

Fluidodinamica delle macchine

AA 2017-2018

Numerical solution of quasi-one dimensional nozzle flow



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Consegna

L'esercitazione riportata in questa dispensa è da considerarsi parte integrante dell'esame di fluidodinamica delle macchine (AA 2016-2017). Rappresenta la condizione necessaria (ma non sufficiente) per il superamento dell'esame per cui andrà inviata due giorni prima del sostenimento dell'esame scritto. L'esercitazione andrà inviata a nicola.casari@unife.it mettendo in copia il docente (pier.ruggero.spina@unife.it). Se l'esame non viene superato la prima volta non è necessario re-inviare il report per le volte successive: verrà tenuta buona la relazione inviata la prima volta. Vi si chiede di inviare una relazione in cui sono riportate, per ciascuno dei due casi affrontati,

- Equazioni implementate
- Risultati
- Codice

Inoltre andrà riportato lo schema numerico implementato nei suoi passaggi principali come visto in classe. Vi chiedo di inviarmi anche i codici a parte: 3 file .m o script se programmate in un linguaggio diverso. Il report deve obbligatoriamente contenere la validazione del caso, confrontando graficamente il risultato con i grafici riportati in questa dispensa (sovrapporre il vostro risultato ai grafici proposti è una buona idea). Inoltre, ogni elaborato deve affrontare i seguenti punti (commentati e documentati opportunamente):

- Prove di sensibilità alla griglia
- Variazione geometria condotto. Il condotto convergente divergente è una parabola nell'applicazione che vediamo. Lo studente dovrà variare il vertice della parabola di

$$1 - (\#matricola/10^5)$$

Di conseguenza andranno aggiornate le condizioni dell'inizializzazione.

- Variazione della condizione al contorno nel caso con shock: la condizione da imporre è:

$$p_{Nx} = 0.6784 - (\#matricola/10^6)$$

Se il numero risultante è minore di 0.4 usate $p_{Nx} = 0.5$

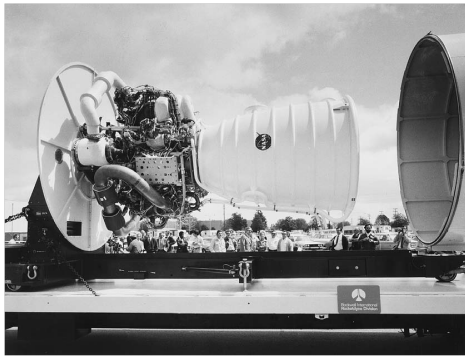
- Variazione della viscosità artificiale
- Sensibilità al numero di Courant (provate il Courant massimo a cui il codice rimane stabile, dovrebbe essere attorno a 1.1)
- Effetto del gas reale: il fluido da scegliere è da selezionare nell'elenco del NIST (vedi paragrafo 4.3), secondo le ultime due cifre del numero di matricola (dividere per due se le cifre sono $i \geq 85$). Ad esempio il numero di matricola 123456 sceglierà il fluido 56 = R134a, il numero 123498 sceglierà il fluido 46 = R23. La scelta delle condizioni a cui calcolare $\gamma(T)$ andrà opportunamente giustificata

Per qualsiasi dubbio contattatemi liberamente (allegate il pdf della relazione se avete bisogno di mostrarmi qualcosa).

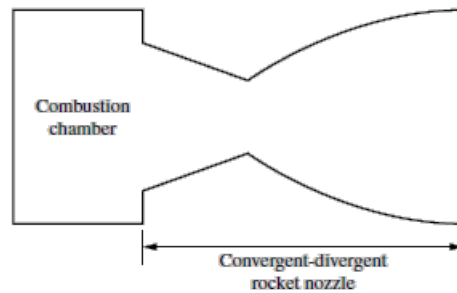
Chapter 1

Introduction

One of the most fascinating example of the harnessing of nature by engineers is shown in Fig. 1.1a, which is a photograph of the main rocket engine for the space shuttle. This engine produces over 1.5 MN of thrust. Note the large bell-like divergent nozzle of the rocket engine. Why this shape instead of some convergent shape? In reality, in Figure 1.1a, we are seeing only part of the rocket nozzle; hidden behind all the plumbing to the left of the divergent duct in is a combustion chamber that feeds the hot, high-pressure gas into a convergent duct that transitions to the divergent part, as sketched in Fig. 1.1b.



(a) Space shuttle main rocket engine (NASA)



(b) Shuttle engine sketch

Figure 1.1: Typical converging diverging nozzle problem

In the first part of the notes we will deal with the isentropic steady-state flow through the converging-diverging nozzle reported in Fig. 2.1. Later on we will present the case of shock wave and the numerical techniques able to capture the discontinuities.

Chapter 2

Problem statement - isentropic flow

Assuming that the air is flowing according to the positive x-axis, at the inlet we consider the flow coming from a reservoir. Here the pressure and temperature are p_0 and T_0 . These quantities can be considered as stagnation value, since the area is theoretically $A \rightarrow \infty$.

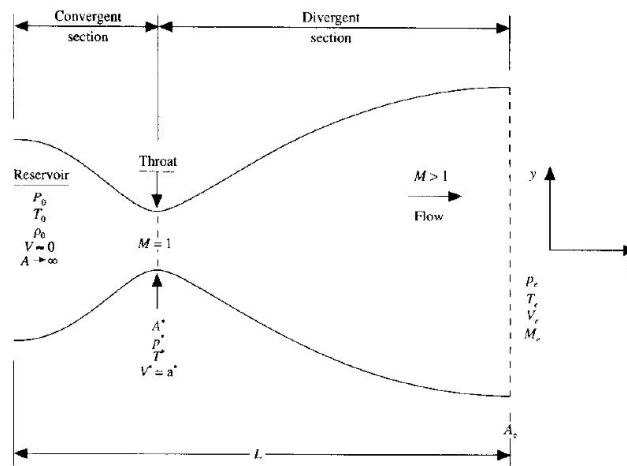


Figure 2.1: Sketch of the nozzle under investigation

An additional assumption is to consider the problem as one-dimensional. This hypothesis actually does not reflect the reality since during both the converging as well as the diverging part of the duct the flow will have motion even along the y-axis. By considering the properties as uniform across any cross section we are dealing with a *quasi-one-dimensional* flow.

The problem under investigation has an analytic solution, that states that the Mach number variation along the duct depends only on the area ratio A/A^* . With the notation of Fig. 2.1, where the * denotes the sonic section,

we have that the mass flow rate that flows through the duct is the same whatever section we consider. Thus:

$$\rho^* A^* V^* = \rho A V \quad (2.1)$$

Since $V^* = a^*$, we can express the area variation with respect to the sonic throat in the following fashion:

$$\frac{A}{A^*} = \frac{\rho^* V^*}{\rho V} = \frac{\rho^*}{\rho_0} \frac{\rho_0 a^*}{\rho V} \quad (2.2)$$

Where the subscript 0 denotes the stagnation quantities (equal to the value in the reservoir, since the flow is isentropic). Having this fact in mind, from the definition of the stagnation quantities one has

$$\frac{\rho_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{1}{\gamma - 1}} \quad (2.3)$$

$$\frac{\rho^*}{\rho_0} = \left(\frac{2}{\gamma + 1}\right)^{\frac{1}{\gamma - 1}} \quad (2.4)$$

From the conservation of the total enthalpy one can derive the following formulation for the Mach number

$$\frac{V}{a^*} = M^{*2} = \frac{[(\gamma + 1)]M^2}{2 + [(\gamma - 1)]M^2} \quad (2.5)$$

Substituting equations (2.3) to (2.5) into Eqn. (2.2), we obtain

$$\left(\frac{A}{A^*}\right)^2 = \frac{1}{M^2} \left[\frac{2}{\gamma + 1} \left(1 + \frac{\gamma - 1}{2} M^2\right)\right]^{\frac{\gamma + 1}{\gamma - 1}} \quad (2.6)$$

Equation (2.6) is called the area–Mach number relation. It states that $M = f(A/A^*)$ that is, the Mach number at any location in the duct is a function of the ratio of the local duct area to the sonic throat area.

In this assignment we will derive the approximated solution through the numerical study of the problem.

