High-Fidelity Simulation for Turbulent Flows

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1 Solution of the advection-diffusion equation

Consider the steady-state 1D advection-diffusion equation

$$a\frac{\partial w}{\partial x} = \nu\frac{\partial^2 w}{\partial x^2} \qquad \text{with} \quad w \in [0, L], \quad a > 0, \quad \nu > 0 \tag{1}$$

with boundary conditions $w(0) = \alpha$ and $w(L) = \beta$.

1. Show that the analytical solution of equation (1) reads

$$w(x) = \alpha + (\beta - \alpha)\frac{\exp(\mathrm{Re}_x) - 1}{\exp(\mathrm{Re}_L) - 1} \tag{2}$$

   with $\mathrm{Re}_x = \dfrac{ax}{\nu}$ and $\mathrm{Re}_L = \dfrac{aL}{\nu}$, respectively.
   Hint: The general form of the solution is $w(x) = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x}$, where λ_1 and λ_2 are the roots of the characteristic equation.

2. We consider the simple case for which α=0 and β=1. A Cartesian regular mesh is considered, such that x_j=$j\Delta x$, for j∈$[0, N]$. Express the formula of the exact solution on the discretized mesh as a function of j, N and $R_m = \dfrac{a\Delta x}{\nu}$, where R_m is the mesh Reynolds number.

3. Equation (1) is now discretized by means of the following numerical scheme:

$$a\frac{w_j - w_{j-1}}{\Delta x} = \nu\frac{w_{j+1} - 2w_j + w_{j-1}}{\Delta x^2} \tag{12}$$

   Show that the analytical solution of the discretized equation reads:

$$w_j = \frac{1 - (1 + R_m)^j}{1 - (1 + R_m)^N} \tag{13}$$

4. Repeat the analysis by considering the following scheme:

$$a\frac{w_{j+1}-w_{j-1}}{2\Delta x}=\nu\frac{w_{j+1}-2w_j+w_{j-1}}{\Delta x^2} \tag{24}$$

   and show that the analytical solution reads

$$w_j=\frac{\left(\frac{2+R_m}{2-R_m}\right)^j-1}{\left(\frac{2+R_m}{2-R_m}\right)^N-1} \tag{25}$$

5. Compute the relative error of the two chosen discretizations with respect to the exact solution, at the grid point x_{N-1} for R_m=1.5 and R_m=2.5. Consider $N=1000$.
6. Does the value of N change the relative errors? What should be done to remove the oscillating solution for the centred scheme?

2 Semi-implicit Lax-Wendroff scheme

We want to study the linear advection equation

$$\frac{\partial w}{\partial t}+a\frac{\partial w}{\partial x}=0 \qquad a\in\mathbb{R} \tag{1}$$

To this aim, we consider the semi-implicit Lax-Wendroff scheme:

$$\frac{w_j^{n+1}-w_j^n}{\Delta t}+a\frac{w_{j+1}^n-w_{j-1}^n}{2\Delta x}=|a|^2\Delta t\frac{w_{j+1}^{n+1}-2w_j^{n+1}+w_{j-1}^{n+1}}{2\Delta x^2} \tag{2}$$

1. Perform a stability analysis of the chosen discretization.
2. By using the standard finite difference operators:

$$\delta(\bullet)_j=(\bullet)_{j+\frac{1}{2}}-(\bullet)_{j-\frac{1}{2}} \qquad \mu(\bullet)_j=\frac{1}{2}\left[(\bullet)_{j+\frac{1}{2}}+(\bullet)_{j-\frac{1}{2}}\right] \tag{9}$$

   Rewrite the scheme in Δ-form as:

$$A_{\mathrm{LW}}\Delta w_j^n=\Delta w_{\mathrm{exp},j}^{\mathrm{LW},n} \tag{10}$$

   and give the expressions of the mass matrix A_{LW} and of the explicit phase $\Delta w_{\mathrm{exp},j}^{\mathrm{LW},n}$.
3. Specify the form of the mass matrix A_{LW}. Verify if it is diagonal dominant.
4. Is the scheme appropriate for computing the steady-state solution of the problem? Why? For unsteady problems, would it be more suited for slow or rapid cases?

