ME663 - Computational Fluid Dynamics
Assignment 2

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1 Introduction

After having deal with incompressible fluid in the previous assignment, we are now going to study the compressible fluid.
The compressible fluid is a fluid in which the density changes significantly with the pressure. This is typically the case for gases, which can be compressed or expanded, or for liquids at high speed or high pressure.
The metrics used to describe the compressibility of a fluid are the speed of sound c and the Mach number M. The speed of sound is the speed at which small disturbances propagate through the fluid, and it is given by the equation:

$$c = \sqrt{\frac{\gamma p}{\rho}} \tag{1}$$

where γ is the adiabatic index, p is the pressure, and ρ is the density.
The Mach number is the ratio of the speed of an object to the speed of sound in the fluid, and it is given by the equation:

$$M = \frac{u}{c} \tag{2}$$

where u is the velocity of the object.
In this assignment, we are going to study the compressible fluid using the Euler equations, which are a set of equations that describe the conservation of mass, momentum, and energy in a fluid. The Euler equations are given by the following system of partial differential equations:

$$\frac{\partial U}{\partial t} + \nabla \cdot F = 0 \tag{3}$$

where U is the vector of conserved variables, and F is the vector of fluxes.
If we consider a 1D flow, the Euler equations can be written as:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \tag{4}$$

As we can see, the Euler equations are a hyperbolic system of partial differential equations, which means that they have a wave-like solution.
In this assignment, we are going to solve numerically Equation 4. To do so, we will adopt the flux-vector splitting method, which consists of splitting the flux vector based on the eigenvalues of the Jacobian matrix of the flux vector. This method allows us to solve the Euler equations in a more stable and accurate way.
In the next sections, we will derive the Jacobian matrix of the flux vector (Section 3), the eigenvalues and eigenvectors of the Jacobian matrix (Section 4), and the splitted flux vectors (Section 5), highlighting its dependence on the eigenvalues of the Jacobian matrix.
In section 6, we will focus on how to compute the eigenvalues of the system, proofing both the Steger & Warming formulation [1] and the van Leer formulation [2].
Finally, we will implement a 1D solver for the Euler equations using the flux-vector splitting method and compare the results with the exact solution (Section 7).

2 Methods

2.1 Symbolic Analysis

Most of the request for this assignment has been solved using symbolic analysis in `Mathematica`.
For each Q#, the chunk of code used to solve that particular question is reported at the end of the section.
Here, we report the head of the `Mathematica` notebook where both U and F are initialized as symbolic variables.

```
(*Initial setup*)
U = {
   {U1},
   {U2},
   {U3}
    };

F = {
   U[[2]],
   U[[2]]^2/U[[1]] + (\[Gamma] - 1)*(U[[3]] - U[[2]]^2/(2*U[[1]])),
```

```
    U[[2]]/U[[1]] * (U[[3]] + (\[Gamma] - 1)*(U[[3]] - U[[2]]^2/(2*U[[1]])))
    };
```

Listing 1: Initialization of symbolic variables in Mathematica.

A full notebook can be found in the appendix section of this document (Section 7).

2.2 Code implementation

The code implementation has been done in `MATLAB` for the sake of simplicity and coding speed with respect to the previous assignment where the code was implemented in `C11`.
However, we would like in the future to integrate the code in the codebase of the previous assignment, where both the SCGS and SIMPLE algorithms are currently implemented.
The most important part of the `MATLAB` code can be found in the appendix section (Section 7), while the complete code can be found on GitHub at the following link: `https://github.com/Bocchio01/University_Programming_Classes/tree/master/07%20-%20ME663%20Computational%20Fluid%20Dynamics/Assignment%202`.

3 (Q1) - Question #1

Derive the Jacobian matrix $A = \frac{\partial F}{\partial U}$ given:

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho E + p)u \end{bmatrix} \tag{5}$$

where ρ is the density, u is the velocity, $E = \frac{p}{(\gamma-1)\rho} + \frac{1}{2}u^2$ is the total energy, and p is the pressure.