2.1 Governing Euler Equations

In the following we will consider the reservoir as containing an inviscid fluid and so the Euler equations are the governing system of partial differential equations (PDEs). Since we are doing such a strong assumption, that is to consider the properties of the flow uniform over the area, the physics of the problem is different from the real physics of the flow. Under such a perspective it is compulsory to ensure that the conservation of mass, momentum and energy is satisfied. Let's derive the corresponding relations for the case of quasi-one dimensional fluid.

Continuity equation

Recalling the integral form of the continuity equation

$$\frac{\partial}{\partial t} \iiint_{\Omega} \rho d\Omega + \iint_S \rho \mathbf{V} \cdot d\mathbf{S} = 0 \quad (2.7)$$

Equation (2.7) is applied to the control volume shaded in Fig. 2.2. If we consider the volume as vanishing ($dx \rightarrow 0$), the volume integral of Eqn. (2.8) can be approximated by:

$$\frac{\partial}{\partial t} \iiint_{\Omega} \rho d\Omega = \frac{\partial(\rho A dx)}{\partial t} \quad (2.8)$$

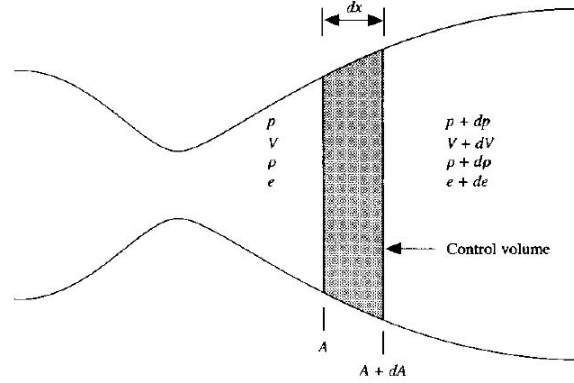


Figure 2.2: Control Volume for the derivation of the governing equations of the quasi-one-dimensional case

Equation (2.8) can be written because The control volume $\Omega \simeq A dx$ for $dx \rightarrow 0$. On the other hand the case of surface integral of Eqn. (2.7) can be written as:

$$\iint_S \rho \mathbf{V} \cdot d\mathbf{S} = -\rho AV + (\rho + d\rho)(A + dA)(V + dV) \quad (2.9)$$

OSS: The minus sign before the first term on the right hand side of equation (2.9) is due to the fact that \mathbf{S} and \mathbf{V} point in opposite directions since the surface normal vector points outward the volume by convention.

Expanding the triple product a series of term involving the product of differentials (e.g. $\rho dV dA$ or $A d\rho dV$) appears. Such terms go to zero faster than the terms which have only one differential and thus can be neglected. In the limit dx tends to zero, equation (2.7) becomes Eqn. (2.10):

$$\frac{\partial(\rho A dx)}{\partial t} + d(\rho AV) = 0 \quad (2.10)$$

Dividing by dx and keeping in mind that $d(\rho AV)/dx$ is the partial derivative with respect to x when dx vanishes, one has:

$$\frac{\partial \rho A}{\partial t} + \frac{\partial \rho AV}{\partial x} = 0 \quad (2.11)$$

that represents the continuity equation for an unsteady quasi-one-dimensional flow.

Momentum equation

For what concerns the x-component of the momentum equation, for an inviscid flow and without body forces one has:

$$\frac{\partial}{\partial t} \int \int \int_{\Omega} (\rho u) d\Omega + \int \int_S (\rho u \mathbf{V}) \cdot d\mathbf{S} = - \int \int_S (p dS)_x \quad (2.12)$$

A treatise analogous to the one done for the derivation of Eqns. (2.8) and (2.10) can be done here, obtaining :

$$\frac{\partial}{\partial t} \int \int \int_{\Omega} \rho u d\Omega = \frac{\partial \rho V A dx}{\partial t} \quad (2.13)$$

and:

$$\int \int_S (\rho u \mathbf{V}) \cdot d\mathbf{S} = -\rho AV^2 + (\rho + d\rho) (A + dA) (V + dV)^2 \quad (2.14)$$

For what concerns the term on the right hand side of Eqn. (2.12), namely the pressure force in x direction, the reader is referred to Fig. 2.3. The balance leads to Eqn.

$$\int \int_S (p dS)_x = -pA + (p + dp) (A + dA) - 2p \left(\frac{dA}{2} \right) \quad (2.15)$$

Substituting Eqns. (2.14), (2.13) and (2.15), doing the operations on the right hand side of equation (2.15) and ignoring the terms involving the product of differentials, one finds:

$$\frac{\partial(\rho V A dx)}{\partial t} + d(\rho AV^2) = -A dp \quad (2.16)$$

Again, as done for equation (2.11), we get the conservation form of the momentum equation for a quasi-one-dimensional nozzle:

$$\frac{\partial(\rho V A)}{\partial t} + \frac{\partial(\rho AV^2)}{\partial x} = - \frac{\partial(pA)}{\partial x} \quad (2.17)$$

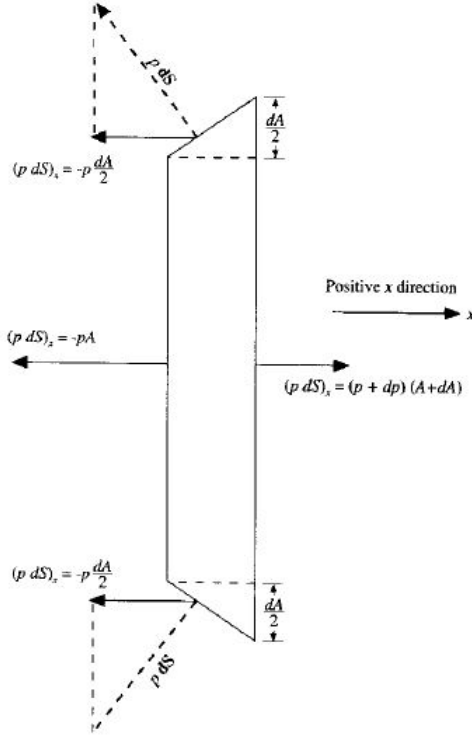


Figure 2.3: Control Volume for the derivation of the governing equations of the quasi-one-dimensional case

Equation (2.17) could be used as is for our purposes. Nonetheless, the numerical scheme we are setting up is based on the nonconservative form of the governing equations. Thus, to obtain that form of the momentum equation, we have to multiply the continuity equation (2.11) by V and subtract the so-obtained equation from (2.17). Expanding the derivatives and cancelling the equal terms and dividing by A we get the final form of the momentum equation in the nonconservative form, as we were seeking:

$$\rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial x} = -\frac{\partial p}{\partial x} \quad (2.18)$$

Energy equation

If we neglect the body forces and considering an adiabatic flow ($\dot{q} = 0$), the general Euler equation is:

$$\frac{\partial}{\partial t} \int \int \int_{\Omega} \rho \left(e + \frac{V^2}{2} \right) d\Omega + \int \int_S \rho \left(e + \frac{V^2}{2} \right) \mathbf{v} \cdot d\mathbf{S} = - \int \int_S (p \mathbf{v}) \cdot d\mathbf{S} \quad (2.19)$$

Again, referring to Fig. 2.2, one can write:

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho \left(e + \frac{V^2}{2} \right) A dx \right] - \rho \left(e + \frac{V^2}{2} \right) V A \\ + (p + dp) \left[e + de + \frac{(V + dV)^2}{2} \right] (V + dV)(A + dA) \\ = - \left[-pVA + (p + dp)(V + dV)(A + dA) - 2 \left(pV \frac{dA}{2} \right) \right] \end{aligned} \quad (2.20)$$

Expanding the products and neglecting the products of differentials we derive:

$$\frac{\partial}{\partial t} \left[\rho \left(e + \frac{V^2}{2} \right) A dx \right] + d(\rho e V A) + \frac{d(\rho V^3 A)}{2} = -d(pVA) \quad (2.21)$$

or, equivalently, as dx approaches zero:

$$\frac{\partial}{\partial t} \left[\rho \left(e + \frac{V^2}{2} \right) A \right] + \frac{\partial}{\partial x} \left[\rho \left(e + \frac{V^2}{2} \right) V A \right] = -\frac{\partial(pVA)}{\partial x} \quad (2.22)$$

Which is the conservation form of the energy equation in its conservative form expressed in terms of total energy $(e + V^2/2)$. To obtain the non conservative form in terms of internal energy e , let us multiply the conservation form of the momentum equation (2.17) by V , and subtract it from (2.22) obtaining:

$$\frac{\partial(\rho e A)}{\partial t} + \frac{\partial(\rho e V A)}{\partial x} = -p \frac{\partial(AV)}{\partial x} \quad (2.23)$$