3 Adams-Bashforth 3-step

We consider the semi-discrete ODE

$$\frac{\mathrm{d}w}{\mathrm{d}t} = R(w) \tag{1}$$

The three-step explicit Adams-Bashforth method can be written under the form:

$$w^{n+1} = w^n + a\Delta t R(w^n) + b\Delta t R(w^{n-1}) + c\Delta t R(w^{n-2}) \tag{2}$$

1. Derive the coefficients of the method by equating the coefficients of the Taylor series for the l.h.s. and r.h.s. of equation (2).

2. Compute the temporal order of accuracy of the discretization.

4 Analysis of a finite element scheme

By applying the Galerkin method with linear elements to the conservation equation

$$\frac{\partial w}{\partial t} + \frac{\partial f}{\partial x} = 0 \tag{1}$$

one obtains the following implicit formulation:

$$\frac{1}{6}\left[\frac{\mathrm{d}w_{j-1}}{\mathrm{d}t} + 4\frac{\mathrm{d}w_j}{\mathrm{d}t} + \frac{\mathrm{d}w_{j+1}}{\mathrm{d}t}\right] = \frac{f_{j+1} - f_{j-1}}{2\Delta x} \tag{2}$$

Using a central time integration (leapfrog) and considering the linear equation $f = aw$, the following scheme is obtained:

$$(w_{j-1}^{n+1} - w_{j-1}^{n-1}) + 4(w_j^{n+1} - w_j^{n-1}) + (w_{j+1}^{n+1} - w_{j+1}^{n-1}) + 6\dot{a}(w_{j+1}^n - w_{j-1}^n) = 0 \tag{3}$$

with $\dot{a} = \dfrac{a\Delta t}{\Delta x}$.

1. Compute the amplification factor of the scheme and obtain a stability condition of the type

$$\dot{a}^2 \leq f(\beta) \tag{4}$$

   where $f(\beta)$ is a function of $\beta = k\Delta x$.

2. Derive the most restrictive condition for satisfying equation (4). *Hint*: compute the minimum of the function $f(\beta)$.

3. Compute the dispersion and diffusion errors of the scheme.

5 Stability of the Leapfrog scheme

We apply the Leapfrog scheme (central difference in time) for the general semi-discrete ODE:

$$\frac{\partial w}{\partial t} = R(w) \quad \Longrightarrow \quad \frac{w_j^{n+1} - w_j^{n-1}}{2\Delta t} = R(w) \tag{1}$$

1. First, we consider the heat-conduction equation (thus $R(w) = \dfrac{\partial^2 w}{\partial x^2}$) where the space operator is discretized by centred second-order finite differences, giving:

$$w_j^{n+1} - w_j^{n-1} = 2\nu \frac{\Delta t}{\Delta x^2}(w_{j+1}^n - 2w_j^n + w_{j-1}^n) \tag{2}$$

   Discuss the stability of the numerical discretization.

2. Now we consider the advection equation (thus $R(w) = -a\dfrac{\partial w}{\partial x}$, with $a > 0$), where the space operator is discretized by upwind first-order differences, giving:

$$w_j^{n+1} - w_j^{n-1} = -2a\frac{\Delta t}{\Delta x}(w_j^n - w_{j-1}^n) \tag{14}$$

   Discuss the stability of the numerical discretization. (*Hint:* what happens for $k\Delta x{=}\beta{=}\pi$?)

3. Justify the previous results by sketching the absolute stability region of the leapfrog scheme. What properties should have $R(w)$?

6 2D Burgers equation

We aim to solve the coupled system of Burgers' equations:

$$\frac{\partial w}{\partial t} + \frac{\partial f(w)}{\partial x} + \frac{\partial g(w)}{\partial y} = \nu\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right) \tag{1}$$

with

$$w = \begin{bmatrix} u \\ v \end{bmatrix}, \quad f = \begin{bmatrix} u^2 \\ uv \end{bmatrix}, \quad g = \begin{bmatrix} uv \\ v^2 \end{bmatrix}, \quad \nu \geq 0 \tag{2}$$

