Outline

LabDF Tutorial: Investigating CFD Methods with DEMOFLOW

- Nozzle Flow
- Conservation Equations
- Grids
- Schemes
  - Explicit Runge-Kutta with Roe flux
  - Explicit Runge-Kutta with Jameson flux
  - Implicit Euler with Roe flux
  - Implicit Euler with Jameson flux
- Boundary Conditions
- Convergence to steady state

Introduction & Objectives

Objectives:

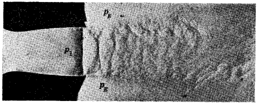
- compute solutions to quasi-1D Euler eqs using 4 different schemes with several different parameter settings,
- compare computed results with exact solution & draw conclusions about effect of varying these parameters.

In particular you are to:

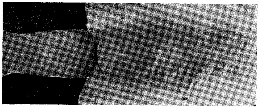
- Test the philosophy of time marching to obtain steady flow solutions
- Gain practical experience with time-integration methods
- Illustrate effects of mesh refinement and artificial viscosity
- Understand better the stability limits of the various schemes.

Nozzle Experiment

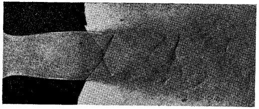
$\frac{p_1}{p_E} < 0.4$



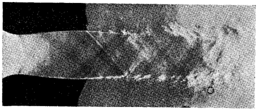
$\frac{p_1}{p_E} = 0.66$



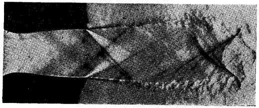
$\frac{p_1}{p_E} = 0.85$



$\frac{p_1}{p_E} = 1.00$

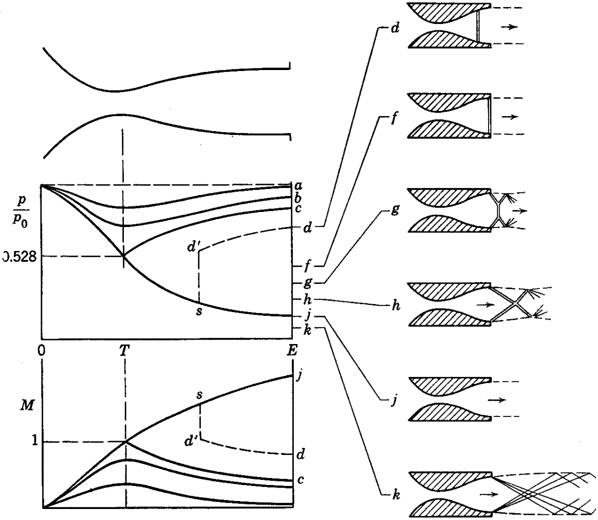


$\frac{p_1}{p_E} = 1.50$



Convergent-Divergent Nozzle Flow

- flow subsonic at inlet, can reach sonic speed at throat, return to subsonic speed across shock, depending on exit pressure
- exit pressure (or velocity) determines flow downstream of throat (T), subsonic or mixed supersonic-subsonic with shock
- Upstream of shock flow given by subsonic-supersonic isentropic eq., downstream by subsonic eq.

