Compressible Flow - TME085

Lecture 13

Niklas Andersson

Chalmers University of Technology
Department of Mechanics and Maritime Sciences
Division of Fluid Mechanics
Gothenburg, Sweden

niklas.andersson@chalmers.se

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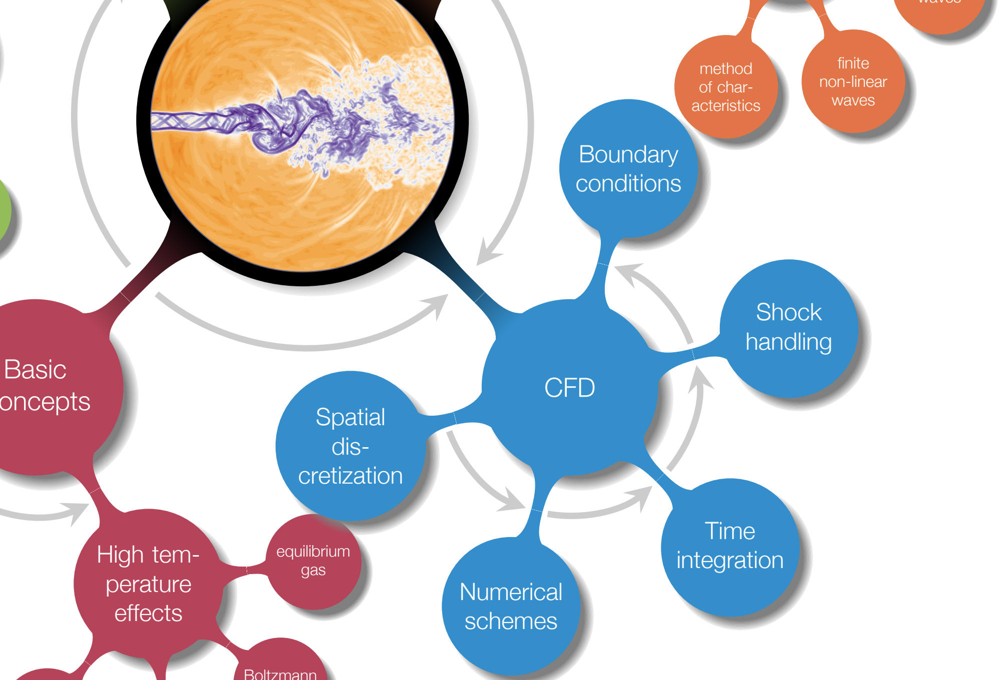
Chapter 12
The Time-Marching Technique

Overview



method of char-acteristics
finite non-linear waves
Boundary conditions
Shock handling
CFD
Spatial dis-cretization
Time integration
Numerical schemes
Basic oncepts
High tem-perature effects
equilibrium gas
Boltzmann

Learning Outcomes

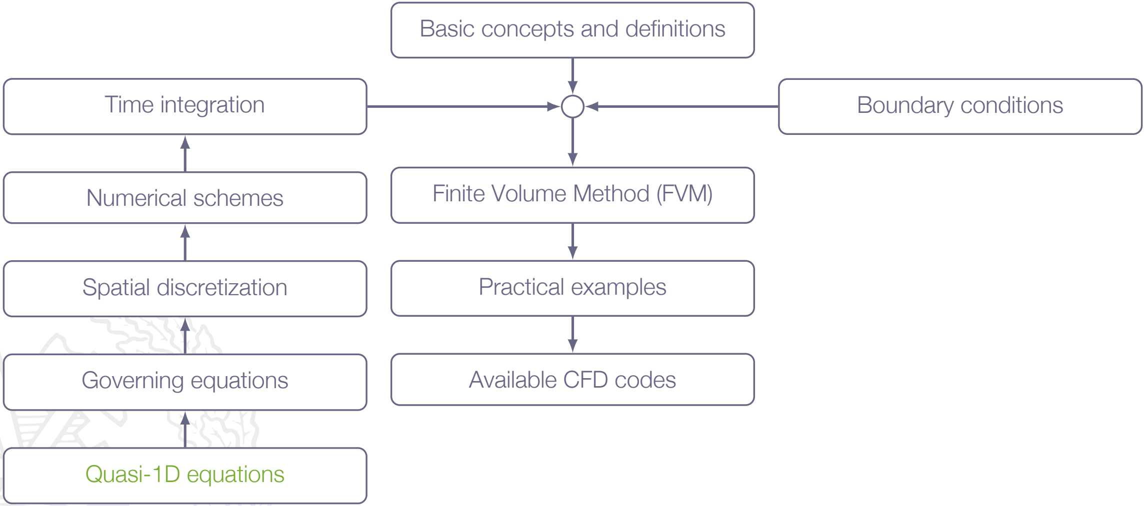
12 Explain the main principles behind a modern Finite Volume CFD code and such concepts as explicit/implicit time stepping, CFL number, conservation, handling of compression shocks, and boundary conditions

14 Analyze and verify the quality of the numerical solution

15 Explain the limitations in fluid flow simulation software

time for CFD!