As you can easily see the form of Eqn. (2.23) is exactly the same of (2.22), but the transported variable is e instead of $(e + V^2/2)$. To obtain the non conservative form of the sought equation, we have to multiply the continuity equation (2.11) by e and subtract it from (2.23), expanding the right hand side and dividing by A , it yields to:

$$\rho \frac{\partial e}{\partial t} + \rho V \frac{\partial e}{\partial x} = -p \frac{\partial V}{\partial x} - p \frac{V}{A} \frac{\partial(A)}{\partial x} \quad (2.24)$$

or, noticing that on the right hand side the last term is actually the derivative of a logarithm,

$$\rho \frac{\partial e}{\partial t} + \rho V \frac{\partial e}{\partial x} = -p \frac{\partial V}{\partial x} - pV \frac{\partial \ln(A)}{\partial x} \quad (2.25)$$

Which is the nonconservation form of the energy equation for a quasi-one-dimensional flow. All the effort put in deriving such equation is due to the fact that from Eqn.(2.25) is straightforward to obtain a relation where the primitive variable T appears as is. To deal with the primary dependent

variable is thus sufficient recalling the relation valid for a calorically perfect gas (c_v constant with respect to the temperature):

$$e = c_v T \quad (2.26)$$

And thus Eqn. (2.25), becomes:

$$\rho c_v \frac{\partial T}{\partial t} + \rho V c_v \frac{\partial T}{\partial x} = -p \frac{\partial V}{\partial x} - p V \frac{\partial \ln(A)}{\partial x} \quad (2.27)$$

Which ends the system of equations that rule the problem. If you take a deeper look into Eqs. (2.11), (2.18) and (2.27), you might note that we have three equations in four variables : ρ , V , p and T . We can call a fourth equation to get help in order to reduce the number of unknowns. That is the equation of state for a perfect gas:

$$p = \rho R T \quad (2.28)$$

which, along with its derivative with respect to the spatial coordinate,

$$\frac{\partial p}{\partial x} = R \left(\rho \frac{\partial T}{\partial x} + T \frac{\partial \rho}{\partial x} \right) \quad (2.29)$$

allows us to rewrite the governing set of Euler equations in the case of quasi-one-dimensional nozzle flow in the following fashion (expanding the derivatives):

$$\frac{\partial \rho A}{\partial t} + \rho A \frac{\partial V}{\partial x} + \rho V \frac{\partial A}{\partial x} + A V \frac{\partial \rho}{\partial x} = 0 \quad (2.30)$$

$$\rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial x} = -R \left(\rho \frac{\partial T}{\partial x} + T \frac{\partial \rho}{\partial x} \right) \quad (2.31)$$

$$\rho c_v \frac{\partial T}{\partial t} + \rho V c_v \frac{\partial T}{\partial x} = -\rho R T \left[\frac{\partial V}{\partial x} + V \frac{\partial \ln(A)}{\partial x} \right] \quad (2.32)$$

Chapter 3

Finite Difference Method - Implementation Remarks

Both the numerical methods presented in this notes are explicit in time. This means that a stability criterion is required. To have a clearer view of the meaning of this sentence, the following section presents a few remarks and analysis are carried out. The treatise is carried out with an upwind scheme in order to better focus on the idea behind the numerical method rather on the method itself.

This paragraph is reported for giving a general idea of the meaning of the Courant number and the CFL condition. This condition is very important in the solution of CFD problems and allow to discern between stable schemes (e.g. Forward-Backward, Lax-Friedrich) and unstable ones (e.g. Forward-Forward). Nonetheless this paragraph is NOT part of the assignment. Since the focus is on the physical meaning, the treatise is not rigorous.

3.1 Upwind Scheme - General Features

Let us consider a linear convection equation: a typical first-order hyperbolic equation.

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad (3.1)$$

This equations, represent the transport of the unknown property $u = u(x, t)$ by the convection with a speed a . Two partial derivatives appears in Eqn. (3.1), with respect to the time an to the space. The choice of the discretisation must keep into account both the derivatives at the same time. So, for having an explicit scheme, we must evaluate the spatial derivative terms at the time n and not $n + 1$, which would lead to an implicit scheme. The choice of such an approach would lead to a more accurate and stable solution, but the implementation of such a technique is more complicate and involves the solution of the system of equations using the properties of the

linear systems. This approach is used in the more complicate CFD codes, where the problem of inhomogeneous distribution of the nodes usually leads to too much small time steps for stability reason. By the moment, let's stay with a simpler code.

In such a scenario the space derivative can be approximated by the central, forward or backward (rearward) difference and according to the choice the order of the approximation (i.e. the truncation error) would respectively the 2nd or 1st. For instance, if we choose the forward difference, the equation (3.1) is discretised in the following fashion:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -a \frac{u_{i+1}^n - u_i^n}{\Delta x} \quad (3.2)$$

Such a discretisation lead to a fist order approximate equation both in space and time. The order of the approximation can be increased by simply consider a central difference approximation on the left hand side of equation (3.2).

The name upwind derives from the fact that actually the choice of backward rather than forward difference is not arbitrary. In this case, it is natural to select the points in the solution at the time-level n that are upwind of the solution at the position i and at the time-level $n + 1$, as these are the ones causally connected with u_i^{n+1} . Depending then on the direction in which the solution is translated, and thus on the sign of the velocity a , equation (3.2) can be written in two different way

$$\left\{ \begin{array}{ll} \frac{u_i^{n+1} - u_i^n}{\Delta t} = -a \frac{u_{i+1}^n - u_i^n}{\Delta x} & \text{if } a < 0 \\ \frac{u_i^{n+1} - u_i^n}{\Delta t} = -a \frac{u_i^n - u_{i-1}^n}{\Delta x} & \text{if } a > 0 \end{array} \right. \quad (3.3)$$

$$\left. \begin{array}{l} \\ \end{array} \right\} \quad (3.4)$$

Stability analysis

The upwind scheme is a stable one in the sense that the solution will not have exponentially growing modes. This can be seen through a von Neumann stability analysis, a useful tool which allows a first simple validation of a given numerical scheme. It is important to underline that the von Neumann stability analysis is local in the sense that: a) it does not take into account boundary effects; b) it assumes that the coefficients of the finite difference equations are sufficiently slowly varying to be considered constant in time and space (this is a reasonable assumptions if the equations are linear). Under these assumptions, the solution can be seen as a sum of eigenmodes which at each grid point have the form:

$$u_i^n = \xi^n e^{ikx} \quad (3.5)$$

where k is the spatial wave number and $\xi = \xi(k)$ is a complex number. If one consider the symbolic representation of the finite difference equation for the next time step as:

$$u_i^{n+1} = G(\Delta t^p, \Delta x^q)u_i^n \quad (3.6)$$

Where $G(\Delta t^p, \Delta x^q)$ is the evolution operator of order p in time and q in space. It can be seen that the time evolution of a single eigenmode is nothing but a succession of integer powers of the complex number ξ which is therefore named amplification factor. This naturally leads to a criterion of stability as the one for which the modulus of the amplification factor is always less than 1 and so:

$$|\xi|^2 = \xi\xi^* \leq 1 \quad (3.7)$$

Applying Eqn. (3.5) to Eqs. (3.3)(3.4) the amplification factor is:

$$\xi = 1 - |\alpha|(1 - \cos(k\Delta x)) - i\alpha \sin(k\Delta x) \quad (3.8)$$

Where

$$\alpha \equiv \frac{a\Delta t}{\Delta x} \quad (3.9)$$

and therefore $|\xi|^2$:

$$|\xi|^2 = 1 - 2|\alpha|(1 - |\alpha|)(1 - \cos(k\Delta x)) \quad (3.10)$$

and the stability criterion (3.6) is satisfied as long as we chose

$$|\alpha| \leq 1 \quad (3.11)$$

Equation (3.11) is usually referred to as Courant condition or CFL (form Courant-Friedrichs-Loewy condition). Equation (3.11) is translated in a maximum value for the time step Δt since Δx is known from the discretization and a is known from the former time step:

$$\Delta t = C \frac{\Delta x}{|a|} \quad (3.12)$$

With C is the CFL number. From Eqn.(3.12) and Fig. 3.1, on can observe that:

- From a mathematical standpoint, the stability is ensured if the numerical domain of dependence of the solution is larger than the physical one.
- From a physical standpoint, the respecting of the CFL condition ensures that the propagation speed of any physical perturbation (in the cases of our interest is the speed of sound) is smaller of a grid cell.