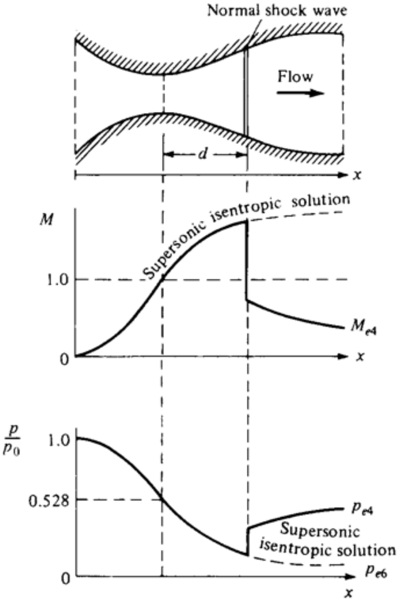


Description of Test Case

- Solve unsteady quasi-1D Euler equations for a steady flow through a convergent-divergent nozzle (flow properties vary only with the coordinate x along the nozzle)
- Flow is driven by fixed pressure ratio between exit &inlet, invariant with time
- Computing case with shock wave standing inside the nozzle illustrates well:
    1. conservation form of the governing equations capturing the shock wave correctly
    2. efficiency of large time steps with implicit time integration to reach steady state
    3. role of added dissipation to obtain a quality solution
    4. effect of grid size on accuracy.
- important case because it illustrates the technique of capturing a **steady shock** within numerical solution that marches forward in time until steady solution obtained

Exact solution

- exact solution determined by isentropic flow eqs & shock jump conditions
- user specifies x location of shock & code determines exact solution upstream & downstream of shock, pressure (or velocity) at exit



The CFD Approach

1. Study physical flow
2. Construct mathematical problem
   - analyze partial differential eqns
   - choose boundary conditions
3. Formulate numerical problem
   - construct a mesh
   - time differencing
   - space differencing
   - initial conditions
   - boundary conditions
   - solve difference eqns, stability ?

Quasi-1D Euler Equations

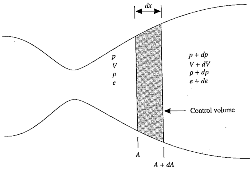
$$-\rho\ V\ A + (\rho + d\rho)(V + dV)(A + dA) = 0$$

$$d(\rho\ V\ A) = 0$$

$$-\rho V^2\ A + (\rho + d\rho)(V + dV)^2 (A + dA) = pA - (p + dp)(A + dA) + p\ dA$$

$$d(\rho V^2\ A) = -A\ dp$$

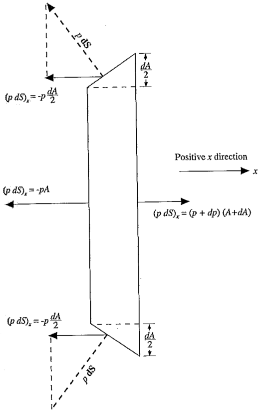
$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = G$$



$$U = A \begin{pmatrix} \rho \\ \rho u \\ \rho(e + u^2/2) \end{pmatrix}, \quad F = A \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho(e + u^2/2)u + pu \end{pmatrix} \quad G = \begin{pmatrix} 0 \\ p\frac{\partial A}{\partial x} \\ 0 \end{pmatrix}$$

and A denotes the nozzle area

$$A(x) = 1 - 4(1 - A_{\text{throat}})x(1 - x), \quad x \in [0, L]$$



Characteristic Variables

$$U_t + F_x = G$$

$B = \partial F / \partial U$
$U_t + B \ U_x = G$
B can be diagonalized

$$\partial_t \hat{W} + \Lambda \partial_x \hat{W} = -\tilde{H}$$

In *Riemann variables* $w_k, k = 1, 2, 3$ reflects best physics of flow, used in BCs

Riemann variables

Elements $\hat{W} = (w_1, w_2, w_3)$ are *Riemann variables* or *characteristic variables*.

$$\begin{aligned} w_1 &= \frac{p}{\rho^\gamma} \\ w_2 &= u + \frac{2c}{\gamma - 1} \\ w_3 &= u - \frac{2c}{\gamma - 1} \end{aligned}$$