Roadmap - The Time-Marching Technique



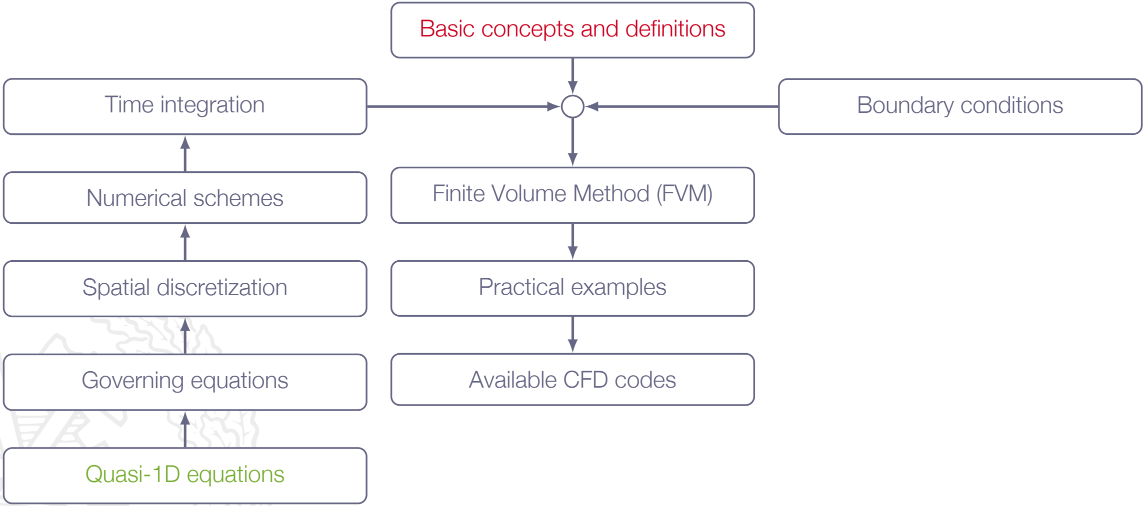
Motivation

Computational Fluid Dynamics (CFD) is the backbone of all practical engineering compressible flow analysis

As an engineer doing numerical compressible flow analyzes it is extremely important to have knowledge about the fundamental numerical principles and their limitations

Going through the material covered in this section will not make you understand all the details but you will get a feeling, which is a good start

Roadmap - The Time-Marching Technique



The Time-Marching Technique

Note!

Anderson's text is here rather out-of-date, it was written during the 70's and has not really been updated since then.
The additional material covered in this lecture is an attempt to amend this.

The Time-Marching Technique

The problems that we like to investigate numerically within the field of compressible flows can be categorized as

- steady-state compressible flows
- unsteady compressible flows

The Time-marching method is a solver framework that addresses both problem categories

The Time-Marching Technique

The time-marching approach is a good alternative for simulating flows where there are both supersonic and subsonic regions

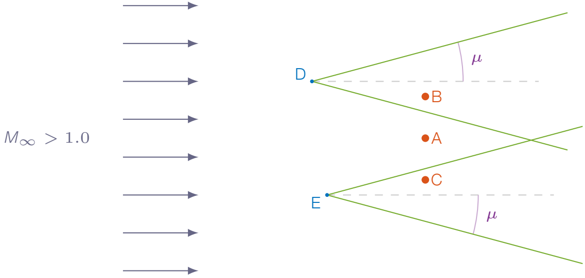
supersonic/hyperbolic:

- perturbations propagate in preferred directions
- zone of influence/zone of dependence
- PDEs can be transformed into ODEs

subsonic/elliptic:

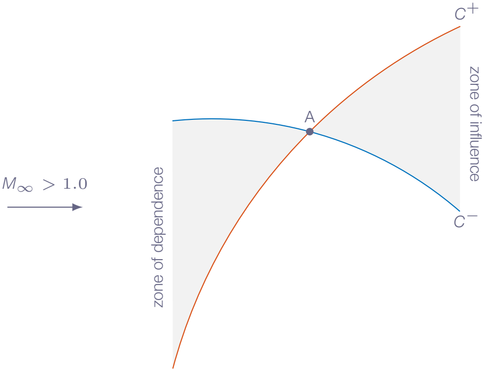
- perturbations propagate in all directions