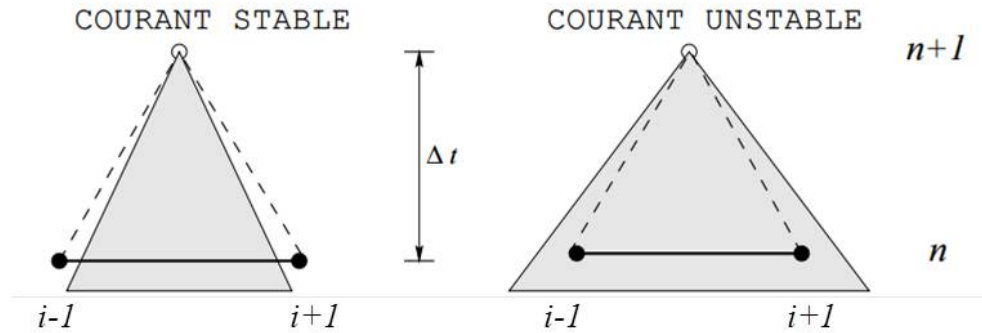


Figure 3.1: Mathematical meaning of Courant stable and unstable conditions: the dashed lines represent the numerical domain of dependence of the solution at x_i^n , if the central difference scheme for the spatial derivative is chosen. The shaded area is the physical domain of dependence. Stability is ensured if the numerical area of dependence includes the physical one

OSS: For the present application, the CFL number criterion does not hold exactly (a stable solution is achievable even with a Courant number of 1.1). In this case in fact we are dealing with a nonlinear hyperbolic partial differential equation and the CFL criterion is formulated for a linear one. In spite of this, the CFL still stands as a good criterion for a reliable estimation of the Δt .

Chapter 4

Finite Difference Methods - Implementation

4.1 Adimensionalisation of the Governing Equations

Although the set of equations (2.30) to (2.32) could directly be implemented in a CFD code, when dealing with nozzle flows it is common practice to make use of nondimensional variables. In this section we will transform the set of Euler equation for having the physical quantities adimensionalised with respect to the reservoir values. In the following the prime represent a nondimensional quantity. Thus, we have:

$$T' = \frac{T}{T_0} \quad \rho' = \frac{\rho}{\rho_0} \quad x' = \frac{x}{L} \quad \text{and} \quad V' = \frac{V}{a_0}, \quad \text{where} \quad a_0 = \sqrt{\gamma RT_0}$$

Where L is the length of the duct. Noticing that L/a_0 has the dimensions of the time, we can write the dimensionless time as $t' = t/(L/a_0)$. Eventually, the reference area for the adimensionalisation is the sonic throat area A^* and thus $A' = A/A^*$.

These relations given, we can proceed in order to obtain the equivalent of Eqs. (2.30), (2.31) and (2.32) in terms of prime quantities. Starting from the continuity equation, one has:

$$\begin{aligned} \frac{\partial \rho' A'}{\partial t'} \left(\frac{\rho_0 A^*}{L/a_0} \right) + \rho' A' \frac{\partial V'}{\partial x'} \left(\frac{\rho_0 A^* a_0}{L} \right) + \rho' V' \frac{\partial A'}{\partial x'} \left(\frac{\rho_0 A^* a_0}{L} \right) \\ + A' V' \frac{\partial \rho'}{\partial x'} \left(\frac{\rho_0 A^* a_0}{L} \right) = 0 \end{aligned} \quad (4.1)$$

Noticing that A' is constant (does not depend on time but only on the space), and all the terms between brackets are equal, the very final form of the continuity equation that will be used is:

$$\boxed{\frac{\partial \rho'}{\partial t'} = -\rho' \frac{\partial V'}{\partial x'} - \rho' V' \frac{\partial \ln(A)}{\partial x'} - V' \frac{\partial \rho'}{\partial x'}} \quad (4.2)$$

For what concerns the momentum equation, from (2.31), we have

$$\begin{aligned} \rho' \frac{\partial V'}{\partial t'} \left(\frac{\rho_0 a_0}{L/a_0} \right) + \rho' V' \frac{\partial V'}{\partial x'} \left(\frac{\rho_0 a_0^2}{L} \right) = \\ - R \left(\rho' \frac{\partial T'}{\partial x'} + T' \frac{\partial \rho'}{\partial x'} \right) \left(\frac{\rho_0 T_0}{L} \right) \end{aligned}$$

Carrying out the proper algebra and noticing that:

$$\frac{RT_0}{a_0^2} = \frac{\gamma RT_0}{\gamma a_0^2} = \frac{a_0^2}{\gamma a_0^2} = \frac{1}{\gamma}$$

One has:

$$\boxed{\frac{\partial V'}{\partial t'} = -V' \frac{\partial V'}{\partial x'} - \frac{1}{\gamma} \left(\frac{\partial T'}{\partial x'} + \frac{T'}{\rho'} \frac{\partial \rho'}{\partial x'} \right)} \quad (4.3)$$

Lastly, recalling Eqn. (2.32) and introducing the adimensionalisations we have:

$$\begin{aligned} \rho' c_v \frac{\partial T'}{\partial t'} \left(\frac{\rho_0 T_0}{L/a_0} \right) + \rho' V' c_v \frac{\partial T'}{\partial x'} \left(\frac{\rho_0 a_0 T_0}{L} \right) = \\ \rho' R T' \left[\frac{\partial V'}{\partial x'} + V' \frac{\partial \ln(A')}{\partial x'} \right] \left(\frac{\rho_0 a_0 T_0}{L} \right) \end{aligned}$$

Keeping in mind the relation

$$\frac{R}{c_v} = \frac{R}{R/(\gamma - 1)} = \gamma - 1$$

We have the last equation needed for the numerical resolution of the problem:

$$\boxed{\frac{\partial T'}{\partial t'} = -V' \frac{\partial T'}{\partial x'} - (\gamma - 1) T' \left[\frac{\partial V'}{\partial x'} + V' \frac{\partial \ln(A')}{\partial x'} \right]} \quad (4.4)$$

For clearness sake, from now on we will deal only with nondimensional quantities and the prime will be omitted.

Before starting with the implementation of the numerical method, the geometry and the boundary condition are presented.

4.1.1 Geometry of the nozzle

No matter what scheme is to be implemented, one first needs to create the computational grid. To keep the things easy, let's implement a parabolic nozzle. The specified shape is held fixed in time and it is given by the relation:

$$A = 1 + 2.2(x - 1.5)^2 \quad 0 \leq x \leq 3 \quad (4.5)$$

In this way the first part of the duct up to $x = 1.5$ is convergent and then is divergent. The throat section is in $x = 1.5$. With the topology reported in Fig. 2.1, the inlet (reservoir) is on the left and the outlet on the right.

4.1.2 Boundary and initial conditions for isentropic flow

In this section we will formulate the boundary conditions for a subsonic-supersonic isentropic solution, where the flow inside the duct is free of developing without constraints (i.e. no back pressure imposed). For what concerns the boundary condition, on a physical basis we know that the mass flow through the nozzle must be allowed to adjust to the proper steady state. Thus a variable must be let free to float: the choice of V_1 makes the most sense as part of this adjustment. In light of this the following conditions are imposed at the inlet:

- $\rho_1=1$
- $T_1=1$
- V_1 Neumann condition (null velocity gradient)

For what concerns the outlet, from the method of the characteristics all the variable must be let free to float. Thus a Neumann condition must be applied to all the quantities ρ_2, T_2 and V_2 .

