COMPUTATIONAL FLUID DYNAMICS (CFD): DISCRETIZATION, STABILITY, DISPERSION AND DISSIPATION

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1. Overall Context

Computational Fluid Dynamics is the ability of simulating complex flow features by use of computers when analytical solutions are not accessible which is the case for a lot of flow problems. Since computers can only produce a set of mathematical operations (addition, substraction, multiplication, division and logical operations) to be operated on discrete numbers of various types (booleans, integer, real, double...), the notion of *discretization* is needed to transform the original governing equations. Different procedures can be employed to transform the evolution equations into a set of discrete values onto which operations can be applied by the computer. However all of these schemes suffer from the same problems that any CFD specialist is supposed to handle before addressing any type of simulation by use of a commercial or preferred Fortran/C++ code.

The aim of this lecture is thus to illustrate and introduce readers to the notion of:

- **Stability**: the ability of a discretization to produce approximations that are bounded or why does my code sometimes gives me nice numbers and others NAN's (Not A Number) in my solution file?
- **Dispersion and Dissipation**: the ability or inability for a discretization to attenuate oscillations or scramble a nice and continuous signal.

2. Stability of CFD Solvers

2.1. **Model Equation.** To ease the analysis, the simple $1D$ problem of convection in an infinitely long domain is proposed and for which the governing differential equation reads:

$$\frac{\partial \phi}{\partial t} + u_0 \frac{\partial \phi}{\partial x} = 0. \tag{1}$$

In the above governing equation, u_0 is the constant convection velocity of the scalar function $\phi(x,t)$ to be found and which evolves in space, x and time t. The problem is supposed infinite and an arbitrary length of 1 m with periodic boundary conditions is retained for the spatial discretization. Supposing an initial condition for $\phi(x, t = 0) = \Phi_0$, the analytical solution to this problem is known, 1, and reads: $\phi(x,t) = \Phi_0(x - u_0\, t)$ (*i.e.*: the initial profile translated by $u_0\, t$).

Figure 1. Representation of the convection problem.

Although the analytical solution is here easily accessible, the first step to the analysis is how can I discretize Eq. (1)? Different approaches exists but in the following, only Finite Difference (FD) is discussed. Other common methods in CFD are discussed in an other dedicated lecture.

2.2. **Discretization by Finite Difference.** First the notion of spatial and temporal discretization is introduced by simply considering the representation of the continuous function $\phi(x,t)$ at specific instants in time (noted t^n and locations in space (noted x_i): *i.e.* $\phi(x,t) \approx \bigcup_{i,n} \phi(x_i, t^n) = \bigcup_{i,n} \phi_i^n$. If the discrete representation of this unknown continuous function is taken at regular intervals in time and space, let's say Δt for time and Δx for space, we have a time-line represented by M points and $N+1$ points in space such that:

$$t^n = n \times \Delta t \text{ with, } \Delta t = T/N \text{ and, } n \in \{0, ..., N\}, \tag{2}$$

$$x_i = i \times \Delta x \text{ with, } \Delta x = 1/M \text{ and, } i \in \{0, ..., M\}. \tag{3}$$

Note that with the previous notation and because of peridictiy, $\phi_0^n = \phi_M^n$. Likewise at $t = 0$, $\phi_i^0 = \Phi_0(x_i) = \Phi_0(i\Delta x)$.

Figure 2. Representation of discretized problem.

FD relies on the mathematical notion of limits applied to continuous functions or by the application of Taylor expansions,

$$\left.\frac{\partial \phi}{\partial x}\right|_{t_n} \approx \lim_{\Delta x \to 0} \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\,\Delta x} \approx \lim_{\Delta x \to 0} \frac{\phi_{i+1}^n - \phi_i^n}{\Delta x} \approx \lim_{\Delta x \to 0} \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} \approx ... \tag{4}$$

(5) $$\left.\frac{\partial \phi}{\partial t}\right|_{x_i} \approx \lim_{\Delta t \to 0} \frac{\phi_i^{n+1} - \phi_i^{n-1}}{2\,\Delta t} \approx \lim_{\Delta t \to 0} \frac{\phi_i^{n+1} - \phi_i^{n}}{\Delta t} \approx \lim_{\Delta t \to 0} \frac{\phi_i^{n} - \phi_i^{n-1}}{\Delta t} \approx ...$$

Of course the discretized version of Eq. (1) and hence the associated set of operations will defer depending on the approximation retained to represent the set of partial differentiation operators present in the original governing equation. For instance, taking the first expression proposed for space and the second one for time, one obtains the so-called *Forward Euler* operator for time and the *Second ordered Centered* scheme for space:

(6) $$\frac{\phi_i^{n+1} - \phi_i^{n}}{\Delta t} + u_0 \frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\,\Delta x} = 0.$$

Note that the notion of order relates to the higher order terms introduced by the Taylor expansion upon which the discrete operators rely. Re-ordering the discrete expression obtained in Eq. (7), one clearly sees the chain of operations to be coded for the computer to apply such a scheme:

(7) $$\phi_i^{n+1} = \phi_i^{n} - u_0 \frac{\Delta t}{2\,\Delta x} \left[\phi_{i+1}^{n} - \phi_{i-1}^{n}\right].$$

Hands-on:

```
Go to the 1D CFD simulator and test the above discretization...

What do you observe after a certain number of turns?
Is the solution comparable to the exact (initial) solution?
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Note: the following differentiation schemes are possible and readers are referred to more advanced CFD books for details.

$\frac{\partial \phi}{\partial t}$	$\frac{\partial \phi}{\partial x}$	Name of the scheme
$\frac{\phi_i^{n+1} - \phi_i^{n}}{\Delta t}$	$\frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\,\Delta x}$	First order explicit in time and Centered in space
-	$\frac{\phi_i^{n} - \phi_{i-1}^{n}}{\Delta x}$	First order explicit in time and Upwind in space
-	$\frac{\phi_i^{n+1} - \phi_{i-1}^{n+1}}{\Delta x}$	First order implicit in time and Upwind in space
-	$\frac{\phi_{i+1}^{n+1/2} - \phi_{i-1}^{n+1/2}}{2\,\Delta x}$	Centered Crank Nicholson
-	$\frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\,\Delta x}$	First order explicit in time and Centered in space
$\frac{\phi_i^{n+1} - \phi_i^{n-1}}{2\,\Delta t}$	$\frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\,\Delta x}$	Explicit Leap Frog

TABLE 1. Typical numercial set ups used in CFD codes.

2.3. **Stability Analysis of a FD Scheme.** Based on the previous series of tests, one observes that the proposed scheme never produces statisfactory results and oscillations are always present. We are faced with a problem of numerical stability of the scheme: *i.e.* any approximation (truncation error, ...) are amplified by the iterative loop cooresponding to the numercial scheme resulting in an unphysical solution. In extreme cases (long time duration of the simulation and/or given spatial to time ratios), the code crashes and no physical solution can be visualized... Such a behavior, although deceptive, could have been apprehended before-hand by use of the "Von-Newmann" analysis.

The "Von-Newmann" analysis studies mathematically the future of a harmonic perturbation when injected into the scheme. Defining the perturbation of period $2\pi/k$ as, $\phi_i^n = A^n\, e^{j\,k\,x_i}$, where $j^2 = -1$) and A^n is the perturbation amplitude at instant t^n. A scheme is thus characterized by its amplification coefficient, $A = \frac{A^{n+1}}{A^n}$, which needs to remain inferior to 1 in absolute value to ensure a none exponential growth of perturbations. Injecting the expression of the harmonic perturbation in Eq. (7), one obtains:

$$\frac{A^{n+1} - A^n}{\Delta t} + u_0\, A^n\, \frac{e^{j\,k\Delta x} - e^{-j\,k\Delta x}}{2\,\Delta x} = 0, \tag{8}$$

or,

$$A = 1 - u_0\, \frac{\Delta t}{\Delta x}\, j\, sin(k\,\Delta x). \tag{9}$$

Clearly, $|A| = \sqrt{1 + [u_0\, \frac{\Delta t}{\Delta x}]^2\, sin^2(k\,\Delta x)} \geq 1$, indicating an exponential growth of any perturbation if this scheme is to be used.

Although specifically derived in the context of the scheme proposed in Eq. (7), any stability analysis results in an amplification coefficient that is essentially a function of $u_0, \Delta t, \Delta x$ and k (the amplification is a function of the perturbation period). The critical parameter that governing the absolute behavior of the scheme is express by the "Courant-Friedrich-Lewy" number:

$$\text{CFL} = \frac{u_0\, \Delta t}{\Delta x}. \tag{10}$$

Hands-on:

```
Go to the 1D CFD simulator and test various discretizations...