Zone of Influence and Zone of Dependence



- A, B and C at the same axial position in the flow
- D and E are located upstream of A, B and C
- Mach waves generated at D will affect the flow in B but not in A and C
- Mach waves generated at E will affect the flow in C but not in A and B
- The flow in A is unaffected by the both D and E

Zone of Influence and Zone of Dependence



The zone of dependence for point A and the zone of influence of point A are defined by C^+ and C^- characteristic lines

The Time-Marching Technique

Steady-state problems:

1. define simple initial solution
2. apply specified boundary conditions
3. march in time until steady-state solution is reached

Unsteady problems:

1. apply specified initial solution
2. apply specified boundary conditions
3. march in time for specified total time to reach a desired unsteady solution

   establish fully developed flow before initiating data sampling

Characterization of CFD Methods - Discretization

Discretization in space and time:

- most common approach: Method of Lines
    1. discretize in space $\Rightarrow$
       system of ordinary differential equations (ODEs)
    2. discretize in time $\Rightarrow$
       time-stepping scheme for system of ODEs

Spatial discretization techniques:

- Finite-Difference Method (FDM)
- Finite-Volume Method (FVM)
- Finite-Element Method (FEM)

Characterization of CFD Methods - Time Stepping

Temporal discretization techniques:

1. Explicit
   - mostly for transonic/supersonic steady-state and unsteady flows
   - short time steps
   - usually very stable
2. Implicit
   - mostly for subsonic/transonic steady-state flows
   - longer time steps possible

for high-supersonic flows, explicit solvers may very well outperform implicit solvers

Characterization of CFD Methods - Equations

Equations solved:

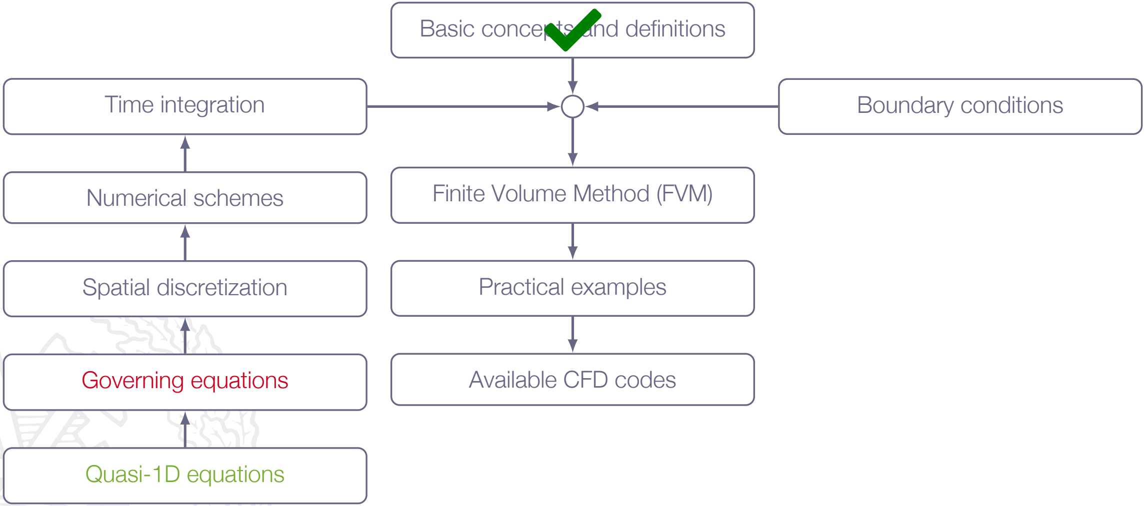
1. Density-based
   - solve for density in the continuity equation
   - mostly for transonic/supersonic steady-state and unsteady flows
2. Pressure-based
   - the continuity and momentum equations are combined to form a pressure correction equation
   - mostly for subsonic/transonic steady-state flows

Characterization of CFD Methods - Solver Approach

Solution procedure:

1. Fully coupled
   - all equations (continuity, momentum, energy, ...) are solved simultaneously
   - mostly for transonic/supersonic steady-state and unsteady flows
2. Segregated
   - solve the equations in sequence
   - mostly for subsonic steady-state flows