We will consider a regular Cartesian grid with sizes $\Delta x, \Delta y$ such that the coordinates for a generic grid point (i,j) are $x_{i,j} = j\Delta x$ and $y_{i,j} = j\Delta y$. The spatial derivatives are discretized by means of finite-difference centred second-order operator:

$$\left.\frac{\partial f(w)}{\partial x}\right|_{i,j} \approx \frac{\delta_x \mu_x f_{i,j}}{\Delta x} + \mathcal{O}(\Delta x^2) \qquad \left.\frac{\partial g(w)}{\partial y}\right|_{i,j} \approx \frac{\delta_y \mu_y f_{i,j}}{\Delta y} + \mathcal{O}(\Delta y^2) \tag{3}$$

$$\left.\frac{\partial^2 w}{\partial x^2}\right|_{i,j} \approx \frac{\delta_x^2 w_{i,j}}{\Delta x^2} + \mathcal{O}(\Delta x^2) \qquad \left.\frac{\partial^2 w}{\partial y^2}\right|_{i,j} \approx \frac{\delta_y^2 w_{i,j}}{\Delta y^2} + \mathcal{O}(\Delta y^2) \tag{4}$$

with the directional difference operators

$$\delta_x(\bullet)_{i,j} = (\bullet)_{i+\frac{1}{2},j} - (\bullet)_{i-\frac{1}{2},j} \qquad \mu_x(\bullet)_{i,j} = \frac{1}{2}[(\bullet)_{i+\frac{1}{2},j} + (\bullet)_{i-\frac{1}{2},j}] \tag{5}$$

$$\delta_y(\bullet)_{i,j} = (\bullet)_{i,j+\frac{1}{2}} - (\bullet)_{i,j-\frac{1}{2}} \qquad \mu_y(\bullet)_{i,j} = \frac{1}{2}[(\bullet)_{i,j+\frac{1}{2}} + (\bullet)_{i,j-\frac{1}{2}}] \tag{6}$$

First, we will use the following semi-implicit scheme for the time integration:

$$\frac{w_{i,j}^{n+1} - w_{i,j}^n}{\Delta t} = -R(w_{i,j}^n) + \nu\left[\frac{\delta_x^2 w}{\Delta x^2} + \frac{\delta_y^2 w}{\Delta y^2}\right]_{i,j}^{n+1} \tag{7}$$

where $R(w) = \dfrac{\partial f(w)}{\partial x} + \dfrac{\partial g(w)}{\partial y}$ and the index n refers to the time instant $t^n = n\Delta t$.

1. Compute the temporal order of accuracy of the scheme (7).
2. Write the scheme 7 in Δ-form by introducing the increment $\Delta w_{i,j}^n = w_{i,j}^{n+1} - w_{i,j}^n$.
3. Show that, at each time step, the computation of the increment $\Delta w_{i,j}^n$ requires the inversion of a linear system with a scalar band matrix. Give the expression of the matrix.
4. In order to speed up the computation, we rewrite the scheme in the factorized form:
$$(\mathcal{I} - \dot{\nu}_x \delta_x^2)(\mathcal{I} - \dot{\nu}_y \delta_y^2)\Delta w_{i,j}^n = -\Delta t R(w_{i,j}^n) + \nu \Delta t \left[\frac{\delta_x^2 w}{\Delta x^2} + \frac{\delta_y^2 w}{\Delta y^2} \right]_{i,j}^n \tag{20}$$
where $\dot{\nu}_x = \dfrac{\nu \Delta t}{\Delta x^2}$ and $\dot{\nu}_y = \dfrac{\nu \Delta t}{\Delta y^2}$, which allows to compute the increment $\Delta w_{i,j}^n$ by means of the inversion of a tridiagonal scalar matrix in each direction. Show that the factorization generates an error of order Δt^2, and give the expression of the error term.
5. Now, we want to make implicit also the nonlinear operator $R(w_{i,j}^n)$. Write the fully-implicit version of the scheme by using the Δ-form.
6. Recall two possible methods that one can apply to compute the solution at the time t^{n+1} for the fully-implicit scheme.
7. In order to end up with a linear system, we decide to linearize $R(w_{i,j})$ at the time t^n, *i.e.* we introduce the approximation
$$R(w_{i,j}^{n+1}) = R(w_{i,j}^n) + \left.\frac{\partial R}{\partial w}\right|_{i,j}^n \Delta w_{i,j}^n + \mathcal{O}(\Delta t^2) \tag{24}$$
To simplify the problem, we consider the inviscid case ($\nu = 0$). Give the expression of the linearized scheme as a function of the operator R and of its derivative.
8. Compute the Jacobian matrix of the operator R for the numerical scheme considered.
9. Specify the type of linear system to be solved (band matrix or not? How many non-zero diagonals?) and suggest a suitable algorithm for solving the problem.