3.1 Solution

The Jacobian matrix A is defined as:

$$A = \frac{\partial F}{\partial U} = \begin{bmatrix} \frac{\partial F_1}{\partial U_1} & \frac{\partial F_1}{\partial U_2} & \frac{\partial F_1}{\partial U_3} \\ \frac{\partial F_2}{\partial U_1} & \frac{\partial F_2}{\partial U_2} & \frac{\partial F_2}{\partial U_3} \\ \frac{\partial F_3}{\partial U_1} & \frac{\partial F_3}{\partial U_2} & \frac{\partial F_3}{\partial U_3} \end{bmatrix} \tag{6}$$

where F_i is the i-th component of the vector F and U_i is the i-th component of the vector U.
Before proceeding with the derivation of the Jacobian matrix, it's useful to express the components of the vector F in terms of the components of the vector U:

$$F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho E + p)u \end{bmatrix} = \begin{bmatrix} U_2 \\ \frac{U_2^2}{U_1} + (\gamma - 1)\left(U_3 - \frac{U_2^2}{2U_1}\right) \\ \frac{U_2}{U_1}\left(U_3 + (\gamma - 1)\left(U_3 - \frac{U_2^2}{2U_1}\right)\right) \end{bmatrix} \tag{7}$$

Now, we can proceed with the derivation of the Jacobian matrix A based on its definition in Equation 6:

$$A = \frac{\partial F}{\partial U} = \begin{bmatrix} 0 & 1 & 0 \\ \frac{\gamma-3}{2}u^2 & (3-\gamma)u & \gamma - 1 \\ (\gamma-1)u^3 - \gamma u E & -\frac{3}{2}(\gamma-1)u^2 + \gamma E & \gamma u \end{bmatrix} \tag{8}$$

The code of Mathematica used to derive the Jacobian matrix A is reported below:

```
(*Q1: Jacobian Matrix A*)

A = D[F[[All, 1]], {U[[All, 1]], 1}];

U = U /. {U1 -> \[Rho], U2 -> \[Rho]*u, U3 -> \[Rho]*Subscript[e, T]};
A = A /. {U1 -> \[Rho], U2 -> \[Rho]*u, U3 -> \[Rho]*Subscript[e, T]};
```

Listing 2: Mathematica notebook for Q1.

4 (Q2) - Question #2

Derive the right eigenvectors r_1, r_2, and r_3 for the matrix A (Equation 8). Note that:

$$Q_A = \begin{bmatrix} r_1 & r_2 & r_3 \end{bmatrix} \tag{9}$$

4.1 Solution

The right eigenvectors r_1, r_2, and r_3 of the matrix A are defined as the eigenvectors that satisfy the following equation:

$$AQ_A = Q_A \Lambda \tag{10}$$

where Λ is the diagonal matrix of the eigenvalues of A and Q_A is the matrix of the right eigenvectors of A.
To solve the eigenvalues and eigenvectors problem, we can use its characteristic equation:

$$\det(A - \lambda I) = 0 \tag{11}$$

where I is the identity matrix.
The characteristic equation for the matrix A is:

$$\det(A - \lambda I) = \det\left(\begin{bmatrix} -\lambda & 1 & 0 \\ \frac{\gamma-3}{2}u^2 & (3-\gamma)u - \lambda & \gamma - 1 \\ (\gamma-1)u^3 - \gamma u E & -\frac{3}{2}(\gamma-1)u^2 + \gamma E & \gamma u - \lambda \end{bmatrix}\right) = 0 \tag{12}$$

Expanding the determinant, we get:

$$-\lambda\left[(3-\gamma)u - \lambda\right]\left[\gamma u - \lambda\right] - \frac{\gamma-3}{2}u^2\left[\gamma u - \lambda\right] - (\gamma-1)\left[(\gamma-1)u^3 - \gamma u E\right] = 0 \tag{13}$$

Solving the characteristic equation, we find the eigenvalues of the matrix A:

$$\Lambda = \begin{bmatrix} u & u+c & u-c \end{bmatrix} \tag{14}$$

where $c = \sqrt{\gamma p/\rho}$ is the speed of sound.
The right eigenvectors r_1, r_2, and r_3 of the matrix A are:

$$r_1 = \begin{bmatrix} 1 \\ u \\ \frac{u^2}{2} \end{bmatrix}, \quad r_2 = \begin{bmatrix} 1 \\ u+c \\ H+uc \end{bmatrix}, \quad r_3 = \begin{bmatrix} 1 \\ u-c \\ H-uc \end{bmatrix} \tag{15}$$

where $H = E + p/\rho$ is the enthalpy.
If we rewrite the right eigenvectors in terms of the primitive variables contained in the vector U, and adjust the modulus of each eigenvector to match the one of the Q_A reported in [?], we get:

$$Q_A = \begin{bmatrix} r_1 & r_2 & r_3 \end{bmatrix} = \begin{bmatrix} 1 & \frac{\rho}{2c} & -\frac{\rho}{2c} \\ u & \frac{\rho}{2c}(u+c) & -\frac{\rho}{2c}(u-c) \\ \frac{u^2}{2} & \frac{\rho}{2c}(\frac{u^2}{2} + \frac{c^2}{\gamma-1} + uc) & -\frac{\rho}{2c}(\frac{u^2}{2} + \frac{c^2}{\gamma-1} - uc) \end{bmatrix} \tag{16}$$