Roadmap - The Time-Marching Technique

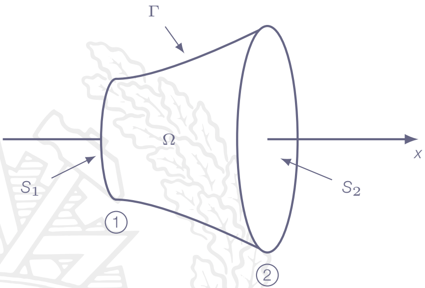


Governing Equations

Quasi-One-Dimensional Flow - Conceptual Idea

Introduce cross-section-averaged flow quantities $\Rightarrow$
all quantities depend on x only

$$A = A(x),\ \rho = \rho(x),\ u = u(x),\ p = p(x),\ \dots$$



Ω	control volume
S_1	left boundary (area A_1)
S_2	right boundary (area A_2)
Γ	perimeter boundary

$$\partial\Omega = S_1 \cup \Gamma \cup S_2$$

Quasi-One-Dimensional Flow - Governing Equations

Governing equations (general form):

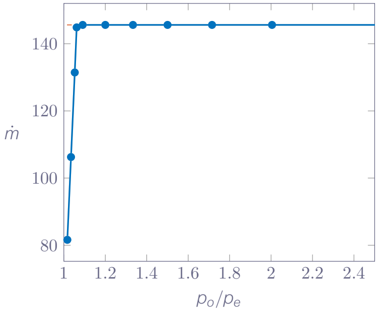
$$\frac{d}{dt}\iiint\limits_{\Omega}\rho d\mathscr{V} + \oiint\limits_{\partial\Omega}\rho\mathbf{v}\cdot\mathbf{n}dS = 0$$

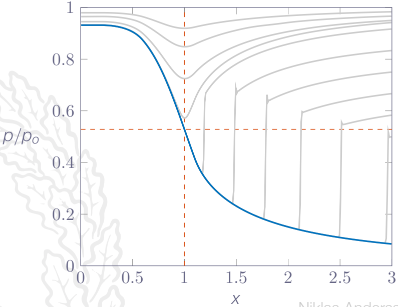
$$\frac{d}{dt}\iiint\limits_{\Omega}\rho u d\mathscr{V} + \oiint\limits_{\partial\Omega}\left[\rho(\mathbf{v}\cdot\mathbf{n})u + p(\mathbf{n}\cdot\mathbf{e}_x)\right]dS = 0$$

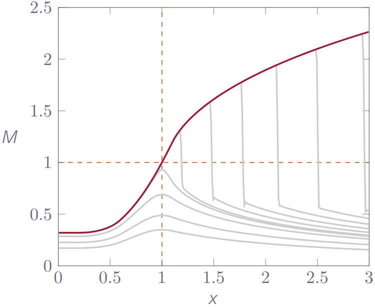
$$\frac{d}{dt}\iiint\limits_{\Omega}\rho e_o d\mathscr{V} + \oiint\limits_{\partial\Omega}\rho h_o(\mathbf{v}\cdot\mathbf{n})dS = 0$$

Example: Nozzle Simulation

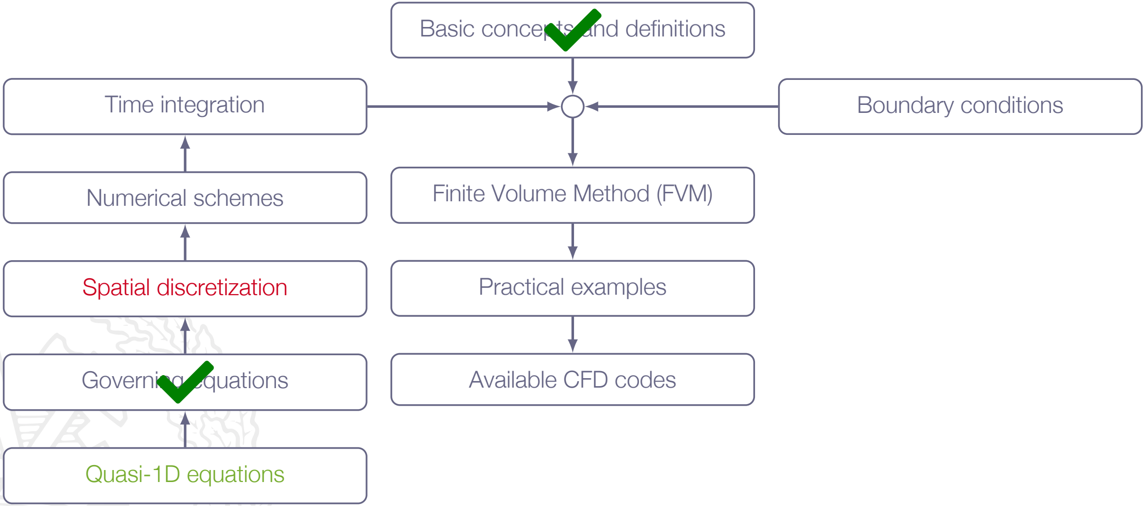
p_o	1.20 [bar]
p_e	0.50 [bar]
p_o/p_e	11.8
$\dot{m}$	145.6 [kg/s]
M_{max}	2.26







