Compressible Flow - TME085

Chapter 12

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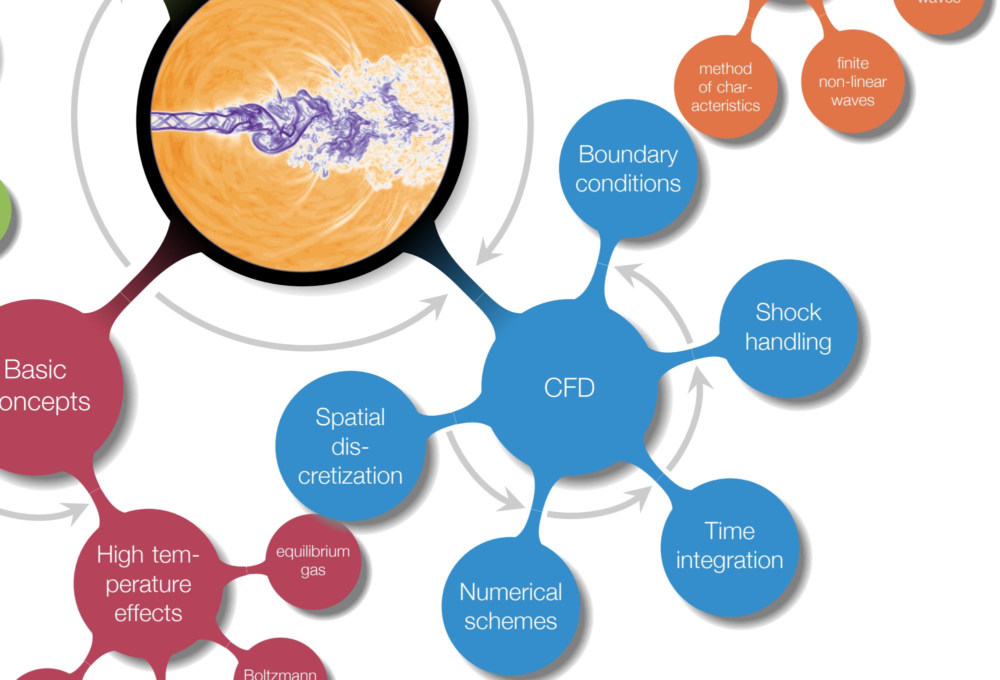
```
#undef __FUNCT__
#define __FUNCT__ "RungeKutta::fwd"
PetscErrorCode RungeKutta::fwd(Domain *dom){
    PetscErrorCode ierr=0;

    ierr=G3DCopy(dom->cons,cons0);CHKERRQ(ierr);

    /* RK1 */

    dom->update();

    dcons->evaluate(dom);

    ierr=G3DWAXPY(dom->cons,1.0,dcons,cons0);CHKERRQ(ierr);
    ierr=G3DAXPBY(cons0,0.5,0.5,dom->cons);CHKERRQ(ierr);

    /* RK2 */

    dom->update();
    dcons->evaluate(dom);

    ierr=G3DWAXPY(dom->cons,0.5,dcons,cons0);CHKERRQ(ierr);

    /* RK3 */
```

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

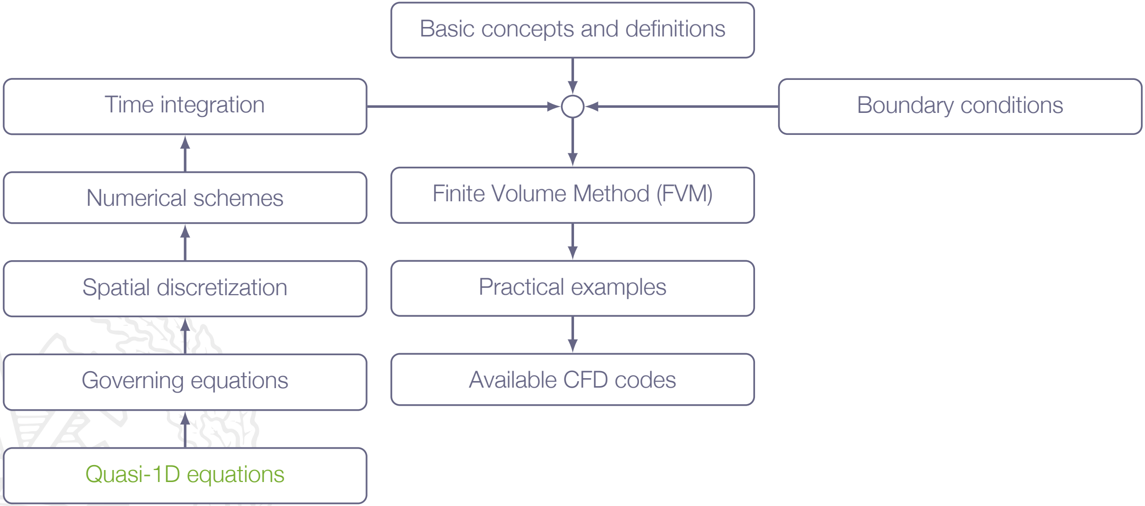
12 **Explain** the main principles behind a modern Finite Volume CFD code and such concepts as explicit/implicit time stepping, CFL number, conservation, handling of compression shocks, and boundary conditions

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



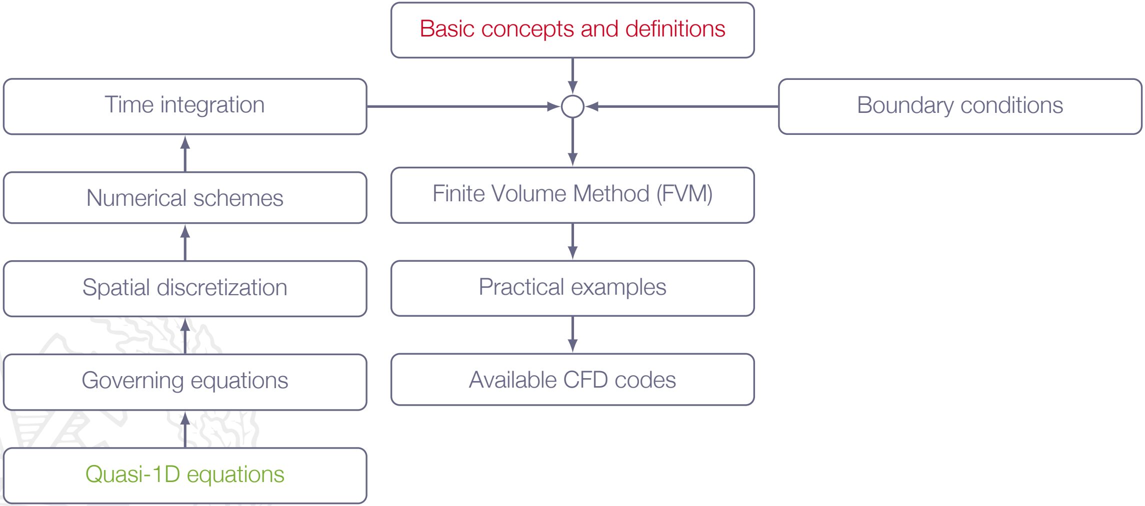
Motivation

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

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 technique** is a solver framework that addresses both problem categories

