Note that this will require an additional argument for ϕ^{n-1}.

5. Change the file `timeloop.F90` so that it calls the forward scheme only in the first timestep:

   ```
   IF (IT==1) THEN
     CALL TIMESTEP_FORWARD(PHI0,PHI1)
   ELSE
     CALL TIMESTEP_LEAPFROG(PHI9,PHI0,PHI1)
   ENDIF
   ```

   Don't forget to declare the array `PHI9`, and to store the current solution as the previous solution at the end of the timestep:

   ```
   ! swap results
   PHI9=PHI0
   PHI0=PHI1
   ```

6. Change the compilation command in the run script `run.sh` so that it includes the files `timestep_forward.F90` and `timestep_leapfrog.F90`. Run the program, and review the results.

7. Leapfrog is accelerating, centered differences are decelerating. Is the combination accelerating or decelerating?

8. What are the phase speed and group speed for very short waves? Check the wavenumber-dependency of the phase speed with your model.

9. The group speed can be visualized by considering a field composed of two harmonics in the file `exact_solution.F90`:

$$\psi_j^0 = \cos\left(2\pi k_1 \frac{j}{n_x}\right) + \cos\left(2\pi k_2 \frac{j}{n_x}\right)$$

where k_1 and k_2 are the wavenumbers of the two harmonics and n_x is the number of gridpoints. Take $k_1 = n_x/2 - 1$ and $k_2 = n_x/2 - 2$ for a clear view of the group speed of short waves.

5 Heun and Matsuno with centered spatial differences

(this section can be skipped if you want)

The Heun scheme is given by

$$\tilde{\phi}_j = \phi_j^n - c\Delta t \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x}$$
$$\phi_j^{n+1} = \phi_j^n - c\frac{\Delta t}{2}\left(\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} + \frac{\tilde{\phi}_{j+1} - \tilde{\phi}_{j-1}}{2\Delta x}\right)$$

The Matsuno scheme is given by

$$\tilde{\phi}_j = \phi_j^n - c\Delta t \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x}$$
$$\phi_j^{n+1} = \phi_j^n - c\Delta t \frac{\tilde{\phi}_{j+1} - \tilde{\phi}_{j-1}}{2\Delta x}$$

Exercise:

1. Implement and visualize these schemes (in separate directories). Are they stable?
(the Heun scheme is only weakly unstable, so you may need many timesteps to detect the instability)

2. Check that Matsuno is more damping for waves with an intermediate wavenumber ($k \sim n_x/4$) than for longer ($k \sim 1$) or shorter ($k \sim n_x/2$) waves.

6 Spectral model

Exercises:

1. Think about switching from the upstream scheme (see above) to a trapezium scheme:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\frac{1}{2}\left(\frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x} + \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x}\right) = 0$$

Why would this be quite difficult?

2. Copy the spectral model with forward timestepping to your H-drive with

```
$   cd ${HOME}/numtech/adveq/
$   cp -r /user/gent/407/vsc40744/ugent/numtech/practica/practicum2-adveq/src/forward_spectral
```

The scheme is formulated in spectral space like

$$\frac{\hat{\phi}_k^{n+1} - \hat{\phi}_k^n}{\Delta t} + ikc\hat{\phi}_k^n = 0$$

or

$$\hat{\phi}_k^{n+1} = (1 - ikc\Delta t)\hat{\phi}_k^n$$

The code for this equation is found in the file `timestep.F90`

3. Go to this directory, compile and run with

```
$   cd ${HOME}/numtech/adveq/forward_spectral/
$   ./run.sh
```

4. Review the results in Jupyter like for previous exercises.

   Compare these results with those of the upstream scheme. Both models use a forward time scheme. How is it possible that changing to a more accurate space discretization (spectral is more accurate than 1st order decentered) gives worse results?

5. Try to implement trapezium timestepping. In spectral space, it looks like

$$\frac{\hat{\phi}_k^{n+1} - \hat{\phi}_k^n}{\Delta t} + \frac{ikc}{2}\left(\hat{\phi}_k^{n+1} + \hat{\phi}_k^n\right) = 0$$

   or

$$\hat{\phi}_k^{n+1} = \frac{1 - ikc\Delta t/2}{1 + ikc\Delta t/2}\hat{\phi}_k^n$$

   Try to destabilize this scheme by increasing the timestep. Try to explain what you see by considering the dispersion relation for this scheme:

$$\omega = \frac{2}{\Delta t}\arctan\left(\frac{ck\Delta t}{2}\right)$$