To start the time-marching procedure, the variables must be set up with values for every x at the time $t = 0$. Theoretically the conditions could be purely as you wish. Practically, you must be aware that:

- The closer you are to the expected final solution, the faster your simulation will converge
- If you are too far from the final conditions, the timewise gradient can be too big and the program can go unstable

Intelligent choice of the initial conditions is given from any knowledge you have of the problem. Since density and temperature must decrease passing through the nozzle and the velocity, on the other hand, increases. Thus a clever guess for the initial state is

- $\rho = 1 - 0.3146x$
- $T = 1 - 0.2314x$
- $V = (0.1 + 1.09x)T^{1/2}$

4.1.3 MacCormack's technique

MacCormack's technique is a variant of the Lax-Wendroff method, but easier to be implemented. Such a method is second - order - accurate both in time and space. This method is based on a predictor - corrector approach. With regards to the continuity equation, the density in the node i at the next time step is derived from the actual one in the following fashion:

$$\rho_i^{n+1} = \rho_i^n + \left(\frac{\partial \rho}{\partial t} \right)_{ave} \Delta t \quad (4.6)$$

where $(\partial \rho / \partial t)_{ave}$ is a representative "mean" value for $(\partial \rho / \partial t)$ between times n and $n + 1$. This expedient allow us to avoid the computation of $(\partial^2 \rho / \partial t^2)$ which is not difficult but is very time consuming. The way $(\partial \rho / \partial t)_{ave}$ is calculated is so to preserve the second order accuracy. The procedure for the evaluation of this term, in the case of quasi-one-dimensional nozzle flow, is reported in the following.

The first step of the calculation is named *predictor* step and deals with the idea of predict the properties in the next time step according to the values of the quantities at the current time step. In other words, expanding the time derivative with the second order truncated Taylor series:

$$\bar{\rho}_i^{n+1} = \rho_i^n + \left(\frac{\partial \rho}{\partial t} \right)_i^n \Delta t \quad (4.7)$$

Where the barred quantities stands for the predicted values. You can easily see that $\bar{\rho}_i^{n+1}$ from Eqn. (4.7) is only first - order accurate since in its definition only the first - order terms in the Taylor series appear. For the calculation of the term $(\partial \rho / \partial t)_i^n$, the discretized form of the continuity equation (4.2) is used and, with the recommendation of using the *forward* differences in the spatial derivative, equation (4.8) is derived.

$$\left(\frac{\partial \rho}{\partial t} \right)_i^n = \rho_i^n \frac{V_{i+1}^n - V_i^n}{\Delta x} + \rho_i^n V_i^n \frac{\ln(A_{i+1}) - \ln(A_i)}{\Delta x} + V_i^n \frac{\rho_{i+1}^n - \rho_i^n}{\Delta x} \quad (4.8)$$

Computed $(\partial \rho / \partial t)_i^n$ and thus $\bar{\rho}_i^{n+1}$ from Eqn.(4.8) and (4.7) respectively, we can move to the *corrector* step. The idea is obtaining a predicted value of the time derivative at time $n + 1$ (denoting it with the bar sign) by substituting the predicted values of the flow quantities, as shown in Eqn. (4.9)

$$\begin{aligned} \left(\overline{\frac{\partial \rho}{\partial t}}\right)_i^{n+1} = & \bar{\rho}_i^{n+1} + \frac{\bar{V}_i^{n+1} - \bar{V}_{i-1}^{n+1}}{\Delta x} + \bar{\rho}_i^{n+1} \bar{V}_i^{n+1} \frac{\ln(A_i) - \ln(A_{i-1})}{\Delta x} \\ & + \bar{V}_i^{n+1} \frac{\bar{\rho}_i^{n+1} - \bar{\rho}_{i-1}^{n+1}}{\Delta x} \end{aligned} \quad (4.9)$$

The recommendation is here to use the *backward* differences in the spatial derivative. Now the term $(\partial \rho / \partial t)_{ave}$ is easily computed, calling the first term of (4.10) from Eqn. (4.8) and the second one from Eqn. (4.9)

$$\left(\frac{\partial \rho}{\partial t}\right)_{ave} = \frac{1}{2} \left[\left(\frac{\partial \rho}{\partial t}\right)_i^n + \left(\overline{\frac{\partial \rho}{\partial t}}\right)_i^{n+1} \right] \quad (4.10)$$

The quantities at the next time step can be finally computed through (4.6).

The predictor-corrector sequence described above, because a two-step difference is used with forward differences on the predictor and backward differences on the corrector, is a second - order - accurate method. The order presented is not compulsory though.

```

1 % MacCormack's explicit technique for the resolution
2 % of 1d euler equation
3
4 %Imposition of initial condition
5 rho = 1-0.3146*X;
6
7 %Time marching technique
8
9 endTime =100;
10
11 while(t<endTime)
12
13 %Loop over the internal nodes
14
15 rhobartdt(1)=1;
16
17 for i=2:Nx-1
18
19 %% Predictor step
20
21 %forward differencing in space at time t
22 rhoPred(i) = (rhot(i+1)-rhot(i))/dx;
23
24 %computation of the time derivative at time t
25 drhodt(i) = -rhot(i)*uPred(i)-rhot(i)*ut(i)*sPred(i)-ut(i)*rhoPred(i);
26
27 %predicted value for rho
28 rhobartdt(i)= rhot(i)+ drhodt(i)*dt;
29
30 %compute the next time step
31 rho(i)= rho(i) + drhodt(i)*dt;
32
33 %% Corrector step
34 % backward differencing of bar quantities at time t+dt
35 rhoCorr(i)= (rhobartdt(i)-rhobartdt(i-1))/dx;
36
37 %computation of the time derivative at time t+dt
38 drhodtdtdt(i) = -rhobartdt(i)*uCorr(i)-rhobartdt(i)*ubartdt(i)*sCorr(i)
39 -ubartdt(i)*rhoCorr(i);
40
41 %% Rho value at next time step
42
43 %MacCormack average
44 drhodtav(i) = 0.5*(drhodt(i)+drhodtdtdt(i));
45

```

```

46         rhotdt(i)= rhot(i)+drhodtav(i)*dt;
47
48 %Calculation of adimensional sound speed and dt
49         atdt(i)=sqrt(Ttdt(i));
50
51         dtlocal(i)=0.9*dx/(atdt(i)+utdt(i));
52     end
53
54 %Residual monitoring
55     %refreshdata
56         a=a+1;
57         if (mod(a,5)==0)
58             residual(n,:)=drhodtav(:);
59             y(n)=sum(abs(residual(n,:)));
60             a=0;
61             semilogy(time,y)
62             drawnow
63         end
64
65
66 %impose boundary conditions
67         rhotdt(1) = 1;
68         atdt(1)=sqrt(Ttdt(1));
69         dtlocal(1)=0.9*dx/(atdt(1)+ut(1));
70
71         rhotdt(Nx)= 2*rhotdt(Nx-1)-rhotdt(Nx-2);
72         atdt(Nx) = sqrt(Ttdt(Nx));
73         dtlocal(Nx)=0.9*dx/(atdt(Nx)+utdt(Nx));
74
75         dt=min(dtLocal);
76
77         t=t+dt;
78
79     end

```

Results

To validate your code, compare the outcome of your simulation with the Fig. 4.1.

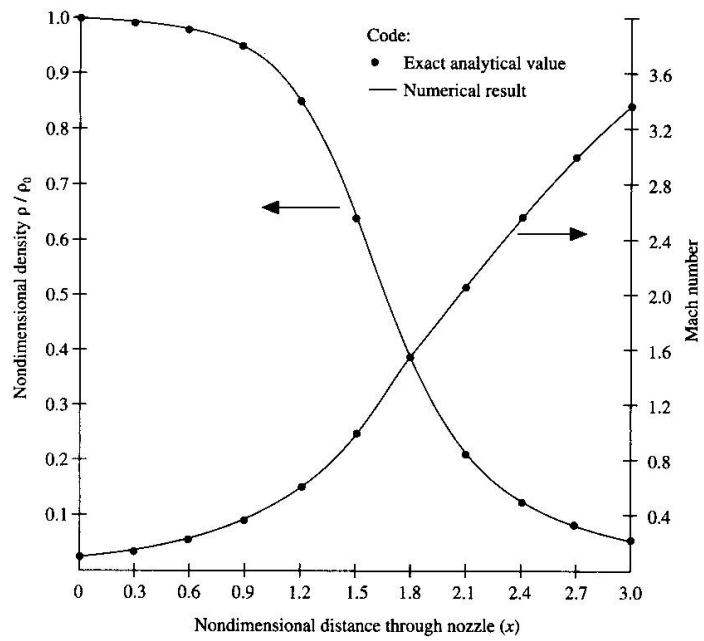


Figure 4.1: Analytical result for the comparison with the outcome of the numerical simulation

4.2 Conservative Euler equations

In flow fields involving shock waves, there are sharp, discontinuous change in the primitive flow-field variables (ρ, p, V, T) across the shocks. In the following we will deal with a shock-capturing technique (opposite to the shock-fitting approach). In this framework, the scheme let the shock wave to appear naturally within the computation space as a direct result of the overall flow solution. If the nonconservation form of the governing equation is used in case of shock-capturing technique, the computed flow field results shows oscillation (wiggles) upstream and downstream of the shock wave that may appear in the wrong location. The solution can even become unstable. For this reason the first part of this section is devoted to the derivation of adimensional-conservation equations.