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

The Time-Marching Technique

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

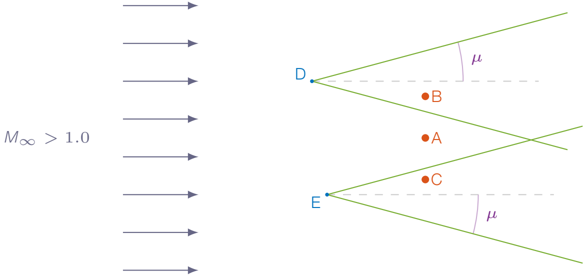
supersonic/hyperbolic:

- 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

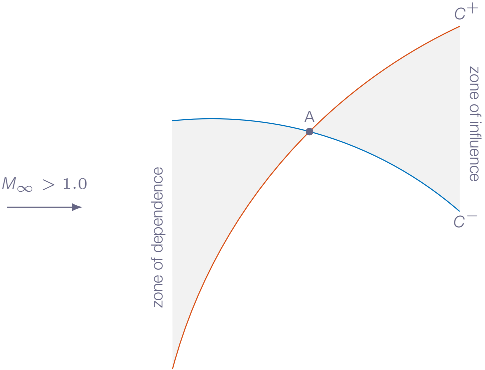
D and E are located upstream of A, B and C

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

Characterization of CFD Methods

Density-based	**Pressure-based**
Fully coupled	**Segregated**
Structured	**Unstructured**
Explicit	**Implicit**

Characterization of CFD Methods

Approach taken in this presentation

Density-based	Pressure-based
Fully coupled	Segregated
Structured	Unstructured
Explicit	Implicit

Characterization of CFD Methods - Equations

Density-based

- solve for density in the continuity equation
- suitable for transonic/supersonic flows

Pressure-based

- the continuity and momentum equations are combined to form a pressure correction equation
- suitable for subsonic/transonic flows

Characterization of CFD Methods - Solver Approach

Fully coupled

all equations (continuity, momentum, energy, ...) are solved simultaneously

suitable for transonic/supersonic flows

Segregated

the governing equations are solved in sequence

suitable for subsonic flows

Characterization of CFD Methods - Time Stepping

Explicit

- \- short time steps
- \+ very stable

Implicit

- \+ longer time steps possible

Characterization of CFD Methods - Time Stepping

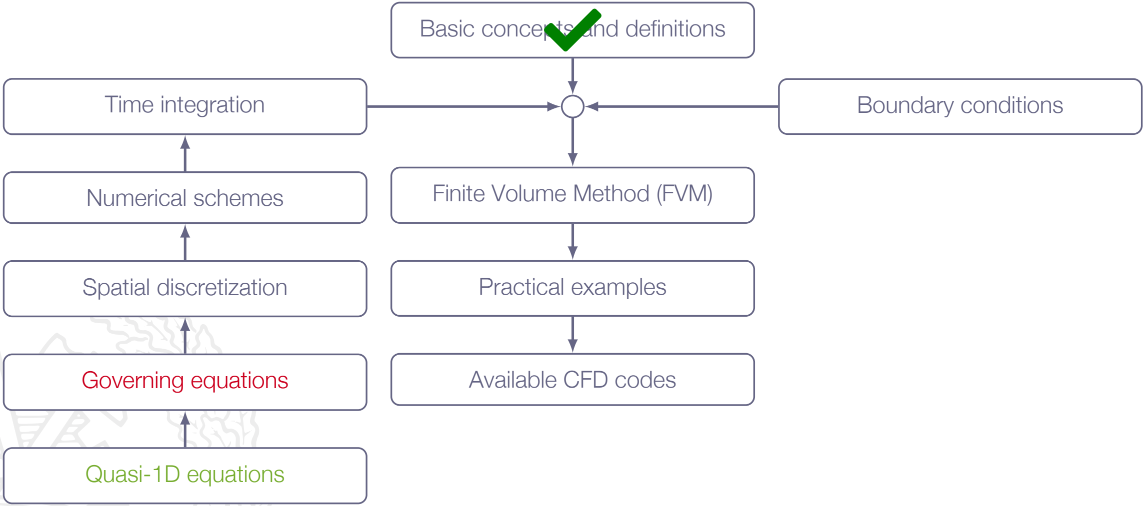
Explicit Time Stepping

Implicit Time Stepping

In general implicit solvers are more efficient than explicit solvers

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

Roadmap - The Time-Marching Technique

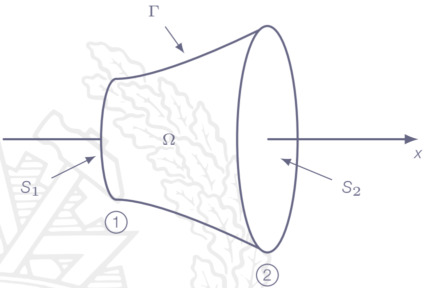


Governing Equations

Quasi-One-Dimensional Flow - Conceptual Idea

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

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



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

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

Governing equations (general form):

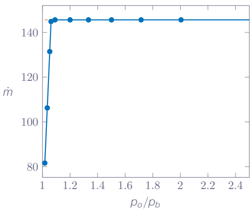
$$\frac{d}{dt}\iiint_{\Omega}\rho d\mathscr{V}+\oiint_{\partial\Omega}\rho\mathbf{v}\cdot\mathbf{n}dS=0$$

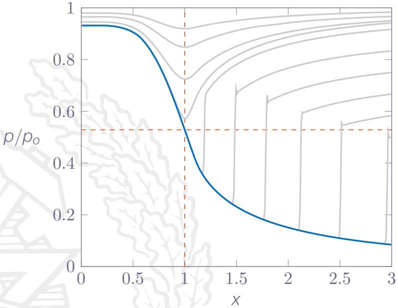
$$\frac{d}{dt}\iiint_{\Omega}\rho u d\mathscr{V}+\oiint_{\partial\Omega}\left[\rho(\mathbf{v}\cdot\mathbf{n})u+p(\mathbf{n}\cdot\mathbf{e}_x)\right]dS=0$$

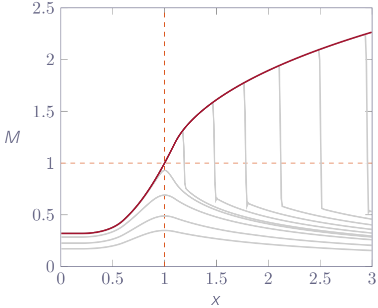
$$\frac{d}{dt}\iiint_{\Omega}\rho e_o d\mathscr{V}+\oiint_{\partial\Omega}\rho h_o(\mathbf{v}\cdot\mathbf{n})dS=0$$