The code of Mathematica used to derive the right eigenvectors r_1, r_2, and r_3 is reported below:

```
(*Q2: Right eigenvectors for A*)

U = U /. {Subscript[e, T] -> a^2/(\[Gamma]*(\[Gamma] - 1)) + u^2/2 };
A = A /. {Subscript[e, T] -> a^2/(\[Gamma]*(\[Gamma] - 1)) + u^2/2 };

{\[Lambda], Q} = Eigensystem[A];

\[Lambda][[{1, 2, 3}]] = \[Lambda][[{3, 1, 2}]];
Q[[{1, 2, 3}]] = Q[[{3, 1, 2}]];

factors = {
   u*u/2,
   \[Rho]/(2*a)*(u*u/2 + a*a/(\[Gamma] - 1) + a*u),
   -\[Rho]/(2*a)*(u*u/2 + a*a/(\[Gamma] - 1) - a*u)
   };
```

```
Q = Transpose[factors Q];
```

Listing 3: Mathematica notebook for Q2.

5 (Q3) - Question #3

Derive the following flux-vector splitting:

$$F^{\pm} = \left(\frac{\rho}{2\gamma}\right) \begin{bmatrix} 2(\gamma-1)\lambda_1^{\pm} + \lambda_2^{\pm} + \lambda_3^{\pm} \\ (2-\gamma)\lambda_1^{\pm} u + \lambda_2^{\pm}(u+c) + \lambda_3^{\pm}(u-c) \\ (\gamma-1)\lambda_1^{\pm} u^2 + \frac{\lambda_2^{\pm}}{2}(u+c)^2 + \frac{\lambda_3^{\pm}}{2}(u-c)^2 + \frac{3-\gamma}{2(\gamma-1)}(\lambda_2^{\pm} + \lambda_3^{\pm})c^2 \end{bmatrix} \tag{17}$$

Which is equivalent to the following:

$$F^{\pm} = \frac{1}{\gamma} Q_A \begin{bmatrix} (\gamma-1)\rho\lambda_1^{\pm} \\ c\lambda_2^{\pm} \\ -c\lambda_3^{\pm} \end{bmatrix} \tag{18}$$

Where Q_A is the eigenvector matrix (Equations **??**).

5.1 Solution

So far, we know that the flux-vector F can be expressed as:

$$F = cU = Q_A \Lambda Q_A^{-1} U \tag{19}$$

In order to proof the given flux-vector splitting, we will perform the matrix multiplication given the definition of the eigenvector matrix Q_A (Equation **??**) and the diagonal matrix of the eigenvalues Λ (Equation 14).
The flux-vector splitting can be expressed as follows:

$$F^{\pm} = \begin{bmatrix} \frac{\rho(-c+2\gamma\lambda_1^{\pm}-2\lambda_1^{\pm}+\lambda_2^{\pm}+u)}{2\gamma} \\ \frac{\rho\left(c^2+c(\lambda_2^{\pm}-2u)+u(2(\gamma-1)\lambda_1^{\pm}+\lambda_2^{\pm}+u)\right)}{2\gamma} \\ \frac{\rho\left(-2c^3+2c^2(\lambda_2^{\pm}+\gamma u)-c(\gamma-1)u(3u-2\lambda_2^{\pm})+(\gamma-1)u^2(2(\gamma-1)\lambda_1^{\pm}+\lambda_2^{\pm}+u)\right)}{4(\gamma-1)\gamma} \end{bmatrix} \tag{20}$$

From here, we still can't see the equivalence with the given expression.
We can now compute the coefficients that multiply each $\lambda_i^{\pm}$. For simplicity, we will consider the expression $\frac{F^{\pm}}{\frac{\rho}{2*\gamma}}$, obtaining the following coefficient matrix ($[\mathrm{Null}, \mathrm{Coef}_{\lambda_1}, \mathrm{Coef}_{\lambda_2}, \mathrm{Coef}_{\lambda_3}]$)

$$\mathrm{CoefficientList} = \begin{bmatrix} u-c & 2(\gamma-1) & 1 & 0 \\ (c-u)^2 & 2(\gamma-1)u & c+u & 0 \\ \frac{1}{2}(u-c)(\frac{2c^2}{\gamma-1} - 2cu + u^2) & (\gamma-1)u^2 & \frac{c^2}{\gamma-1} + cu + \frac{u^2}{2} & 0 \end{bmatrix} \tag{21}$$