Characteristic lines

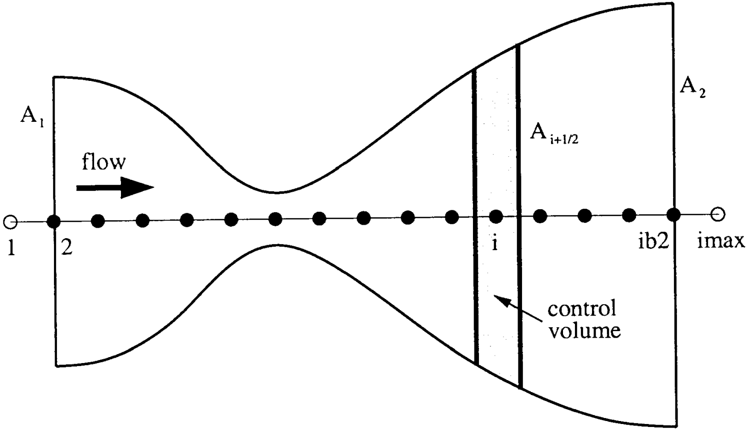
w_j propagate along three *characteristic lines* C_0, C_+, C_- given by

$$\begin{aligned} C_0 &: \frac{dx}{dt} = u \\ C_+ &: \frac{dx}{dt} = u + c \\ C_- &: \frac{dx}{dt} = u - c \end{aligned}$$

When $\tilde{H}$ is zeroRiemann variables constant along characteristic lines - *Riemann invariants*.

Construct Grid

- Equi-spaced mesh $t^n = n\Delta t$, $x_j = j\Delta x$
- Space Discretization: Jameson added scalar dissipationflux, or Roe-MUSCL matrix limited
- Time integration: explicit Runge-Kutta or implicit Euler scheme.
- Boundary conditions at inlet/outlet implemented in characteristic variables
- ‘ghost’ cells are used



Finite-Volume Discretization

Semi-discrete formulation
$\frac{d}{dt}\mathbf{U}_j(t) =$
$-\frac{1}{\Delta x}\left(\hat{\mathbf{F}}^n_{j+1/2} - \hat{\mathbf{F}}^n_{j-1/2} + \mathbf{G}^n_j\right)$
Define *residual* $\mathbf{R}^n_j =$
$-\frac{1}{\Delta x}\left(\hat{\mathbf{F}}^n_{j+1/2} - \hat{\mathbf{F}}^n_{j-1/2} + \mathbf{G}^n_j\right)$
where numerical flux
$\hat{\mathbf{F}}^n_{j+\frac{1}{2}} = \frac{1}{2}(\mathbf{F}^n_{j+1} + \mathbf{F}^n_j) - \hat{\mathbf{D}}^n_{j+\frac{1}{2}}$
Generic dissipation flux function $\hat{\mathbf{D}}^n_{j+\frac{1}{2}}$ specifies particular spatial discretization scheme: Jameson or Roe.

Time method: Implicit forward Euler
$\frac{U^{n+1}_j - U^n_j}{\Delta t} =$
$-\frac{1}{\Delta x}\left(\hat{\mathbf{F}}^{n+1}_{j+1/2} - \hat{\mathbf{F}}^{n+1}_{j-1/2} + \mathbf{G}^n_j\right)$
Taking $\Delta U^n_j = U^{n+1} - U^n$, use linearization
$\left[\frac{I}{\Delta t} + \frac{1}{\Delta x}(\mathcal{A}^n_{j+1/2} - \mathcal{A}^n_{j-1/2})\right] \Delta U =$
$-\frac{1}{\Delta x}\left(\hat{\mathbf{F}}^n_{j+1/2} - \hat{\mathbf{F}}^n_{j-1/2} + \mathbf{G}^n_j\right)$
linear system $3N$ unknowns $\Delta U^n_j, j = 1 \cdots N$. Coefficient matrix *block tri-diagonal*, solve for ΔU^n_j by Gaussian elimination
$U^{n+1} = U^n + \Delta U^n$ advances solution one step from t^n to t^{n+1}. von Neumann stability analysis unconditionally stable, Δt can be arbitrarily large

Time method: Explicit multistage Runge-Kutta
DEMOFLOW uses five stage scheme with coefficients