Quasi-One-Dimensional Flow - Example: Nozzle Flow

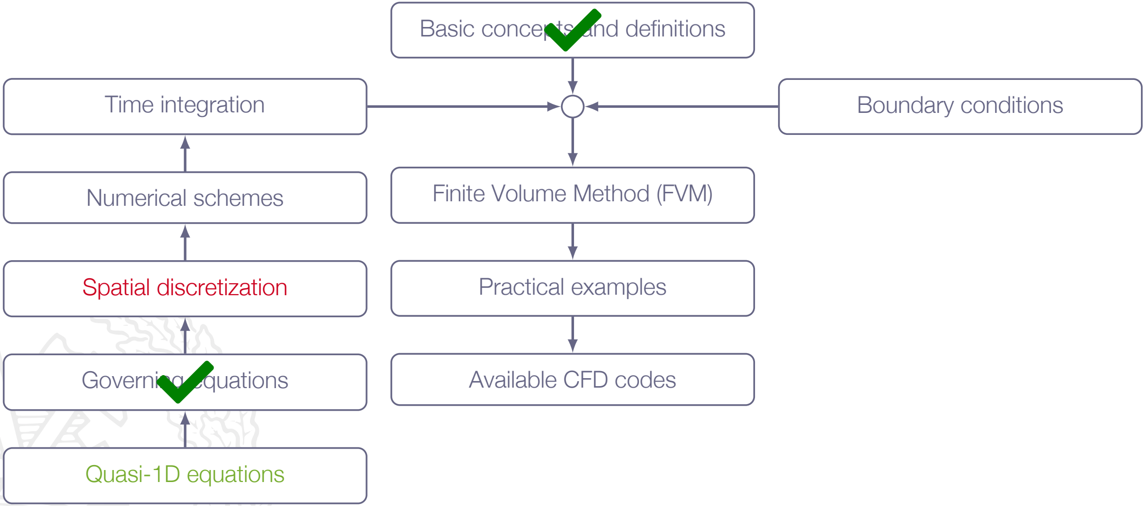
p_o	1.20 [bar]
p_b	0.50 [bar]
p_o/p_b	11.8
$\dot{m}$	145.6 [kg/s]
M_{max}	2.26







Roadmap - The Time-Marching Technique



Spatial Discretization

Spatial Discretization

Discretization in space and time:

Method of Lines (a very common approach):

1. discretize in space $\Rightarrow$ system of ordinary differential equations (ODEs)
2. discretize in time $\Rightarrow$ time-stepping scheme for system of ODEs

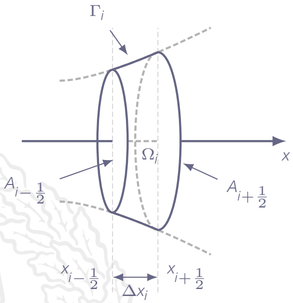
Spatial discretization techniques:

FDM Finite-Difference Method

FVM **Finite-Volume Method**

FEM Finite-Element Method

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



Streamtube with area $A(x)$

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

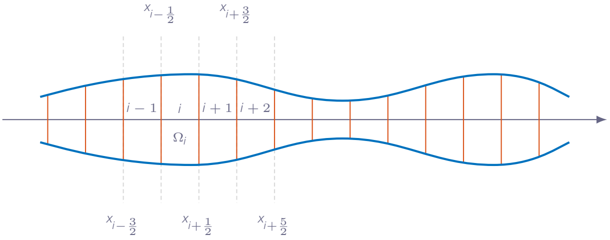
$$A_{i+\frac{1}{2}} = A(x_{i+\frac{1}{2}})$$

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

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



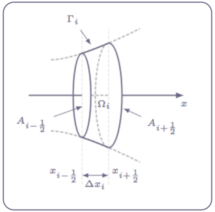
Integer indices: control volumes or **cells**

Fractional indices: interfaces between control volumes or **cell faces**

Apply control volume formulations for mass, momentum, energy to control volume Ω_i

Quasi-One-Dimensional Flow - Spatial Discretization

cell-averaged quantity
face-averaged quantity



Conservation of mass:

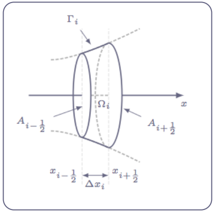
$$\underbrace{\frac{d}{dt}\iiint\limits_{\Omega_i}\rho d\mathscr{V}}_{VOL_i \frac{d}{dt}\bar{\rho}_i} + \underbrace{\iint\limits_{x_{i-\frac{1}{2}}}\rho\mathbf{v}\cdot\mathbf{n}dS}_{-\overline{(\rho u)}_{i-\frac{1}{2}}A_{i-\frac{1}{2}}} + \underbrace{\iint\limits_{x_{i+\frac{1}{2}}}\rho\mathbf{v}\cdot\mathbf{n}dS}_{\overline{(\rho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

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 - Spatial Discretization



cell-averaged quantity

face-averaged quantity

source term

Conservation of momentum:

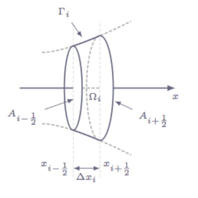
$$\underbrace{\frac{d}{dt}\iiint_{\Omega_i} \rho u \, d\mathscr{V}}_{VOL_i \frac{d}{dt}\overline{(\rho u)}_i} + \underbrace{\iint_{x_{i-\frac{1}{2}}} \left[\rho(\mathbf{v}\cdot\mathbf{n})u + p(\mathbf{n}\cdot\mathbf{e}_x)\right] dS}_{-\overline{(\rho u^2+p)}_{i-\frac{1}{2}} A_{i-\frac{1}{2}}} +$$

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

Quasi-One-Dimensional Flow - Spatial Discretization

cell-averaged quantity

face-averaged quantity

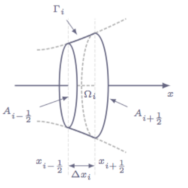


Conservation of energy:

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

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

Quasi-One-Dimensional Flow - Spatial Discretization



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

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

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)
2. Approximate all other quantities in terms of the primary variables

