Fundamentals of Numerical Thermo-Fluid Dynamics 322.061

Exercise 7: Guidelines

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We are interested in the Burger, non-Homogeneous Dirichlet and Homogeneous Neumann Boundary conditions.

$$\begin{cases} \partial_t u + u\,\partial_x u - \nu \partial_{xx} u = 0 \quad , \text{with } t \in \mathbb{R}^+, x \in [0,1], \nu \in \mathbb{R}^+ \\ u(t=0,x) = 1 - x + e^{-\frac{(x-0.5)^2}{0.02}} \\ u(t,x=0) = 1 \quad \dfrac{\partial}{\partial x} u(t,x=1) = 0 \end{cases} \tag{1}$$

To treat this problem, different time marching strategy are possible. We will focus here on the case where Euler Implicit is applied to the problem.

We consider the following discretization of the problem (centered scheme for 1st and 2nd spatial derivatives):

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} - \nu \frac{U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}}{\Delta x^2} + U_i^{n+1} \frac{U_{i+1}^{n+1} - U_{i-1}^{n+1}}{2\Delta x} = 0 \tag{2}$$

One can clearly see that the equation (2) is **non-linear** in U^{n+1} (convection term). Therefore, at each time step, one has to solve a non-linear problem. To solve a non-linear problem different approaches are feasible (e.g. Dichotomy, secant, regula falsi, Newton, Quasi-Newton, fixed point, etc.).

Here we propose to solve this problem using two commonly used method, namely the *fixed point method*, and then with the *Newton method*. In what follows, in order to simplify the notations, U^{n+1} will be noted V. The equation (2) is rewritten in terms of V:

$$\frac{V_i - U_i^n}{\Delta t} - \nu \frac{V_{i-1} - 2V_i + V_{i+1}}{\Delta x^2} + V_i \frac{V_{i+1} - V_{i-1}}{2\Delta x} = 0. \tag{3}$$

Fixed Point Method.

Principle of the Method The principle a fixed point method is the following: Let us consider a function f defined such that $f(x) = x$.

Then let us define a sequence $x^{k+1} = f(x^k)$. Under certain assumptions (not detailed here) on f, this sequence should converge toward a x^* as k increases. Meaning that $x^* = f(x^*)$, and equivalently $|x^{k+1} - x^k| \xrightarrow[k\to\infty]{} 0$.

The idea of the method is to iterate on x^k until $\frac{|x^{k+1}-x^k|}{|x^k||} < \epsilon$, where ϵ is a tolerance.

Applying it to equation 3. To apply the fixed point method, we need to reformulate our problem such that it looks like $f(x) = x$. There is plenty of ways to do it (depending on which V_i one choose to isolate). Let us consider this version :

$$\frac{V_i^{k+1} - U_i^n}{\Delta t} - \nu \frac{V_{i-1}^k - 2V_i + V_{i+1}^k}{\Delta x^2} + V_i^k \frac{V_{i+1}^k - V_{i-1}^k}{2\Delta x} = 0. \tag{4}$$

which is looking like a time marching step. (Note that the first step - when $V = U^n$- is actually Explicit Euler).

One can then isolate V^{k+1} and obtain a function in the form $x^{k+1} = f(x^k)$.

Relaxation factor In reality to get this method to converge, one needs a to introduce a *relaxation factor* θ. Especially at the beginning of the iterations, V^k might vary a lot and diverge. This relaxation factor is introduced such that the new iterate sticks to the previous one.

$$\begin{aligned} V_{intermediary} &= f(x^k) \\ V^{k+1} &= \theta V_{intermediary} + (1-\theta)V^k \end{aligned}$$

The algorithm 1 sums up the method.