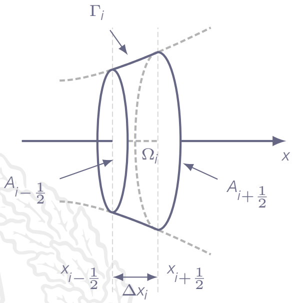
Roadmap - The Time-Marching Technique



Spatial Discretization

Quasi-One-Dimensional Flow - Spatial Discretization

Let's look at a small tube segment with length Δx



Streamtube with area $A(x)$

$$A_{i-\frac{1}{2}} = A(x_{i-\frac{1}{2}})$$

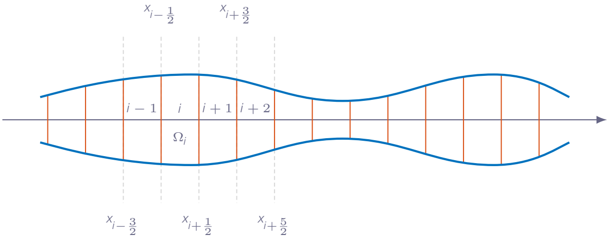
$$A_{i+\frac{1}{2}} = A(x_{i+\frac{1}{2}})$$

$$\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$$

Ω_i - control volume enclosed by $A_{i-\frac{1}{2}}$, $A_{i+\frac{1}{2}}$, and Γ_i

$\Rightarrow$ spatial discretization

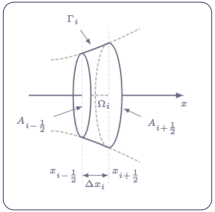
Quasi-One-Dimensional Flow - Spatial Discretization



- Integer indices (i, $i+1$, ...):
  control volumes or cells
- Fractional indices ($i+\dfrac{1}{2}$, $i+\dfrac{3}{2}$, ...):
  interfaces between control volumes or cell faces
- Apply control volume formulations for mass, momentum, energy to control volume Ω_i

Quasi-One-Dimensional Flow

cell-averaged quantity
face-averaged quantity



Conservation of mass:

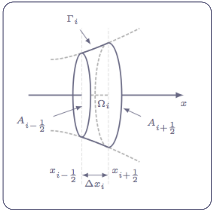
$$\underbrace{\frac{d}{dt}\iiint\limits_{\Omega_i} \rho d\mathscr{V}}_{VOL_i \frac{d}{dt}\bar{\rho}_i} + \underbrace{\iint\limits_{x_{i-\frac{1}{2}}} \rho \mathbf{v}\cdot\mathbf{n} dS}_{-\overline{(\rho u)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}}} + \underbrace{\iint\limits_{x_{i+\frac{1}{2}}} \rho \mathbf{v}\cdot\mathbf{n} dS}_{\overline{(\rho u)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}}} + \underbrace{\iint\limits_{\Gamma_i} \rho \mathbf{v}\cdot\mathbf{n} dS}_{0} = 0$$

where

$$VOL_i = \iiint\limits_{\Omega_i} d\mathscr{V} \qquad \overline{(\rho u)}_{i-\frac{1}{2}} = \frac{1}{A_{i-\frac{1}{2}}} \iint\limits_{x_{i-\frac{1}{2}}} \rho u dS$$

$$\bar{\rho}_i = \frac{1}{VOL_i} \iiint\limits_{\Omega_i} \rho d\mathscr{V} \qquad \overline{(\rho u)}_{i+\frac{1}{2}} = \frac{1}{A_{i+\frac{1}{2}}} \iint\limits_{x_{i+\frac{1}{2}}} \rho u dS$$

Quasi-One-Dimensional Flow



cell-averaged quantity

face-averaged quantity

source term

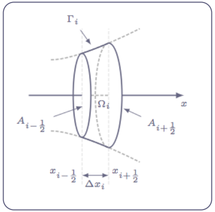
Conservation of momentum:

$$\underbrace{\frac{d}{dt}\iiint\limits_{\Omega_i} \rho u \, d\mathscr{V}}_{VOL_i \frac{d}{dt}\overline{(\rho u)}_i} + \underbrace{\iint\limits_{x_{i-\frac{1}{2}}} \left[\rho(\mathbf{v}\cdot\mathbf{n})u + p(\mathbf{n}\cdot\mathbf{e}_x)\right] dS}_{-\overline{(\rho u^2+p)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}}} +$$

$$+ \underbrace{\iint\limits_{x_{i+\frac{1}{2}}} \left[\rho(\mathbf{v}\cdot\mathbf{n})u + p(\mathbf{n}\cdot\mathbf{e}_x)\right] dS}_{\overline{(\rho u^2+p)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}}} + \underbrace{\iint\limits_{\Gamma_i} \left[\rho(\mathbf{v}\cdot\mathbf{n})u + p(\mathbf{n}\cdot\mathbf{e}_x)\right] dS}_{-\iint_{\Gamma_i} p dA} = 0$$