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

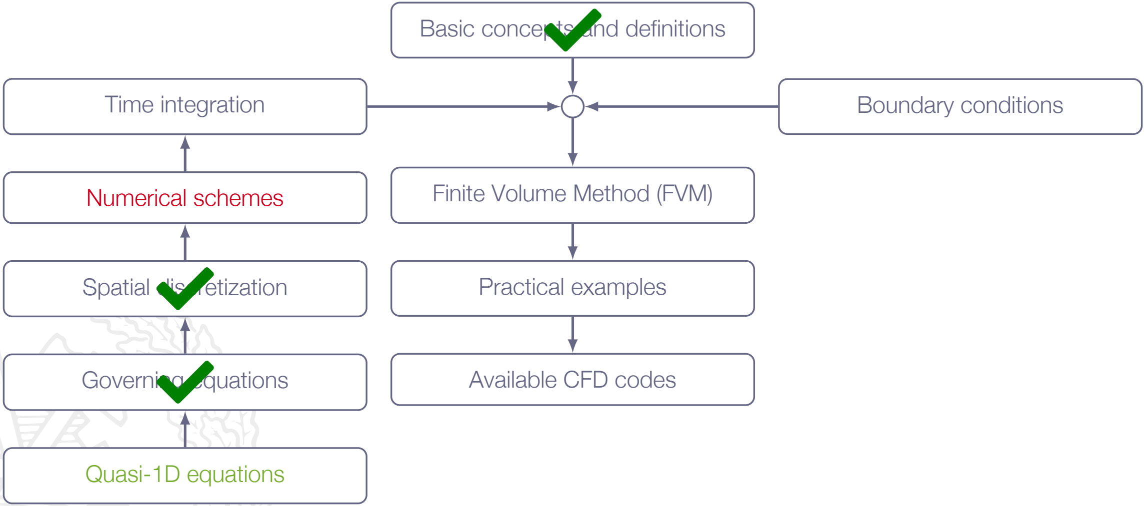
Degrees of freedom:

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

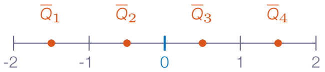
Optimized numerical dissipation:

- upwind type of flux scheme

Shock handling:

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

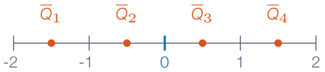
Flux Term Approximation



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

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

Flux Term Approximation

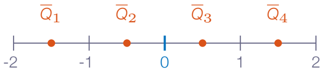


$$\overline{Q}_1 = \frac{1}{VOL_1}\int_{-2}^{-1} Q(x)dx$$

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

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

Flux Term Approximation



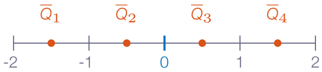
$$\overline{Q}_1 = \int_{-2}^{-1} Q(x)dx = \left[Ax + \frac{1}{2}Bx^2 + \frac{1}{3}Cx^3 + \frac{1}{4}Dx^4\right]_{-2}^{-1}$$

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

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

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

Flux Term Approximation



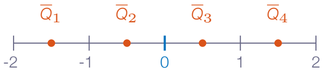
$$\overline{Q}_1 = A - \frac{3}{2}B + \frac{7}{3}C - \frac{15}{4}D$$

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

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

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

Flux Term Approximation



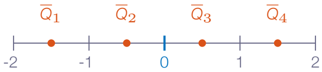
$$A = \frac{1}{12}\left[-\overline{Q}_1 + 7\overline{Q}_2 + 7\overline{Q}_3 - \overline{Q}_4\right]$$

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

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

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

Flux Term Approximation



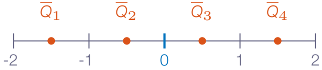
$$Q_0 = Q(0) + \delta Q'''(0) \Rightarrow Q_0 = A + 6\delta D$$

$\delta = 0 \Rightarrow$ 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



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

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

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

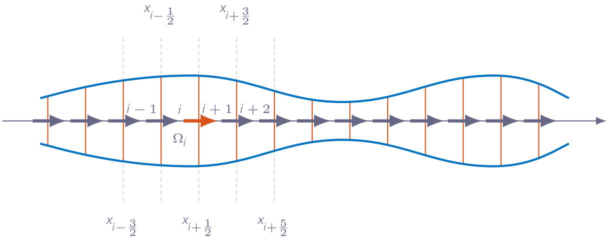
method of characteristics used in order to decide whether left- or right-upwinded flow quantities should be used

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



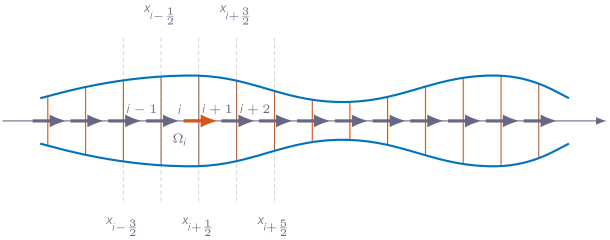
mass conservation:

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

* correct prediction of shocks:
strength
position
velocity

Shock Capturing

Jameson shock detector:

$$\nu_{i+\frac{1}{2}} = max\left\{\nu_i, \nu_{i+1}\right\}$$

where ν_i is a scaled pressure derivative

$$\nu_i = \frac{|p_{i+1} - 2p_i + p_{i-1}|}{p_{i+1} + 2p_i + p_{i-1}}$$

For a smooth pressure field ν $\mathcal{O}(\Delta x^2)$ and near a shock ν $\mathcal{O}(1)$

Artificial damping term (α is a user-defined constant):

$$\alpha\left(|u| + c\right)_{i+\frac{1}{2}} \nu_{i+\frac{1}{2}} A_{i+\frac{1}{2}} \left(Q_{i+1} - Q_i\right)$$

Density Discontinuities

Jameson-type detector:

$$\nu_{i+\frac{1}{2}} = max\left\{\nu_i, \nu_{i+1}\right\}$$

where ν_i is a scaled density derivative

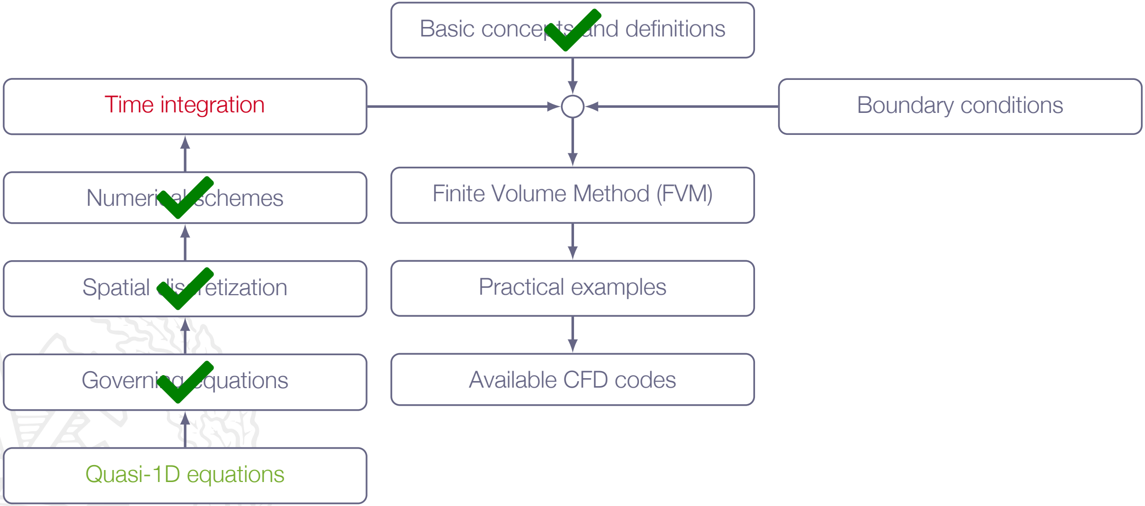
$$\nu_i = \frac{\left|\rho_{i+1} - 2\rho_i + \rho_{i-1}\right|}{\rho_{i+1} + 2\rho_i + \rho_{i-1}}$$