4.2.1 Derivation of adimensional equation

From (2.11), one can see that the equation is already in its conservation form. Thus for the adimensionalisation, the following form is obtained

$$\frac{\partial \left(\frac{\rho}{\rho_0} \frac{A}{A^*} \right)}{\partial \left(\frac{t}{L/a_0} \right)} \left(\frac{\rho_0 A^* a_0}{L} \right) + \frac{\partial \left(\frac{\rho}{\rho_0} \frac{A}{A^*} \frac{V}{a_0} \right)}{\partial \left(\frac{x}{L} \right)} \left(\frac{\rho_0 A^* a_0}{L} \right) = 0 \quad (4.11)$$

And thus in term of prime quantities,

$$\boxed{\frac{\partial \rho' A'}{\partial t'} + \frac{\partial \rho' A' V'}{\partial x'} = 0} \quad (4.12)$$

For what concerns the momentum equation (2.17), adding it to Eqn. (4.12), we have:

$$\frac{\partial(\rho V A)}{\partial t} + \frac{\partial(\rho A V^2 + p A)}{\partial x} = -p \frac{\partial A}{\partial x} \quad (4.13)$$

The nondimensionalisation leads to:

$$\begin{aligned} \frac{\partial \left(\frac{\rho}{\rho_0} \frac{A}{A^*} \frac{V}{a_0} \right)}{\partial \left(\frac{t}{L/a_0} \right)} \left(\frac{\rho_0 A^* a_0^2}{L} \right) + \frac{\partial \left[\frac{\rho}{\rho_0} \frac{A}{A^*} \frac{V^2}{a_0^2} (\rho_0 A^* a_0^2) + \frac{p}{p_0} \frac{A}{A^*} (p_0 A^*) \right]}{\partial \left(\frac{x}{L} \right) L} \\ = \frac{p}{p_0} \frac{\partial(A/A^*)}{\partial(x/L)} \left(\frac{p_0 A^*}{L} \right) \end{aligned} \quad (4.14)$$

or, in prime terms,

$$\frac{\partial(\rho' V' A')}{\partial t'} + \frac{\partial[\rho' A' V'^2 + p' A' (p_0/\rho_0 a_0^2)]}{\partial x'} = p' \frac{\partial A'}{\partial x'} \left(\frac{p_0}{\rho_0 a_0^2} \right) \quad (4.15)$$

And keeping in mind that

$$\frac{p_0}{\rho_0 a_0^2} = \frac{\rho_0 R T_0}{\rho_0 a_0^2} = \frac{\rho_0 R T_0}{\rho_0 \gamma R T_0} = \frac{1}{\gamma} \quad (4.16)$$

And thus:

$$\boxed{\frac{\partial(\rho' V' A')}{\partial t'} + \frac{\partial[\rho' A' V'^2 + (1/\gamma)p' A']}{\partial x'} = \frac{1}{\gamma} p' \frac{\partial A'}{\partial x'}} \quad (4.17)$$

For what concerns energy equation in its conservation form (2.22), combining the x derivatives we have

$$\frac{\partial}{\partial t} \left[\rho \left(e + \frac{V^2}{2} \right) A \right] + \frac{\partial}{\partial x} \left[\rho \left(e + \frac{V^2}{2} \right) V A + p V A \right] = 0 \quad (4.18)$$

Defining the nondimensional internal energy as

$$e' = e/e_0 \quad e_0 = c_v T_0 = \frac{R T_0}{\gamma - 1}$$

Proceeding with the adimensionalisation, we have

$$\begin{aligned} & \frac{\partial \left\{ \frac{\rho}{\rho_0} \left[\frac{e}{e_0} e_0 + \frac{V^2}{2 a_0^2} a_0^2 \right] \frac{A}{A^*} \right\}}{\partial \left(\frac{x}{L/a_0} \right)} \\ & + \frac{\partial \left\{ \frac{\rho}{\rho_0} \left[\frac{e}{e_0} e_0 + \frac{V^2}{2 a_0^2} a_0^2 \right] \frac{A}{A^*} \frac{V}{a_0} (\rho_0 a_0 A^*) + \left(\frac{p}{\rho_0} \frac{A}{A^*} \frac{V}{a_0} \right) (\rho_0 a_0 A^*) \right\}}{\partial \left(\frac{x}{L/a_0} \right)} = 0 \end{aligned} \quad (4.19)$$

Adding the fact that $e_0 = R T_0 / (\gamma - 1)$, equation (4.19) becomes:

$$\begin{aligned} & \frac{\partial \left[\rho' \left(\frac{e'}{\gamma-1} + \frac{\gamma}{2} V'^2 \right) A' \right]}{\partial t'} \left(\frac{\rho_0 A^* a_0 R T_0}{L} \right) \\ & + \frac{\partial \left[\rho' \left(\frac{e'}{\gamma-1} + \frac{\gamma}{2} V'^2 \right) A' V' \left(\frac{\rho_0 A^* a_0 R T_0}{L} \right) + (p' A' V') \left(\frac{p_0 A^* a_0}{L} \right) \right]}{\partial x'} = 0 \end{aligned} \quad (4.20)$$

Adding the fact that $p_0 / (\gamma R T_0) = 1$ for a perfect gas and dividing by $\rho_0 A^* a_0 R T_0 / L$ we obtain:

$$\boxed{\frac{\partial \left[\rho' \left(\frac{e'}{\gamma-1} + \frac{\gamma}{2} V'^2 \right) A' \right]}{\partial t'} + \frac{\partial \left[\rho' \left(\frac{e'}{\gamma-1} + \frac{\gamma}{2} V'^2 \right) A' V' + p' A' V' \right]}{\partial x'} = 0} \quad (4.21)$$

The boxed equations are the governing equations in conservation form for a quasi-one-dimensional nozzle flow. Writing down the system in the usual fashion with column vectors as follow:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{J} \quad (4.22)$$

we shall define the components of the solutions vectors \mathbf{U} , the flux vector \mathbf{F} and source terms vector \mathbf{J} (the prime is omitted, all the terms are nondimensional)

$$\begin{aligned} U_1 &= \rho A \\ U_2 &= \rho AV \\ U_3 &= \rho \left(\frac{e}{\gamma - 1} + \frac{\gamma}{2} V^2 \right) A \\ F_1 &= \rho AV \\ F_2 &= \rho AV^2 + \frac{1}{2} p A \\ F_3 &= \rho \left(\frac{e}{\gamma - 1} + \frac{\gamma}{2} V^2 \right) V A + p AV \\ J_2 &= \frac{1}{\gamma} p \frac{\partial A}{\partial x} \end{aligned} \quad (4.23)$$

The governing equations take the form:

$$\frac{\partial U_1}{\partial t} = - \frac{\partial F_1}{\partial x} \quad (4.24)$$

$$\frac{\partial U_2}{\partial t} = - \frac{\partial F_2}{\partial x} + J_2 \quad (4.25)$$

$$\frac{\partial U_3}{\partial t} = - \frac{\partial F_3}{\partial x} \quad (4.26)$$

The primitive variables can be easily derived

$$\rho = \frac{U_1}{A} \quad (4.27)$$

$$V = \frac{U_2}{U_1} \quad (4.28)$$

$$T = e = (\gamma - 1) \left(\frac{U_3}{U_1} - \frac{\gamma}{2} V^2 \right) \quad \text{remember} \quad e' \equiv \frac{e}{e_0} = \frac{c_v T}{c_v T_0} = T' \quad (4.29)$$

$$p = \rho T \quad (4.30)$$

The implementation of the former equations in a code, pass usually through the expression of the fluxes presented in (4.24) in the way $\mathbf{F} = \mathbf{F}(\mathbf{U})$.

If it weren't done, the code would have some numerical issues. This is basically due to the fact that the dependent variables that appear in Eqn. (4.26), are the conservative and not the primitive variables. The mixing of the two would lead to instabilities and potentially failure in the computation. Therefore a consistent formulation in terms of conservative variables is required. Thus to express the desired formulation of the adimensional conservative equation, a few passages are required.