Can you evaluate a critical CFL number to ensure stability?
```

Hands-on:

```
For the 3rd order Runge-Kutta scheme in time and central
differencing in space, stability is ensure if and only if: CFL $\leq \sqrt{3}

Is this what you observe?
```

3. Dispersion and Dissipation of CFD Solvers

3.0.1. *Time steps.* When the CFL number is altered or the grid size modified, the time step changes as per the inequality $\Delta t < CFL \frac{\Delta x}{|u|+c}$, where u and c are respectively the local flow and local sound speeds. Hence, it is imperative to terminate computations when a pre-specified physical time is reached to obtain comparable results. Being in a fully periodic problem with propagation speeds that are known ($u + c$ for the acoustic wave studied), the time taken by the wave for one turn-around time is known and will be used. In the `run.dat` file, `istore` was set to 2, the `tlast` to $2ms$ and `dtstore` to $1ms$; `nstore` is not read.

4. Presentation of the reference runs and exploitation

4.1. **Results: TTGC and LW schemes.** Figures 3& 4 show the acoustic wave after one turn-around time ($2ms$) for three grid resolutions. For clarity, the exact solution to the problem is also plotted. As observed for this wave length, the grid resolution impacts the numerical solution in two potential ways:

- dispersion: the wave has not travelled the proper distance,
- dissipation: the maxima are not recovered and the predicted signal is "smoother".

The behavior is also found to slightly differ from one scheme to the next. The main idea of the next section is to provide hints on the evaluation of the dissipation and dispersion of both schemes. To do so and to ease the diagnostic, the reader is encouraged to produce simulations with a large number of turn-around times: 10.

4.2. **Dissipation and dispersion.** In order to ease the exploitation of the results, the mathematical concepts of dispersion and dissipation are detailed here. For simplicity, one assumes the temporal integration to be exact (*i.e.*: not temporal discretization) and only spatial operators are studied. In the context of acoustics with a uniform velocity flow, small perturabtions are not distorted and are simply convected at $(u + c)$. This physical behavior is described by the following convection equation,