α_1	α_2	α_3	α_4
0.0695	0.1602	0.2898	0.5060

CFL limit $CFL = 4$

Roe Matrix-limited Flux Scheme

$$\hat{\mathbf{D}}^n_{j+\frac{1}{2}} = -\frac{1}{2}\mathbf{S}_{j+\frac{1}{2}}\Psi_{j+\frac{1}{2}}\mathbf{S}^{-1}_{j+\frac{1}{2}}\left(\mathbf{U}^n_{j+1} - \mathbf{U}^n_j\right)$$

where

$$\boldsymbol{\Psi} = diag(|\lambda_i|\,\psi_i)$$

- uses MUSCL variable interpolation by means of an eigen-analysis, decomposes flux difference into sum of left- and right-running wave contributions
- ψ_i functions of flux limiters ϕ_i and
- λ_i is i^{th} eigenvalue of the matrix $\mathcal{A}$
- limiting MUSCL interpolation this way ensures correct amount of dissipation given to each eigen-component

Jameson flux approximation

Jameson $\hat{\mathbf{D}}^n_{j+\frac{1}{2}}$: in *ad hoc* manner adds second-order diffusion term activated near discontinuities to become 1st order. To achieve 2nd order everywhere else, it is switched off by sensor which turns on a fourth-order dissipation term

Switch to toggle between dissipation modes monitor pressure variation at each node using the normalized second difference $\mu_j = \frac{|p_{j+1}-2p_j+p_{j-1}|}{p_{j+1}+2p_j+p_{j-1}}$ $O(\Delta x^2)$, except in strong pressure gradients Apply smoothing and obtain $\upsilon_j = \frac{1}{2}\mu_j + \frac{1}{4}(\mu_{j-1} + \mu_{j+1})$

Second & fourth order coefficients
Apply sensor υ_j to switch between dissipative modes. Each mode is associated with a coefficient which depends on sensor υ_j, so that 4th order dissipation automatically switched off near shocks

$$\begin{aligned} \varepsilon_j^{(2)} &= k^{(2)}\upsilon_j \\ \varepsilon_j^{(4)} &= max(0, k^{(4)} - \varepsilon_j^{(2)}) \end{aligned}$$

where constants $k^{(2)}$ and $k^{(4)}$, in two variable coefficients $\varepsilon_j^{(2)}, \varepsilon_j^{(4)}$ specified by user and called *Vis*2 and *Vis*4 in DEMOFLOW

Scaling
Scale *numerical* dissipation by spectral radius of $B = \partial F/\partial U$ simplify to $\lambda_j = A_j(|u_j| + c_j)$ where c_j is local speed of sound. Average for final scaling factor $r_{j+1/2} = \frac{1}{2}(\lambda_j + \lambda_{j+1})$

Dissipation flux
$\hat{\mathbf{D}}^n_{j+\frac{1}{2}} = r_{j+\frac{1}{2}}[\ \varepsilon_j^{(2)}(\mathbf{U}_{j+1} - \mathbf{U}_j) - \varepsilon_j^{(4)}(\mathbf{U}_{j+2} - 3\mathbf{U}_{j+1} + 3\mathbf{U}_j - \mathbf{U}_{j-1})\ ]$

Time-Step Size

- Maximum time step, Δt for explicit solution calculated using Courant-Friedrichs-Lewy (CFL) condition

$$\Delta t = CFL \frac{\Delta x_{min}}{|\lambda_{max}|}$$

  where min and max are taken over all cells
- Note that not only the cell size but also the local wave velocities are involved, so it is not possible to choose the time-step in advance
- Motivation for implicit schemes is to relieve severe limitation of CFL condition
- Explicit schemes typically have a CFL limit of 1 while implicit schemes have values in the hundreds.
- Notice that maximum time step Δt can become very small as the mesh becomes finer.
- Time-marching approach requires stepping the solution forward in time until all disturbances have been expelled through the boundaries, and the flow becomes steady. Thus it is important to be able to reach the steady-state flow in a *minimum* number of time steps