Algorithm 1 My fixed point

procedure GETSTEPFIXEDPOINT(U^n,tol,k_{max},θ)
  $V_1 \leftarrow U^n$; $k \leftarrow 0$
  while $tol < \delta$ and $k < k_{max}$ **do**
    $V^{k+1} \leftarrow f(V^k, U^n)$
    $\delta \leftarrow norm(V^{k+1} - V^k)/norm(V^k)$
    $V^{k+1} \leftarrow \theta V^{k+1} + (1-\theta)V^k$
    $k \leftarrow k + 1$
  end do
  return V^{k+1}

Newton Method

Principle of the Method. Let us recall the principle of the Newton method. One consider function F that is non-linear in x, and one wants to find the roots of this function F. The idea of the method relies on a Taylor expand:

$$F(x^k + \delta x) = F(x^k) + J_F(x^k)\delta x + o(\delta x)$$

The only unknown there is the δx, x^k is given from the previous iteration. Assuming that the $F(x + \delta x) = 0$ gives that

$$0 \approx F(x^k) + J_F(x^k)\delta x \tag{5}$$

δx is then the solution of the linear problem $J_F(x^k)\delta x = -F(x^k)$. (Our non linear problem has been linearized, and one search for the solution of the linearized problem.) Once the linear problem is solved one can find the new iterate by simply adding

$$x^{k+1} = x^k + \delta x \tag{6}$$

.

As for the fixed point iteration, one repeats this until a convergence criteria is fulfilled (e.g.$\frac{\|V^{k+1}-V^k\|}{\|V^k\|}$) $< \epsilon$, where ϵ is a given tolerance).

Applying it to Eq. 3 Let us first define our function F .

$$F_i(V) = \frac{V_i - U_i^n}{\Delta t} - \nu \frac{V_{i-1} - 2V_i + V_{i+1}}{\Delta x^2} + V_i \frac{V_{i+1} - V_{i-1}}{2\Delta x}$$

In our case : $F : \mathbb{R}^N \to \mathbb{R}^N$. We notice that F_i depends only on V_{i-1}, V_i, V_{i+1}. Therefore only the partial derivatives of F_i with respect to $V_{i-1}, V_i, Vi + 1$ will be non zero. Then the Jacobian matrix $J_F(x)$ should be a tridiagonal matrix, with

$$\partial_{V_{i-1}} F_i(V), \quad \partial_{V_i} F_i(V), \quad \partial_{V_{i+1}} F_i(V)$$

as coefficients for the first lower diagonal, main diagonal, and first upper diagonal.

Boundary Conditions The boundary conditions of the linear problem defined by Eq. (5) still have to be defined.

Dirichlet Boundary condition The step defined by Eq. (6) in our case reads:

$$V^{k+1} = V^k + \delta V \tag{7}$$

Assuming that $V_1^k = V_{Dirichlet}$, ensuring that $V^{k+1} = V_{Dirichlet}$ as well is equivalent to say that one must have $\delta V_1 = 0$. The linear problem defined by Eq. (5) has then an homogenenous Dirichlet boundary condition.

Neumann Boundary condition If we introduce a ghost point outside of the domain, a Neumann boundary condition can be written for instance as

$$\frac{V_{N+1}^{k+1} - V_{N-1}^{k+1}}{2\Delta x} = \beta \tag{8}$$

where $\beta \in \mathbb{R}$ is the imposed flux. We could have chosen an other approximation of the first derivative, but this one is already the one used for the first derivative approximation in (2).

Injecting Eq. (7) in (8) gives

$$\frac{V_{N+1}^{k+1} - V_{N-1}^{k+1}}{2\Delta x} = \frac{V_{N+1}^{k} - V_{N-1}^{k}}{2\Delta x} + \frac{\delta V_{N+1} - \delta V_{N-1}}{2\Delta x} = \beta \tag{9}$$

Assuming that a condition similar to Eq(8) is also valid at the previous iteration (for V^k), then we obtain the boundary condition for δx :

$$\frac{\delta V_{N+1} - \delta V_{N-1}}{2\Delta x} = 0 \tag{10}$$

The linear problem defined by Eq. (5) has then a homogenenous Neumann boundary condition.

The Algorithm 2 sums up the method.

Algorithm 2 My Newton

procedure GETSTEPNEWTON(U^n,tol,k_{max})
    $V_1 \leftarrow U^n$
    $k \leftarrow 1$
    while $tol < \delta$ and $k < k_{max}$ **do**
        $F \leftarrow createVector_F(V^k, U^n)$
        $J \leftarrow createJacobian(V^k, U^n)$
        $V^{k+1} = V^k - J^{-1}F$
        $\delta \leftarrow norm(V^{k+1} - V^k)/norm(V^k)$
        $k \leftarrow k + 1$
    end do
    $U^{n+1} \leftarrow V^{k+1}$
    return U^{n+1}