4.2.2 Governing equations in terms of $\mathbf{F}=\mathbf{F}(\mathbf{U})$

F_1

From Eqs. (4.24), $F_1 = \rho AV$. Thus, using (4.27) and (4.28), one obtain:

$$F_1 = U_2 \quad (4.31)$$

F_2

From Eqs. (4.24), $F_2 = \rho AV^2 + (1/\gamma)pA$. Thus, using Eqs. (4.30) (4.27) and (4.29), one obtain:

$$F_2 = \frac{U_2^2}{U_1} + \frac{1}{\gamma}U_1(\gamma - 1) \left[\frac{U_3}{U_1} - \frac{\gamma}{2} \left(\frac{U_2}{U_1} \right)^2 \right] \quad (4.32)$$

and eventually:

$$F_2 = \frac{U_2^2}{U_1} + \frac{\gamma - 1}{\gamma} \left(U_3 - \frac{\gamma U_2^2}{2 U_1} \right) \quad (4.33)$$

F_3

From Eqs. (4.24),

$$F_3 = \rho \left(\frac{e}{\gamma - 1} + \frac{\gamma}{2} V^2 \right) VA + pAV \quad (4.34)$$

Recalling Eqs. (4.27) to (4.30), it is straightforward to obtain:

$$\begin{aligned} F_3 &= U_2 \left(\frac{U_3}{U_1} - \frac{\gamma}{2} V^2 + \frac{\gamma}{2} V^2 \right) VA + U_2 T \\ &= \frac{U_2 U_3}{U_1} + (\gamma - 1) U_2 \left[\frac{U_3}{U_1} - \frac{\gamma}{2} \left(\frac{U_3}{U_1} \right)^2 \right] \end{aligned} \quad (4.35)$$

And thus

$$F_3 = \gamma \frac{U_2 U_3}{U_1} - \frac{\gamma(\gamma - 1)}{2} \frac{U_3^2}{U_1^2} V^2 \quad (4.36)$$

J_2

For what concerns the source term,

$$J_2 = \frac{1}{\gamma} p \frac{\partial A}{\partial x} \quad (4.37)$$

Using Eqs. (4.30), (4.27) and (4.29), one has:

$$J_2 = \frac{1}{\gamma} \frac{U_1}{A} (\gamma - 1) \left[\frac{U_3}{U_1} - \frac{\gamma}{2} \left(\frac{U_2}{U_1} \right)^2 \right] \frac{\partial A}{\partial x} \quad (4.38)$$

And finally:

$$J_2 = \frac{\gamma - 1}{\gamma} \left(U_3 - \frac{\gamma U_2^2}{2 U_1} \right) \frac{\partial \ln(A)}{\partial x} \quad (4.39)$$

4.2.3 Boundary and initial conditions for the shock capturing case

On the contrary with the subject of section 4.1.2, here the back pressure is kept under control. If we lower the pressure p_e (with the notation of Fig. 2.1), the following scenarios can occur.

- If p_e/p_0 is greater than the critical ratio $(p_e)_c/p_0$ (i.e. the ratio by which the Mach number in the throat section equals one), there are an infinite number of possible isentropic solution each one corresponding to a specific pressure ratio. The flow is totally subsonic and the specified back pressure make the local flow properties are function of both the local area ratio (as in the former case) and the pressure ratio.
- If $p_e/p_0 < (p_e)_c/p_0$ the duct becomes choked: the flow remains sonic at the throat and, no matter how the pressure is reduced below $(p_e)_c$, the mass flow remain a fixed value.
- If $p_e/p_0 = (p_e)_{is}/p_0$, where $(p_e)_{is}$ is the pressure at the outlet of the domain which come from the solution of the isentropic case, the solution is unique and is given from the analytic solution of equation (2.6)

In this section we are interested in the second case of the list. If the back pressure is lower than the one which causes the Mach number to be 1 in the throat section the isentropic hypothesis for the resolution of the flow field is not acceptable any more.

Particularly what happens is depicted in Fig. 4.2: the final solution tends to be equal to the isentropic one up to a certain point in the divergent nozzle. Here the back pressure, being higher than the value in case of isentropic

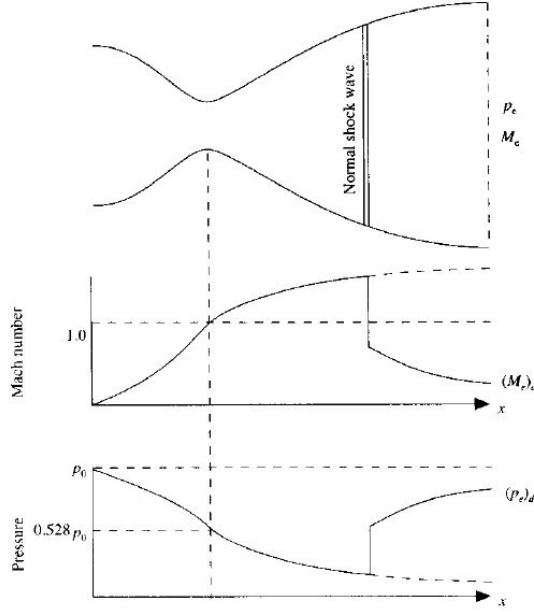


Figure 4.2: Shock in a nozzle: location and variation of relevant quantities

solution, causes the presence of a normal shock wave. The location of the shock is such that the discontinuity in pressure plus the pressure recovery of the subsonic flow downwards the shock is equal to the back pressure value. The solution downward the shock wave is still isentropic for a subsonic flow, but with an entropy value greater than upwards the shock.

It is interesting to note that since the imposed pressure value p_e is lower than the critical one, $(p_e)_c$, the mass flow of the duct is fixed no matter how much this value goes down. In this situation we are dealing with a choked flow, and the only way to change the mass flow is by the modification of the inlet pressure, since the choked throat section and the outlet cannot communicate. Disturbances cannot work their way upstream of the throat and thus the convergent part of the nozzle is frozen in its state.

To obtain such a solution the inlet boundary conditions are theoretically the same described in 4.1.2: two variables are hold fixed and one is let free to float. The application to the conservative variable is done keeping in mind that $U_1 = \rho A$. Thus, if we want ρ to be equal to one at the inlet, it follows:

$$U_{1(i=1)} = (\rho A)_{i=1} = A_{i=1} = const \quad (4.40)$$

For what concerns the momentum equation, the floating value of U_2 is evaluated through a Neumann condition at the end of each time step, and thus:

$$U_{2(i=1)} = 2U_{2(i=2)} - U_{2(i=3)} \quad (4.41)$$

Eventually the value of U_3 is evaluated keeping in mind that

$$U_3 = \rho \left(\frac{e}{\gamma - 1} + \frac{\gamma}{2} V^2 \right) A \quad (4.42)$$

or, equivalently, since $T_{i=1} = 1$ and $e = T$,

$$U_3 = U_1 \left(\frac{1}{\gamma - 1} + \frac{\gamma}{2} V^2 \right) \quad (4.43)$$

For what concerns the outlet, a pressure ratio right to force a normal shock wave is $p_e/p_{01} = 0.6784$. Here, we must specify a variable value at the outlet. Let's obtain U_1 and U_2 in the usual way:

$$U_{1(i=Nx)} = 2U_{1(i=Nx-1)} - U_{1(i=Nx-2)} \quad (4.44)$$

$$U_{2(i=Nx)} = 2U_{2(i=Nx-1)} - U_{2(i=Nx-2)} \quad (4.45)$$

On the other hand the effect of the imposed pressure reflects on U_3 . From Eqn. (4.42), recalling the equation of state, $e = T$ and the definition of $U_2 = \rho AV$:

$$U_{3(i=Nx)} = \frac{p_{Nx} A}{\gamma - 1} + \frac{\gamma}{2} U_{2(i=Nx)} V_{Nx} \quad (4.46)$$