$$\frac{\partial \Phi_i}{\partial t} = -(u+c)\,\frac{\partial \Phi}{\partial x}, \tag{11}$$

for which the solution is known. In particular, if an initial harmonic perturbation is imposed as the initial condition, the exact solution reads:

$$\Phi(t) = \hat{\Phi}(0)\, e^{j\,\omega\,[x-(u+c)t]}. \tag{12}$$

Numerically, the problem is discretized and reads (upwind scheme),

$$\frac{\partial \Phi_i}{\partial t} = -(u+c)\,\frac{\Phi_i - \Phi_{i-1}}{\Delta x}, \tag{13}$$

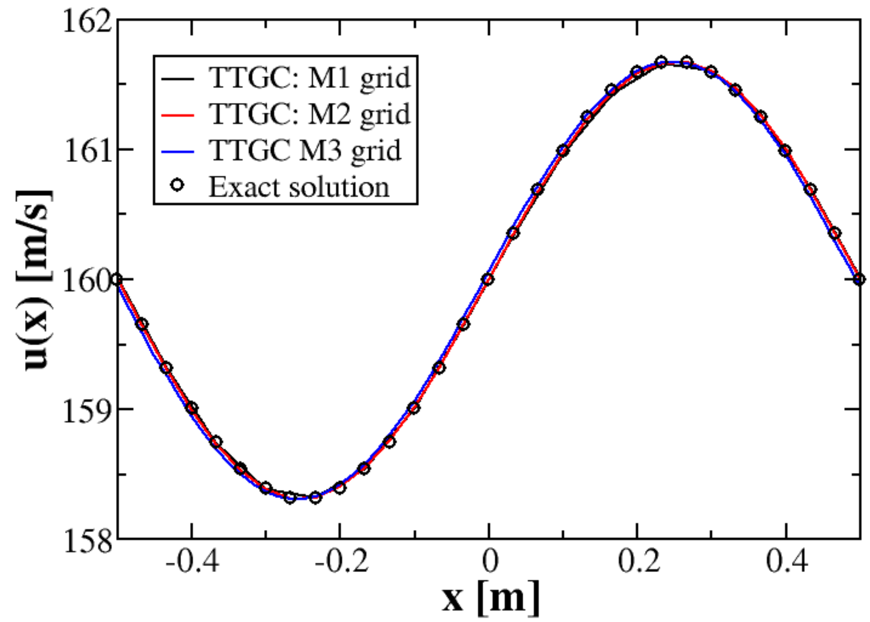

FIGURE 3. Velocity field obtained with TTGC after one turn-around time on three grid resolutions. Symbols correspond to the exact solution.

solving for,

$$\frac{\partial \hat{\Phi}}{\partial t} = -(u+c)\,\hat{\Phi}\,\frac{1-e^{-j\,\omega\,\Delta x}}{\Delta x} \tag{14}$$

$$= -\hat{\Phi}\,j\,\omega\,(u+c)\,\frac{sin(\frac{\omega\,\Delta x}{2})}{\frac{\omega\,\Delta x}{2}}\,e^{-j\,\omega\,\Delta x/2} \tag{15}$$

$$= -\hat{\Phi}\,j\,\omega\,(u+c)A(\omega). \tag{16}$$

The discretized system hence provides a solution of the form: $\hat{\Phi}(\omega,t) = \hat{\Phi}(0)e^{j\,\omega\,[x-(u+c)\,A(\omega)t]}$, the effective convection velocity of the wave being: $(u+c)\,A(\omega)$. The numerical prediction equals the exact solution only if $A(\omega)=1$. The real and imaginary parts of A respectively distort the phase velocity (dispersion) and damp (dissipation) the signal. Manipulation of the exact and approximate solutions allows to retrieve these informations from the different runs obtained previously as illustrated below for the LW scheme.

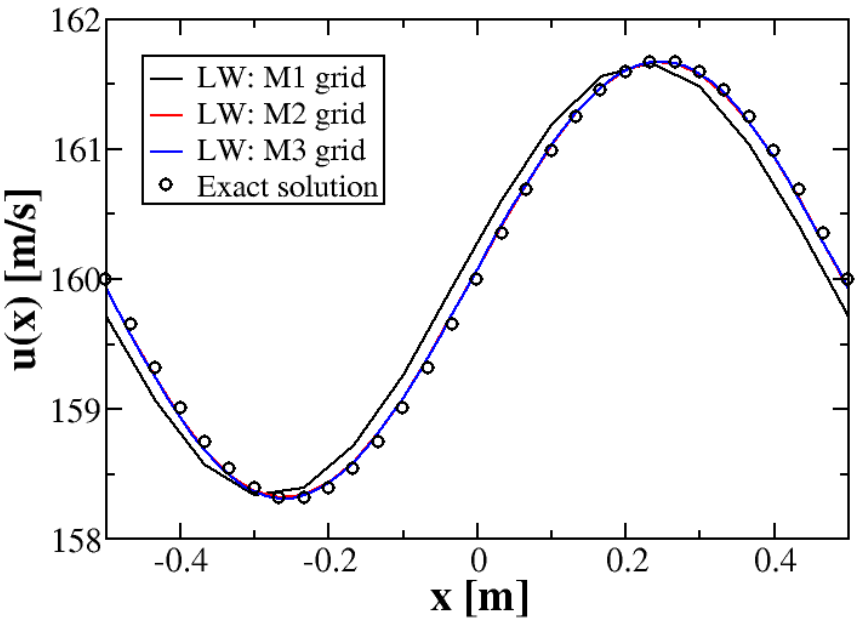

Figure 4. Velocity field obtained with LW after one turn-around time on three grid resolutions. Symbols correspond to the exact solution.

5. Conclusion

One-dimensional acoustic wave propagation computations are obtained with AVBP for two of the classical schemes that are Lax-Wendroff and TTGC. The comparaison of the numerical predictions for different grid resolutions allows to illustrate the notion of dissipation and dispersion as introduced by numerical schemes.

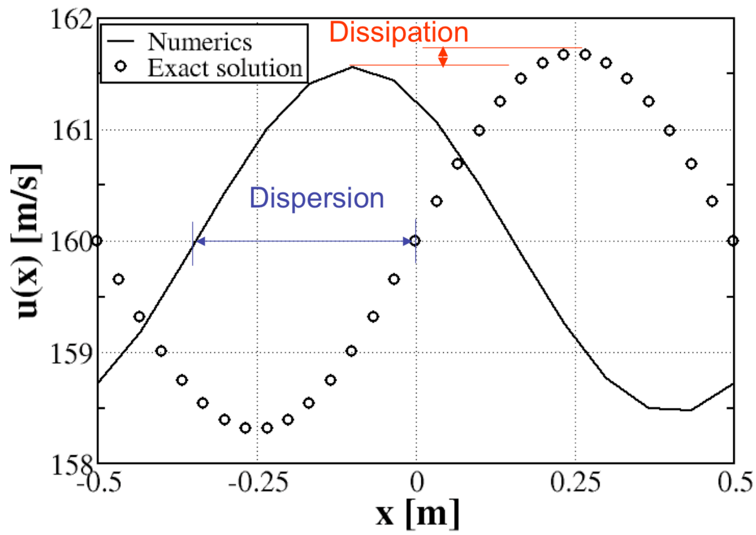

FIGURE 5. Schematic representation of dispersion and dissipation effects on a mono-chromatic harmonic acoustic wave propagated after 10 turn-over times using LW.