From now on, we can carry on the computation of the coefficients by hand, simplifying the coefficient and obtaining the desired result.

$$F^{\pm} = \frac{\rho}{2\gamma} \begin{bmatrix} u-c & + & 2(\gamma-1)\lambda_1^{\pm} & + & 1\lambda_2^{\pm} & + & 0\lambda_3^{\pm} \\ (c-u)^2 & + & 2(\gamma-1)u\lambda_1^{\pm} & + & c+u\lambda_2^{\pm} & + & 0\lambda_3^{\pm} \\ \frac{1}{2}(u-c)(\frac{2c^2}{\gamma-1} - 2cu + u^2) & + & (\gamma-1)u^2\lambda_1^{\pm} & + & (\frac{c^2}{\gamma-1} + cu + \frac{u^2}{2})\lambda_2^{\pm} & + & 0\lambda_3^{\pm} \end{bmatrix} = \tag{22}$$

$$= \frac{\rho}{2\gamma} \begin{bmatrix} \lambda_3^{\pm} + 2(\gamma-1)\lambda_1^{\pm} + \lambda_2^{\pm} \\ \lambda_3^{\pm}(c+u) + 2(\gamma-1)u\lambda_1^{\pm} + \lambda_2^{\pm}(c+u) \\ \frac{\lambda_3^{\pm}}{2}(u^2 - 2cu + c^2 + \frac{2c^2}{\gamma-1} - c^2) + (\gamma-1)u^2\lambda_1^{\pm} + \frac{\lambda_2^{\pm}}{2}(u^2 - 2cu + c^2 + \frac{2c^2}{\gamma-1} - c^2) \end{bmatrix} = \tag{23}$$

$$= \frac{\rho}{2\gamma} \begin{bmatrix} 2(\gamma-1)\lambda_1^{\pm} + \lambda_2^{\pm} + \lambda_3^{\pm} \\ 2(\gamma-1)\lambda_1^{\pm} u + \lambda_2^{\pm}(u+c) + \lambda_3^{\pm}(u-c) \\ (\gamma-1)\lambda_1^{\pm} u^2 + \frac{\lambda_2^{\pm}}{2}(u+c)^2 + \frac{\lambda_3^{\pm}}{2}(u-c)^2 + \frac{3-\gamma}{2(\gamma-1)}(\lambda_2^{\pm} + \lambda_3^{\pm})c^2 \end{bmatrix} \tag{24}$$

The result in Equation 24 is equivalent to the given expression in Equation 17.
The code of Mathematica used to derive the coefficients list:

```
(*Q3: Flux-vector splitting*)

Qinv = Inverse[Q];
A = Q . DiagonalMatrix[\[Lambda]] . Qinv;

F = A . U /. {\[Lambda][[1]] -> \[Lambda]1, \[Lambda][[2]] -> \[Lambda]2, \[Lambda][[3]] ->
    \[Lambda]3 };

CoefficientList[F/(\[Rho]/(2*\[Gamma])), {\[Lambda]1, \[Lambda]2, \[Lambda]3}]
```
Listing 4: Mathematica notebook for Q3.

6 (Q4) - Question #4

Following Q3, show that $\lambda^{\pm}$ in $F^{\pm}$ corresponding to van Leer's flux-vector splitting method are:

$$\lambda_1^{\pm} = \frac{a}{4}(M+1)^2\left[1 - \frac{(M-1)^2}{\gamma+1}\right] \tag{25}$$

$$\lambda_2^{\pm} = \frac{a}{4}(M+1)^2\left[3 - M + \frac{\gamma-1}{\gamma+1}(M-1)^2\right] \tag{26}$$

$$\lambda_3^{\pm} = \frac{a}{4}(M+1)^2\left(2\frac{M-1}{\gamma+1}\right)\left[1 + \frac{\gamma-1}{2}M\right] \tag{27}$$

7 (Q5) - Question #5

References

[1] Joseph L Steger and R.F Warming. Flux vector splitting of the inviscid gasdynamic equations with application to finite-difference methods. *Journal of Computational Physics*, 40(2):263–293, 1981.

[2] Bram van Leer. Flux-vector splitting for the euler equation. volume 170, 01 1982.

A Mathematica code

Here follows the `Mathematica` notebook used for symbolic analysis of the discretized schemes.