Quasi-One-Dimensional Flow

cell-averaged quantity
face-averaged quantity

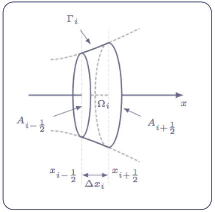


Conservation of energy:

$$\underbrace{\frac{d}{dt}\iiint\limits_{\Omega_i} \rho e_o d\mathscr{V}}_{VOL_i \frac{d}{dt}\overline{(\rho e_o)}_i} + \underbrace{\iint\limits_{X_{i-\frac{1}{2}}} \rho h_o(\mathbf{v}\cdot\mathbf{n})dS}_{-\overline{(\rho u h_o)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}}} +$$

$$+ \underbrace{\iint\limits_{X_{i+\frac{1}{2}}} \rho h_o(\mathbf{v}\cdot\mathbf{n})dS}_{\overline{(\rho u h_o)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}}} + \underbrace{\iint\limits_{\Gamma_i} \rho h_o(\mathbf{v}\cdot\mathbf{n})dS}_{0} = 0$$

Quasi-One-Dimensional Flow



Lower order term due to varying stream tube area:

$$\iint\limits_{\Gamma_i} p dA \approx \bar{p}_i \left(A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} \right)$$

where $\bar{p}_i$ is calculated from cell-averaged quantities (DOFs) $\left\{ \bar{\rho}, \overline{(\rho u)}, \overline{(\rho e_o)} \right\}_i$ as

$$\bar{p}_i = (\gamma - 1) \left(\overline{(\rho e_o)}_i - \frac{1}{2} \bar{\rho}_i \bar{u}_i \right), \; \bar{u}_i = \frac{\overline{(\rho u)}_i}{\bar{\rho}_i}$$

Quasi-One-Dimensional Flow - Spatial Discretization

cell-averaged quantity
face-averaged quantity
source term

$$VOL_i \frac{d}{dt}\bar{\rho}_i - \overline{(\rho u)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}} + \overline{(\rho u)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} = 0$$

$$VOL_i \frac{d}{dt}\overline{(\rho u)}_i - \overline{(\rho u^2 + p)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}} + \overline{(\rho u^2 + p)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} = \bar{p}_i \left(A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}\right)$$

$$VOL_i \frac{d}{dt}\overline{(\rho e_o)}_i - \overline{(\rho u h_o)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}} + \overline{(\rho u h_o)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} = 0$$

Application of these equations to all cells $i \in \{1, 2, ..., N\}$ of the computational domain results in a system of ODEs

Spatial Discretization - Summary

Steps to achieve spatial discretization:

1. Choose primary variables (Degrees of Freedom or DOFs)
2. Approximate all other quantities in terms of DOFs

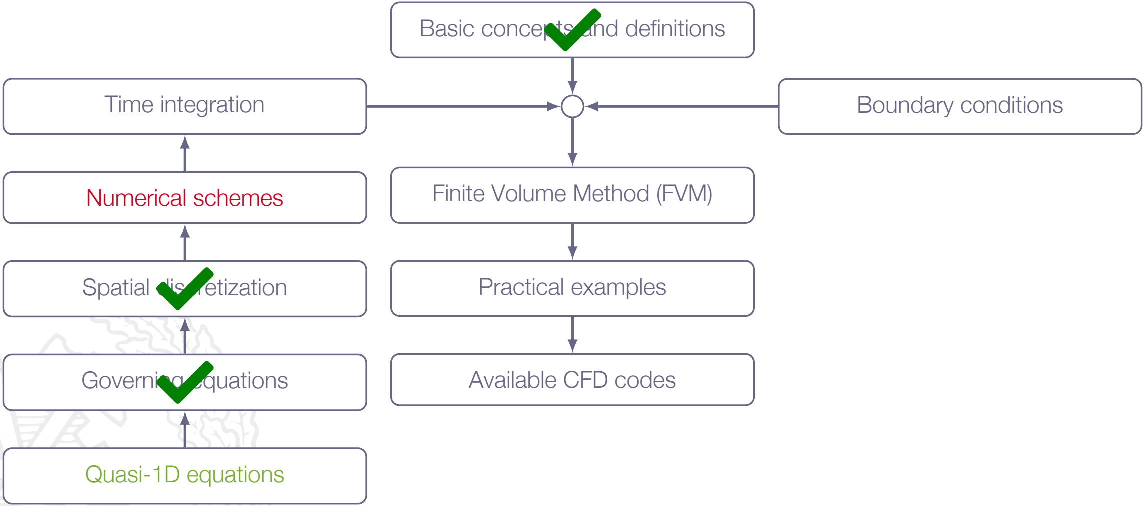
$\Rightarrow$ System of ordinary differential equations (ODEs)