For a smooth density field ν $\mathcal{O}(\Delta x^2)$ and near a density discontinuity ν $\mathcal{O}(1)$

Artificial damping term (β is a user-defined constant):

$$\beta \left|u\right|_{i+\frac{1}{2}} \nu_{i+\frac{1}{2}} A_{i+\frac{1}{2}} \left(Q_{i+1} - Q_i\right)$$

Roadmap - The Time-Marching Technique



Time Stepping

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

Quasi-One-Dimensional Flow - Spatial Discretization

cell-averaged quantity
face-averaged quantity
source term

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

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

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

Quasi-One-Dimensional Flow - Spatial Discretization

cell-averaged quantity
face-averaged quantity
source term

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

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

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

$$\frac{d}{dt}\overline{\mathbf{Q}}_i = \mathbf{F}(\overline{\mathbf{Q}}_i) \text{ where } \overline{\mathbf{Q}}_i = [\overline{\rho},\ \overline{\rho u},\ \overline{\rho e_o}]_i,\ i \in \{1 : NCells\}$$

Time Stepping

The system of ODEs obtained from the spatial discretization in vector notation

$$\frac{d}{dt}\mathbf{Q} = \mathbf{F}(\mathbf{Q})$$

$\mathbf{Q}$ is a vector containing all DOFs in all cells

$\mathbf{F}(\mathbf{Q})$ is the **time derivative** of $\mathbf{Q}$ resulting from above mentioned **flux approximations** - *non-linear vector-valued function*

Time Stepping

Three-stage Runge-Kutta - *one example of many*:

- **Explicit** time-marching scheme
- **Second-order** accurate

Time Stepping - Three-stage Runge-Kutta

$$\frac{d}{dt}\mathbf{Q} = \mathbf{F}(\mathbf{Q})$$

Let $\mathbf{Q}^n = \mathbf{Q}(t_n)$ and $\mathbf{Q}^{n+1} = \mathbf{Q}(t_{n+1})$

t_n is the current time level and t_{n+1} is the next time level
$\Delta t = t_{n+1} - t_n$ is the solver time step

Algorithm:

$$\begin{aligned}
1.\quad & \mathbf{Q}^* &= \mathbf{Q}^n + \Delta t\mathbf{F}(\mathbf{Q}^n) \\
2.\quad & \mathbf{Q}^{**} &= \mathbf{Q}^n + \frac{1}{2}\Delta t\mathbf{F}(\mathbf{Q}^n) + \frac{1}{2}\Delta t\mathbf{F}(\mathbf{Q}^*) \\
3.\quad & \mathbf{Q}^{n+1} &= \mathbf{Q}^n + \frac{1}{2}\Delta t\mathbf{F}(\mathbf{Q}^n) + \frac{1}{2}\Delta t\mathbf{F}(\mathbf{Q}^{**})
\end{aligned}$$

Time Stepping - Three-stage Runge-Kutta

```
void RungeKutta::fwd(Domain *dom){
  G3DCopy(dom->cons,cons0);

  /* Runge-Kutta step 1 */

  dom->update();
  if(!G3DMode::constdt){LocalTimeStep(dom);}
  dcons->evaluate(dom);
  G3DWAXPY(dom->cons,1.0,dcons,cons0);
  G3DAXPBY(cons0,0.5,0.5,dom->cons);

  /* Runge-Kutta step 2 */

  dom->update();
  dcons->evaluate(dom);
  G3DWAXPY(dom->cons,0.5,dcons,cons0);

  /* Runge-Kutta step 3 */

  dom->update();
  dcons->evaluate(dom);
  G3DWAXPY(dom->cons,0.5,dcons,cons0);
}
```

Time Stepping - Explicit Schemes

Properties of explicit time-stepping schemes:

+ **Easy to implement** in computer codes
+ **Efficient execution** on most computers
+ Easy to adapt for **parallel execution** on distributed memory systems (*e.g.* Linux clusters)

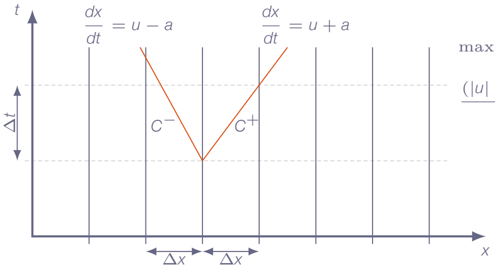
- **Time step limitation** (CFL number)
- Convergence to steady-state **often slow** (there are, however, some remedies for this)

Time Stepping - Explicit Schemes

Courant-Friedrich-Levy **(CFL)** number - *one-dimensional case*:

$$CFL_i = \frac{\Delta t(|u_i| + a_i)}{\Delta x_i} \leq 1$$

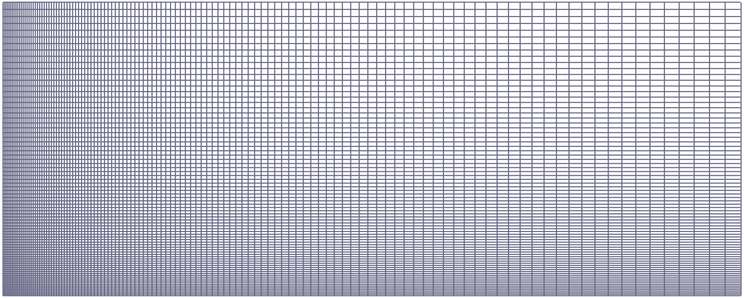
Interpretation: The fastest characteristic (C^+ or C^-) must not travel longer than Δx during one time step



$$\max(|u-a|,|u+a|)\Delta t = (|u|+a)\Delta t \leq \Delta x \Rightarrow$$

$$\frac{(|u|+a)\Delta t}{\Delta x} = CFL \leq 1$$

Time Stepping - Explicit Schemes



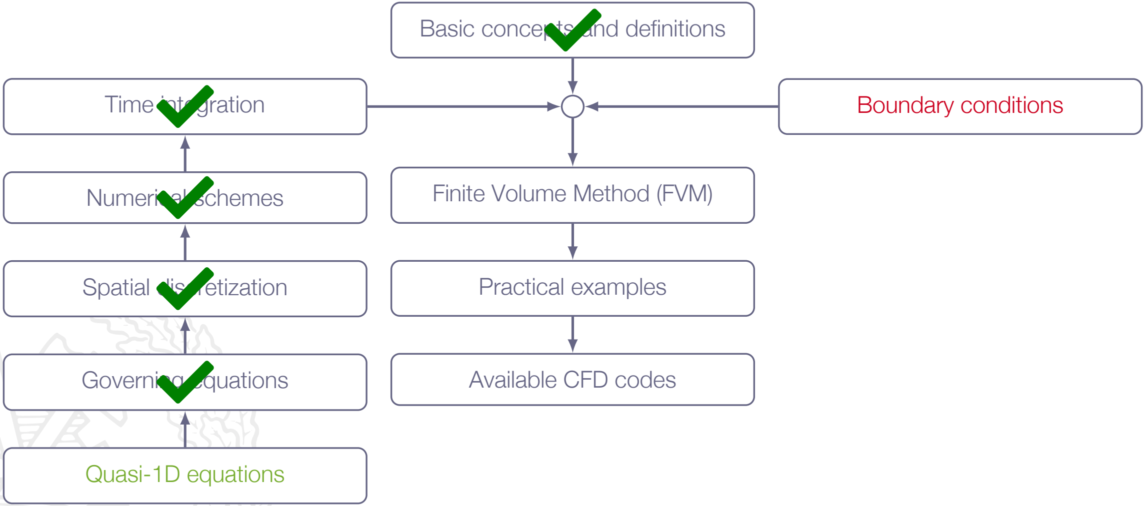
Steady-state problems:

- local time stepping
- each cell has an individual time step
- Δt_i maximum allowed value based on CFL criteria

Unsteady problems:

- time accurate
- all cells have the same time step
- $\Delta t_i = \min\{\Delta t_1, ..., \Delta t_N\}$

Roadmap - The Time-Marching Technique



Boundary Conditions

Boundary Conditions

Boundary conditions are very important for numerical simulation of compressible flows

Main reason: both **flow** and **acoustics** involved!

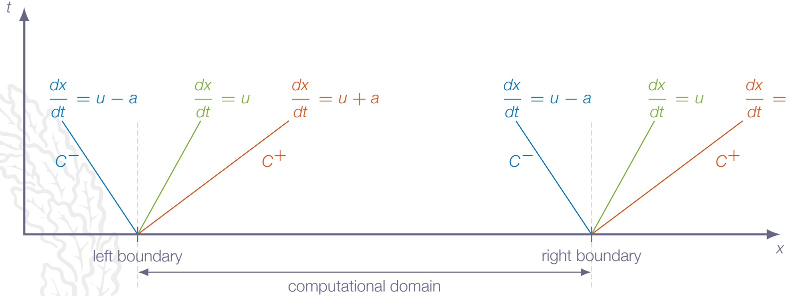
Example 1:
Finite-volume CFD code for Quasi-1D compressible flow (Time-marching procedure)

What boundary conditions should be applied at the left and right ends?

Boundary Conditions

three characteristics:

1. C^+
2. C^-
3. advection



C^+ and C^- characteristics describe the transport of **isentropic pressure waves** (often referred to as **acoustics**)

The advection characteristic simply describes the **transport** of certain quantities **with the fluid itself** (for example **entropy**)

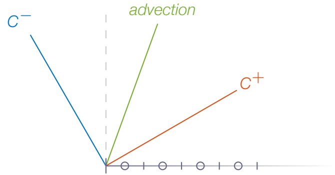
In one space dimension and time, these three characteristics, together with the quantities that are known to be constant along them, give a **complete description** of the time evolution of the flow

We can use the characteristics as a guide to tell us what information that should be specifed at the boundaries

Left Boundary - Subsonic Inflow

we have three PDEs, and are solving for three unknowns

Subsonic inflow: $0 < u < a$



$$u - a < 0$$
$$u > 0$$
$$u + a > 0$$

one outgoing characteristic
two ingoing characteristics

Two variables should be **specified** at the boundary

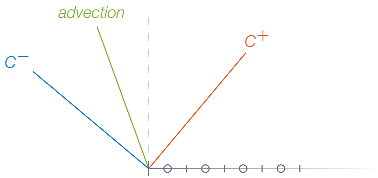
The third variable must be left free

Left Boundary - Subsonic Outflow

we have three PDEs, and are solving for three unknowns

Subsonic outflow: $-a < u < 0$

$$u - a < 0$$
$$u < 0$$
$$u + a > 0$$



two outgoing characteristics
one ingoing characteristic

One variable should be **specified** at the boundary

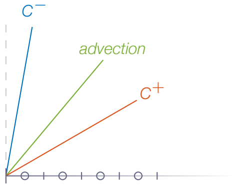
The second and third variables must be left free

Left Boundary - Supersonic Inflow

we have three PDEs, and are solving for three unknowns

Supersonic inflow: $u > a$

$$u - a > 0$$
$$u > 0$$
$$u + a > 0$$



no outgoing characteristics
three ingoing characteristics

All three variables should be **specified** at the boundary

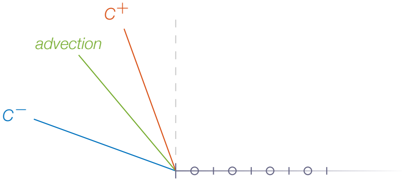
No variables must be left free

Left Boundary - Supersonic Outflow

we have three PDEs, and are solving for three unknowns

Supersonic outflow: $u < -a$

$$u - a < 0$$
$$u < 0$$
$$u + a < 0$$



three outgoing characteristics
no ingoing characteristics

No variables should be **specified** at the boundary

All variables must be left free

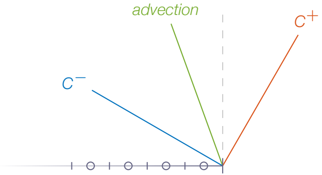
Right Boundary - Subsonic Inflow

we have three PDEs, and are solving for three unknowns

Subsonic inflow: $-a < u < 0$

$$u - a < 0$$
$$u < 0$$
$$u + a > 0$$

two ingoing characteristics
one outgoing characteristic



Two variables should be **specified** at the boundary

The third variables must be left free

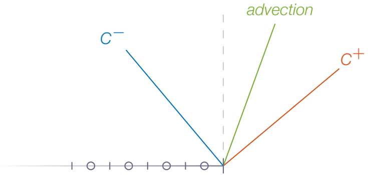
Right Boundary - Subsonic Outflow

we have three PDEs, and are solving for three unknowns

Subsonic outflow: $0 < u < a$

$$u - a < 0$$
$$u > 0$$
$$u + a > 0$$

one ingoing characteristic
two outgoing characteristics



One variable should be **specified** at the boundary

The second and third variables must be left free

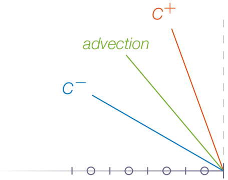
Right Boundary - Supersonic Inflow

we have three PDEs, and are solving for three unknowns

Supersonic inflow: $u < -a$

$$u - a < 0$$
$$u < 0$$
$$u + a < 0$$

three ingoing characteristics
no outgoing characteristics



All three variables should be **specified** at the boundary

No variables must be left free

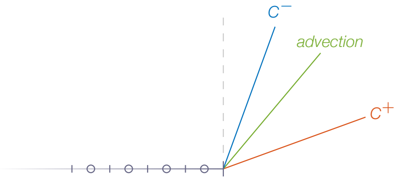
Right Boundary - Supersonic Outflow

we have three PDEs, and are solving for three unknowns

Supersonic outflow: $u > a$

$$u - a > 0$$
$$u > 0$$
$$u + a > 0$$

no ingoing characteristics
three outgoing characteristics



No variables should be **specified** at the boundary

All three variables must be left free

1D Boundary Conditions (Summary)