The boundary condition value is known imposing $p_{Nx} = p_e/p_{01} = 0.6784$. For the initial guess of the flow field we should choose a initial condition that is qualitative similar to the final state. We will implement the following distribution:

$$\left. \begin{array}{l} \rho = 1 \\ T = 1 \end{array} \right\} \text{ for } 0 \leq x \leq 0.5 \quad (4.47)$$

$$\left. \begin{array}{l} \rho = 1 - 0.366(x - 0.5) \\ T = 1 - 0.167(x - 0.5) \end{array} \right\} \text{ for } 0.5 \leq x \leq 1.5 \quad (4.48)$$

$$\left. \begin{array}{l} \rho = 0.634 - 0.702(x - 1.5) \\ T = 0.833 - 0.4908(x - 1.5) \end{array} \right\} \text{ for } 1.5 \leq x \leq 2.1 \quad (4.49)$$

$$\left. \begin{array}{l} \rho = 0.5892 - 0.10228(x - 2.1) \\ T = 0.93968 - 0.0622(x - 2.1) \end{array} \right\} \text{ for } 2.1 \leq x \leq 3 \quad (4.50)$$

4.2.4 Lax–Friedrichs technique

The Lax–Friedrichs method is one of the most stable simple scheme for the discretisation of non linear partial differential equation one can think. To derive this scheme, let's think to the FTCS scheme (Forward Time - Central Space):

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2\Delta x} (f(u_{i+1}^n) - f(u_{i-1}^n)) \quad (4.51)$$

As it is well known the FTCS scheme (4.51) is unconditionally unstable. If one replaces the term u_i^n by $(u_{i+1}^n + u_{i-1}^n)/2$, one obtains the Lax–Friedrichs method:

$$u_i^{n+1} = \frac{1}{2}(u_{i+1}^n + u_{i-1}^n) - \frac{\Delta t}{2\Delta x}(f(u_{i+1}^n) - f(u_{i-1}^n)) \quad (4.52)$$

This method is conservative, consistent and converges to the correct solution as $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$ provided that the CFL condition is satisfied. Furthermore it is first-order accurate in time and space.

```

1
2 % Lax–Friedrich's explicit technique for the resolution
3 % of 1d euler equation – non isentropic case
4
5
6 %initialisation of the conservative variables
7 U1=rho.*s;
8
9
10
11
12 while (t<endTime)
13
14     t=t+dt;
15     time(n)=t;
16
17     for i=1:Nx
18         F1(i)=U2(i);
19     end
20
21
22     U1newt(1)=U1(1);
23
24     U3newt(1)=U3(1);
25     for i=2:Nx-1
26         U1newt(i)=0.5*(U1(i+1)+U1newt(i-1))-dt/dx*(F1(i+1)-F1(i-1));
27
28     end
29
30     U1newt(1) = s(1);
31
32     U1newt(Nx) = 2*U1newt(Nx-1)-U1newt(Nx-2);
33
34 %update the flow field for the next calculation
35 U1=U1newt;
36
37 %evaluation of the CFL condition:
38 dt=min(dtlocal);
39
40 end

```

4.2.5 MacCormack's technique

The first order leads to stable but unsatisfactory results in terms of comparison with the analytical data. The passage to a second order in time and space is therefore suggested. The technique shown in section 4.1.3 can therefore be implemented in this case without major changes. Just keep in mind to use the proper boundary conditions as well as the new conservative variables derived in section 4.2.2. The only major distinction between the isentropic case and the current problem is reported below.

Artificial Viscosity

In the case of shock capturing approach, the need of smoothing and stabilization of the solution arise. If the isentropic case did not ask for any

numerical expedient to smooth the solution. Here the dissipation inherent in the algorithm is not enough to keep the solution under control and thus an extra term of viscosity must be added. We would like this extra viscous term to be a fourth order difference in order not to interfere too much with the actual solution of the problem.

$$(S_j)_i^n = \frac{C_x |(p)_{i+1}^n - 2(p)_i^n + (p)_{i-1}^n|}{(p)_{i+1}^n + 2(p)_i^n + (p)_{i-1}^n} ((U_j)_{i+1}^n - 2(U_j)_i^n + (U_j)_{i-1}^n) \quad (4.53)$$

Where the subscript $j = 1, 2, 3$ represent the variable. So, the implementation of the technique with the add of the new term takes the following form. Starting from the predictor step, for the conserved variable U_1 , we have:

$$(\bar{U}_1)_i^{n+1} = (U_1)_i^n + \left(\frac{\partial U_1}{\partial t} \right)_i^{n+1} \Delta t + (S_1)_i^n \quad (4.54)$$

Moving to the corrector step,

$$(U_1)_i^{n+1} = (U_1)_i^n + \left(\frac{\partial U_1}{\partial t} \right)_{ave}^{n+1} \Delta t + (\bar{S}_1)_i^{n+1} \quad (4.55)$$

where,

$$(\bar{S}_1)_i^{n+1} = \frac{C_x |(\bar{p})_{i+1}^{n+1} - 2(\bar{p})_i^{n+1} + (\bar{p})_{i-1}^{n+1}|}{(\bar{p})_{i+1}^{n+1} + 2(\bar{p})_i^{n+1} + (\bar{p})_{i-1}^{n+1}} \times ((\bar{U}_1)_{i+1}^{n+1} - 2(\bar{U}_1)_i^{n+1} + (\bar{U}_1)_{i-1}^{n+1}) \quad (4.56)$$

Result

To validate your code, compare the outcome of your simulation with Fig. 4.3. The solid line is the numerical result obtained imposing $C_x = 0.2$.

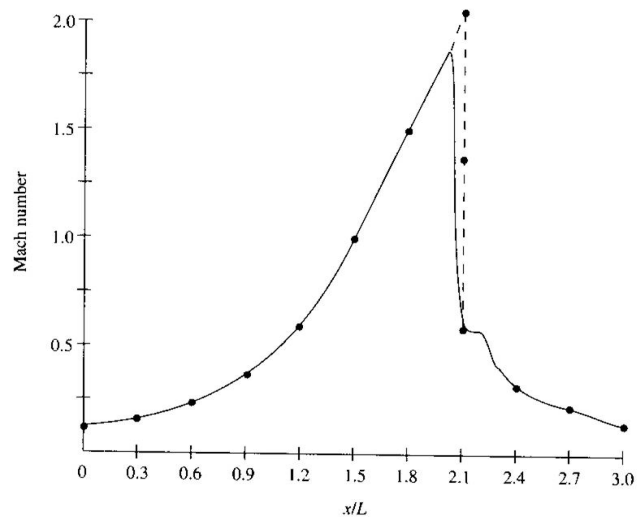


Figure 4.3: Analytical result for the comparison with the outcome of the numerical simulation

4.3 Real Gas Effects

When the working point of the gas is close to the saturated vapour curve, the ideal gas model does not hold any longer. To quantify the amount the operating fluid behaviour deflects from the ideal gas one, the compressibility factor is defined as:

$$Z = \frac{p}{\rho RT} \quad (4.57)$$

If the operating fluid is a refrigerant, or more generally, an organic fluid, the applications of interest involve condition that push the operating point close to (or beyond) the saturated vapor curve. This happens, for example, when dealing with Organic Rankine Cycle (ORC) or refrigerating applications. In all these applications, the compressibility factor is usually quite different from 1, implying the real gas behaviour.

The real gas modeling involve an high complexity in the numerical modeling that is beyond the scope of this assignment. Nonetheless, few simplifications can be made, and in this part the gas will be no longer considered perfect, but rather ideal, implying the variation of the thermophysical properties (e.g the specific heats) with the temperature.

According to the conditions and to the fluid provided, the thermophysical properties can be calculated thanks to the NIST repository <https://webbook.nist.gov/chemistry/fluid/>. An assumption has to be introduced now: both the temperature and the pressure vary along the duct. Keeping into account both the variations would be rather complicate, and thus only the temperature one would be accounted for. This is a common simplification when dealing with gases, and most CFD software allow temperature variation only for this kind of modeling. The user should therefore pick a pressure value that is intermediate among the minimum and the maximum that are registered into the domain. This value is the one at which the property will be evaluated (it is thus an isobaric transformation).

A polynomial (3rd order-) is typically a reasonably good interpolation for the variation $\gamma(T)$. Such value is the one to be used into the CFD code. Typically, the variation in the first time steps is very high, and let the code to calculate the $\gamma(T)$ is not a very good idea. To enforce stability and to ease the code convergence, two expedients should be introduced:

- Under-relaxation factors: a smoother variation is easier to be introduced. By choosing $\alpha=0.1$, the chances of convergence are higher.
- Initialization: the variation of γ might be introduced after the solution with the ideal gas is stable and residuals are low.