7 Analysis of a Dual Time Stepping technique

We aim to solve the linear advection equation:

$$w_t + a w_x = 0 \qquad \text{with} \quad a \in \mathbb{R} \tag{1}$$

To this purpose, we consider a Cartesian grid such that $x_j = j\Delta x$. The following spatial semi-discrete numerical scheme is used:

$$\frac{\partial w}{\partial t} + \frac{a}{\Delta x}\delta\left[\mu w - \frac{1}{6}\delta^2 \mu w\right]_j^n = -\nu |a| \frac{\delta^4 w_j^n}{\Delta x} \qquad \text{with} \quad \nu \in \mathbb{R} \tag{2}$$

Where the classical finite-difference operators δ and μ are used:

$$\delta(\bullet)_j = (\bullet)_{j+\frac{1}{2}} - (\bullet)_{j-\frac{1}{2}} \qquad \text{and} \qquad \mu(\bullet)_j = \frac{1}{2}[(\bullet)_{j+\frac{1}{2}} + (\bullet)_{j-\frac{1}{2}}] \tag{3}$$

1. Determine the order of accuracy of the proposed spatial discretization.
2. We rewrite the semi-discrete scheme under the form of an ordinary differential equation:

   $$\frac{\mathrm{d}w}{\mathrm{d}t} + R(w) = 0 \tag{4}$$

   and solve the equation by means of the Gear (BDF2) scheme, which reads:

   $$\frac{\mathrm{d}w}{\mathrm{d}t} + R(w^{n+1}) = 0 \qquad \text{with} \qquad \frac{\mathrm{d}w}{\mathrm{d}t} = \frac{3w_j^{n+1} - 4w_j^n + w_j^{n-1}}{2\Delta t} \tag{5}$$

   Compute the order of accuracy of the temporal approximation chosen.
3. Knowing that the Gear scheme is A-stable, compute the Fourier symbol of the spatial operator $\widehat{R}$, and comment the conditional (or unconditional) stability (or instability) of the fully-discrete scheme (5), as a function of the sign of the coefficient ν.
4. We now want to solve the equation (5), with the spatial operator shown in equation (2), by means of the Dual Time Stepping (DTS) method. In order to do so, we add to the equation (5) a derivative with respect to a fictitious time τ, obtaining

   $$\frac{\mathrm{d}w}{\mathrm{d}\tau} + R^*(w) = 0 \qquad \text{with} \quad R^*(w) = \frac{Dw}{\Delta t} + R(w) \tag{6}$$

   The ODE (6) is approximated by means of the implicit Euler scheme:

   $$\frac{w^{n+1,m+1} - w^{n+1,m}}{\Delta\tau} + R^*(w^{n+1,m+1}, w^n, w^{n-1}) = 0 \tag{7}$$

   where $w^{n+1,m+1}$ denotes the approximation of w at the physical time step $n+1$, at the iteration $m+1$ with respect to the fictitious time. The approximation in τ becomes then:

   $$\frac{w_j^{m+1} - w_j^m}{\Delta\tau} + \lambda w_j^{m+1} + \dot{a}\left[\delta\mu w_j^{m+1} - \frac{1}{6}\delta^3\mu w_j^{m+1}\right] + \nu|\dot{a}|\delta^4 w_j^{m+1} = C(w^n, w^{n-1}) \tag{8}$$

   where $C(w^n, w^{n-1})$ is a constant (in the pseudo-time) function, λ a numerical constant and $\dot{a} = a\dfrac{\Delta t}{\Delta x}$. Give the expression of λ and $C(w^n, w^{n-1})$.
5. Analyse the linear stability of eq. (8) as a function of the parameter λ, assuming $C = 0$.
6. Does the chosen fictitious time approximation, in combination with the time and space approximations, allow to converge rapidly towards the steady state with respect to τ? Is it more suited for slow or rapid problems? Justify the answer.