Characteristic		1D subsonic inflow (left)	1D subsonic inflow (right)
advection	$\mathbf{v} \cdot \mathbf{n}$	$(u, 0, 0) \cdot (-1, 0, 0) = -u < 0$	$(-u, 0, 0) \cdot (1, 0, 0) = -u < 0$
C^-	$\mathbf{v} \cdot \mathbf{n} - a$	$-u - a < 0$	$-u - a < 0$
C^+	$\mathbf{v} \cdot \mathbf{n} + a$	$-u + a > 0$	$-u + a > 0$
Characteristic		**1D subsonic outflow (left)**	**1D subsonic outflow (right)**
advection	$\mathbf{v} \cdot \mathbf{n}$	$(-u, 0, 0) \cdot (-1, 0, 0) = u > 0$	$(u, 0, 0) \cdot (1, 0, 0) = u > 0$
C^-	$\mathbf{v} \cdot \mathbf{n} - a$	$u - a < 0$	$u - a < 0$
C^+	$\mathbf{v} \cdot \mathbf{n} + a$	$u + a > 0$	$u + a > 0$
Characteristic		**1D supersonic inflow (left)**	**1D supersonic inflow (right)**
advection	$\mathbf{v} \cdot \mathbf{n}$	$(u, 0, 0) \cdot (-1, 0, 0) = -u < 0$	$(-u, 0, 0) \cdot (1, 0, 0) = -u < 0$
C^-	$\mathbf{v} \cdot \mathbf{n} - a$	$-u - a < 0$	$-u - a < 0$
C^+	$\mathbf{v} \cdot \mathbf{n} + a$	$-u + a < 0$	$-u + a < 0$
Characteristic		**1D supersonic outflow (left)**	**1D supersonic outflow (right)**
advection	$\mathbf{v} \cdot \mathbf{n}$	$(-u, 0, 0) \cdot (-1, 0, 0) = u > 0$	$(u, 0, 0) \cdot (1, 0, 0) = u > 0$
C^-	$\mathbf{v} \cdot \mathbf{n} - a$	$u - a > 0$	$u - a > 0$
C^+	$\mathbf{v} \cdot \mathbf{n} + a$	$u + a > 0$	$u + a > 0$

Subsonic Inflow (Left Boundary) - Example

Subsonic inflow: we should specify two variables

Alt	specified variable 1	specified variable 2	well-posed	non-reflective
1	p_o	T_o	X	
2	ρu	T_o	X	
3	s	J^+	X	X

well posed:

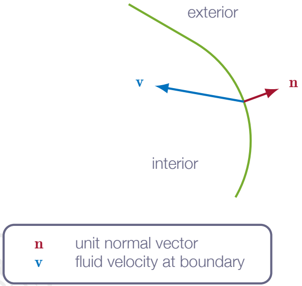
1. the problem has a solution
2. the solution is unique
3. the solution's behaviour changes continuously with initial conditions

Subsonic Outflow (Left Boundary) - Example

Subsonic outflow: we should specify one variable

Alt	specified variable	well-posed	non-reflective
1	p	X	
2	ρu	X	
3	J^+	X	X

Subsonic Inflow 2D/3D



Subsonic inflow

Assumption:

$-a < \mathbf{v} \cdot \mathbf{n} < 0$

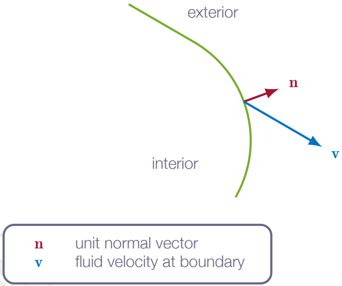
Four ingoing characteristics

One outgoing characteristic

Specify four variables at the boundary:

p_o, T_o, and flow direction (two angles)

Subsonic Outflow 2D/3D



Subsonic outflow

Assumption:

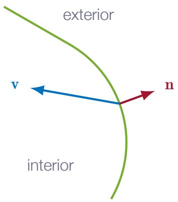
$0 < \mathbf{v} \cdot \mathbf{n} < a$

One ingoing characteristics

Four outgoing characteristic

Specify one variables at the boundary:
static pressure

Supersonic Inflow 2D/3D



$\mathbf{n}$	unit normal vector
$\mathbf{v}$	fluid velocity at boundary

Supersonic inflow

Assumption:

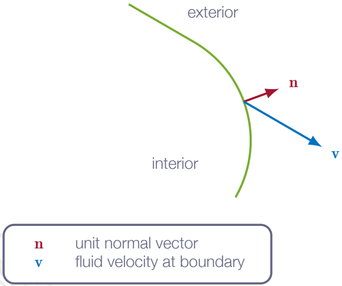
$\mathbf{v} \cdot \mathbf{n} < -a$

Five ingoing characteristics

No outgoing characteristics

Specify five variables at the boundary: solver variables

Supersonic Outflow 2D/3D



Supersonic outflow

Assumption:

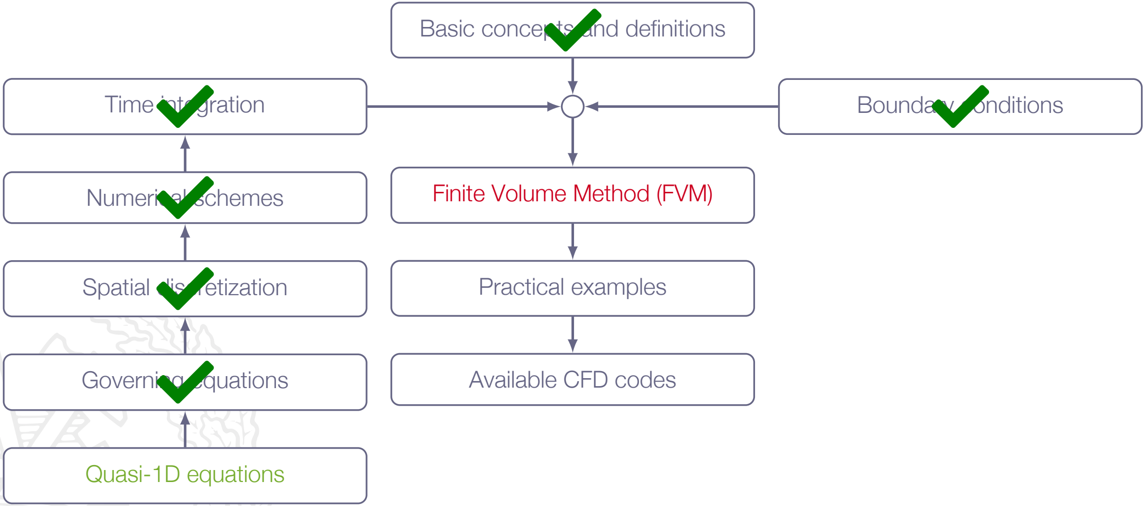
$\mathbf{v} \cdot \mathbf{n} > a$

No ingoing characteristics

Five outgoing characteristics

No variables specified at the boundary

Roadmap - The Time-Marching Technique



Explicit Finite-Volume Method - Summary

The described numerical approach can be categorized as

- Density-based
- Fully coupled
- Structured
- Explicit

with the following features

- High-order convective scheme
- Shock handling (artificial damping)