Boundary Conditions

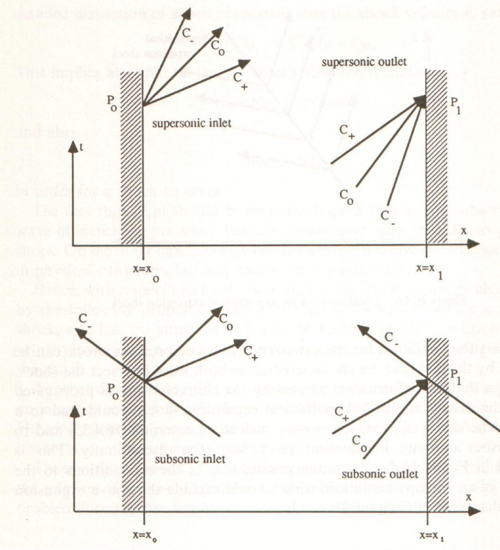
Characteristic lines and boundary conditions
At inlet lines C_0 and C_+ have slope u and $c + u$ *into nozzle* so impose BC. Third characteristic has a slope $u - c$ whose sign depends on the inlet Mach number. If supersonic, information is transported nto flow so impose BC; if subsonic value of w_3 can change so no BC imposed Similar at outlet
Inflow Boundary Conditions (always subsonic)
Two in-going characteristics and one outgoing one. Use Riemann invariants to determine pressure, density and velocity

Outflow Boundary Conditions

- For *supersonic* outflow all characteristics are going out from the domain and physical boundary conditions are neither required nor allowed. Values of the flow variables at the boundary (i.e. numerical boundary conditions) are obtained by linear extrapolation of the Riemann invariants from the interior field points.
- For *subsonic* outflow one characteristic is in-going so one variable should be set, e.g. the pressure is set to the exit pressure $p(L, T) = p_{exit}$. The other two numerical boundary conditions are obtained by linear extrapolation of the Riemann invariants from the interior field points.

Physical Boundary Conditions

	Subsonic	Supersonic
Inlet	Two conditions w_1 and w_2 given	Three conditions w_1, w_2 and w_3 given
Outlet	One condition w_3 given	Zero conditions



Numerical boundary conditions

- Numerical schemes require *all* variables be known at boundaries in order to compute
- *Numerical boundary conditions* consistent with physical properties & compatible with numerical scheme

	Subsonic	Supersonic
Inlet	Physical conditions: w_1, w_2 Numerical conditions: w_3	Physical conditions: w_1, w_2, w_3 Numerical conditions: none
Outlet	Physical conditions: w_3 Numerical conditions: w_1, w_2	Physical conditions: none Numerical conditions: w_1, w_2, w_3

First-order extrapolation Riemann variables W_M^n
where M is the ‘ghost’ cell, i.e. as $W_M^n = 2W_{M-1}^n - W_{M-2}^n$

Reconstitution

After the extrapolation of Riemann variables, the conservation variables U_M^n are determined.

Running DEMOFLOW

Initialization of Flowfield

- **Code initializes the flowfield by linearly interpolating between the exact values at the inlet and at the exit**

'Convergence in time' to steady state

Flow variables change over time step $\frac{U_j^{n+1} - U_j^n}{\Delta t} = \mathbf{R}_j^n$ Steady State is $U_j^{n+1} \longrightarrow U_j^n$ is reached when $\mathbf{R}_j^n \longrightarrow 0$

$\mathbf{L}^2$ residuals using L^2 norm

$$\left|\left(R^\ell\right)_{L^2}\right| = \frac{t_{ref}}{U_{ref}^\ell} \sqrt{\frac{1}{JM} \sum_{j=1}^{JM} \left(R^\ell\right)_j^2}$$

$\mathbf{L}_\infty$ residuals using L_∞ norm

$$\left|\left(R^\ell\right)_{L_\infty}\right| = \frac{t_{ref}}{U_{ref}^\ell} \sup_{j=1,JM} \left|\left(R^\ell\right)_j\right|$$