Degrees of freedom:

- Choose $\left\{\bar{\rho}, \overline{(\rho u)}, \overline{(\rho e_o)}\right\}_i$ in all control volumes Ω_i, $i \in \{1, 2, ..., N\}$ as degrees of freedom, or primary variables
- Note that these are cell-averaged quantities

What about the face values?

Roadmap - The Time-Marching Technique



Numerical Schemes

Flux Term Approximation

$$\left\{\begin{array}{c}\overline{(\rho u)}\\ \\ \overline{(\rho u^2+p)}\\ \\ \overline{(\rho u h_o)}\end{array}\right\}_{i+\frac{1}{2}} = f\left(\left\{\begin{array}{c}\bar{\rho}\\ \\ \overline{(\rho u)}\\ \\ \overline{(\rho e_o)}\end{array}\right\}_i, \left\{\begin{array}{c}\bar{\rho}\\ \\ \overline{(\rho u)}\\ \\ \overline{(\rho e_o)}\end{array}\right\}_{i+1}, \dots\right)$$

cell face values

cell-averaged values

Simple example:

$$\overline{(\rho u)}_{i+\frac{1}{2}} \approx \frac{1}{2}\left[\overline{(\rho u)}_i + \overline{(\rho u)}_{i+1}\right]$$

Flux Term Approximation

More complex approximations usually needed

High-order schemes:

- increased accuracy
- more cell values involved (*wider flux molecule*)
- boundary conditions more difficult to implement

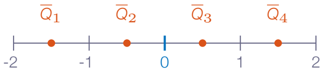
Optimized numerical dissipation:

- upwind type of flux scheme

Shock handling:

- non-linear treatment needed (*e.g.* TVD schemes)
- artificial damping

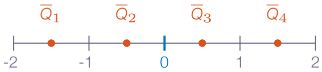
Flux Term Approximation



$$Q(x) = A + Bx + Cx^2 + Dx^3$$

Assume constant area: $A(x) = 1.0$

Flux Term Approximation

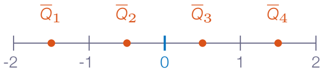


$$\overline{Q}_1 = \frac{1}{VOL_1} \int_{-2}^{-1} Q(x)dx$$

$$VOL_1 = A_1 \Delta x_1 = \{A_1 = 1.0,\ \Delta x_1 = 1.0\} = 1.0$$

$$\Rightarrow \overline{Q}_1 = \int_{-2}^{-1} Q(x)dx$$

Flux Term Approximation



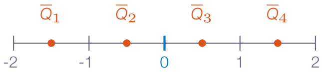
$$\overline{Q}_1 = \int_{-2}^{-1} Q(x)dx = \left[Ax + \frac{1}{2}Bx^2 + \frac{1}{3}Cx^3 + \frac{1}{4}Dx^4\right]_{-2}^{-1}$$

$$\overline{Q}_2 = \int_{-1}^{0} Q(x)dx = \left[Ax + \frac{1}{2}Bx^2 + \frac{1}{3}Cx^3 + \frac{1}{4}Dx^4\right]_{-1}^{0}$$

$$\overline{Q}_3 = \int_{0}^{1} Q(x)dx = \left[Ax + \frac{1}{2}Bx^2 + \frac{1}{3}Cx^3 + \frac{1}{4}Dx^4\right]_{0}^{1}$$

$$\overline{Q}_4 = \int_{1}^{2} Q(x)dx = \left[Ax + \frac{1}{2}Bx^2 + \frac{1}{3}Cx^3 + \frac{1}{4}Dx^4\right]_{1}^{2}$$

Flux Term Approximation



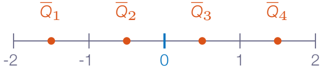
$$\overline{Q}_1 = A - \frac{3}{2}B + \frac{7}{3}C - \frac{15}{4}D$$

$$\overline{Q}_2 = A - \frac{1}{2}B + \frac{1}{3}C - \frac{1}{4}D$$

$$\overline{Q}_3 = A + \frac{1}{2}B + \frac{1}{3}C + \frac{1}{4}D$$

$$\overline{Q}_4 = A + \frac{3}{2}B + \frac{7}{3}C + \frac{15}{4}D$$

Flux Term Approximation



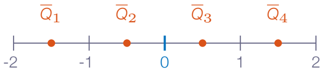
$$A = \frac{1}{12}\left[-\overline{Q}_1 + 7\overline{Q}_2 + 7\overline{Q}_3 - \overline{Q}_4\right]$$

$$B = \frac{1}{12}\left[\overline{Q}_1 - 15\overline{Q}_2 + 15\overline{Q}_3 - \overline{Q}_4\right]$$

$$C = \frac{1}{4}\left[\overline{Q}_1 - \overline{Q}_2 - \overline{Q}_3 + \overline{Q}_4\right]$$

$$D = \frac{1}{6}\left[-\overline{Q}_1 + 3\overline{Q}_2 - 3\overline{Q}_3 + \overline{Q}_4\right]$$

Flux Term Approximation



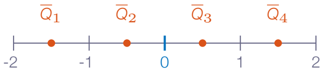
$$Q_0 = Q(0) + \delta Q'''(0) \Rightarrow Q_0 = A + 6\delta D$$

$\delta = 0 \Rightarrow$ fourth-order central scheme

$\delta = 1/12 \Rightarrow$ third-order upwind scheme

$\delta = 1/96 \Rightarrow$ third-order low-dissipation upwind scheme

Flux Term Approximation



$$Q_0 = A + 6\delta D = \{\delta = 1/12\} = -\frac{1}{6}\overline{Q}_1 + \frac{5}{6}\overline{Q}_2 + \frac{1}{3}\overline{Q}_3$$

$$Q_{0_{left}} = -\frac{1}{6}\overline{Q}_1 + \frac{5}{6}\overline{Q}_2 + \frac{1}{3}\overline{Q}_3$$

$$Q_{0_{right}} = -\frac{1}{6}\overline{Q}_4 + \frac{5}{6}\overline{Q}_3 + \frac{1}{3}\overline{Q}_2$$

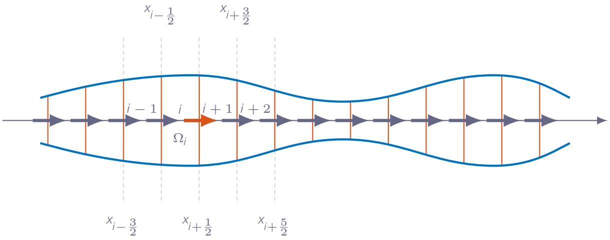
method of characteristics used in order to decide whether left- or right-upwinded flow quantities should be used

Flux Term Approximation

High-order numerical schemes:

- low numerical dissipation (smearing due to amplitudes errors)
- low dispersion errors (wiggles due to phase errors)

Conservative Scheme



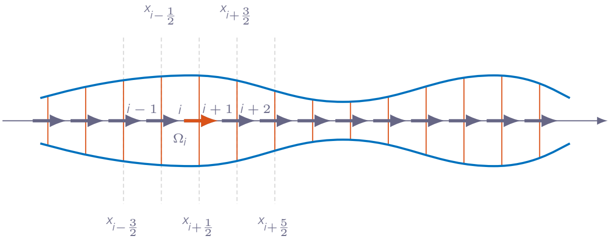
mass conservation:

cell (i): $$VOL_i \frac{d}{dt}\bar{\rho}_i + \overline{(\rho u)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} - \overline{(\rho u)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}} = 0$$

cell ($i+1$): $$VOL_{i+1} \frac{d}{dt}\bar{\rho}_{i+1} + \overline{(\rho u)}_{i+\frac{3}{2}} A_{i+\frac{3}{2}} - \overline{(\rho u)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} = 0$$

(similarly for momentum and energy conservation)

Conservative Scheme



mass conservation:

cell (i): $$VOL_i \frac{d}{dt}\bar{\rho}_i + \overline{(\rho u)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} - \overline{(\rho u)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}} = 0$$

cell ($i+1$): $$VOL_{i+1} \frac{d}{dt}\bar{\rho}_{i+1} + \overline{(\rho u)}_{i+\frac{3}{2}} A_{i+\frac{3}{2}} - \overline{(\rho u)}_{i+\frac{1}{2}} A_{i+\frac{1}{2}} = 0$$

(similarly for momentum and energy conservation)

Conservative scheme

"The flux leaving one control volume equals the flux entering neighbouring control volume"

Conservation property for mass, momentum and energy is crucial for the correct prediction of shocks*

* correct prediction of shocks:
strength
position
velocity