Explicit Finite-Volume Method - Summary

Spatial discretization:

Control volume formulations of conservation equations are applied to the cells of the discretized domain

Cell-averaged flow quantities $(\overline{\rho}, \overline{\rho u}, \overline{\rho e_o})$ are chosen as degrees of freedom

Flux terms are **approximated** in terms of the chosen degrees of freedom

high-order, upwind type of flux approximation is used for optimum results

A **fully conservative** scheme is obtained

the flux leaving one cell is identical to the flux entering the neighboring cell

The result of the spatial discretization is a system of ODEs

Explicit Finite-Volume Method - Summary

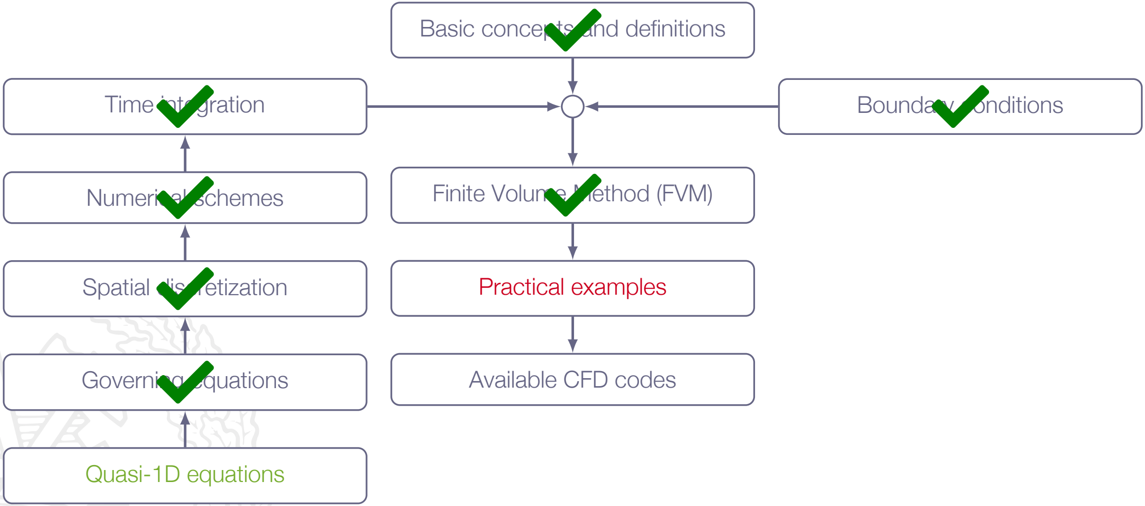
Time marching:

Three-stage, second-order accurate Runge-Kutta scheme

Explicit time-stepping

Time step length **limited by the** *CFL* **condition** ($CFL \leq 1$)

Roadmap - The Time-Marching Technique



Practical Examples: Grid Resolution and Numerical Schemes

Numerical Approach

Code: G3D::Flow (Chalmers in-house CFD code)

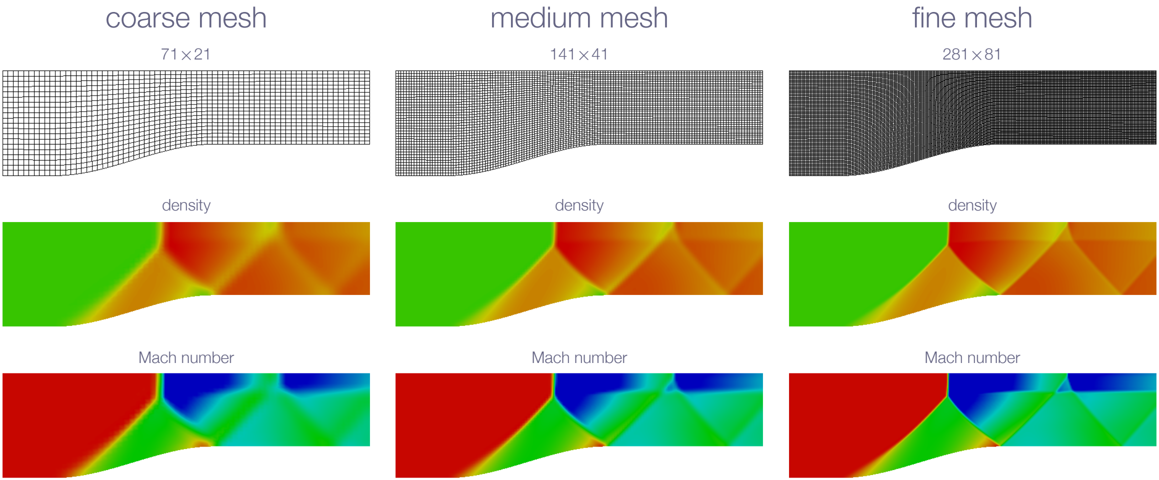
Finite-Volume Method

Three-stage, **second-order** accurate **Runge-Kutta** time stepping

First-order, second-order, and **third-order** characteristic upwinding scheme

Shock handling: TVD and artificial diffusion based on Jameson shock detection

Grid Resolution: Compression Ramp

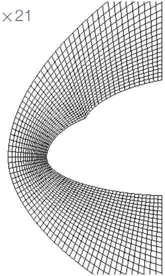


Grid Resolution: Space Shuttle

G3DFLOW

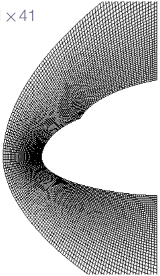
coarse mesh

81×21



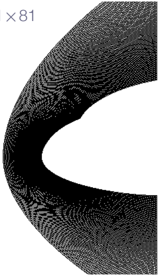
medium mesh

161×41

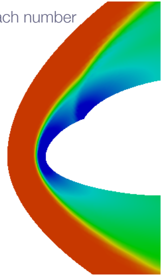


fine mesh

321×81



Mach number



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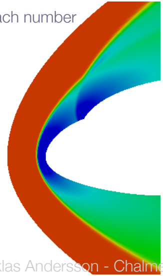
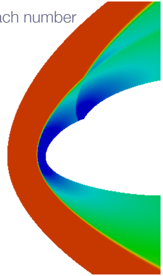


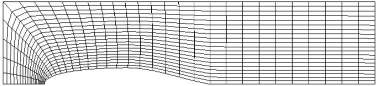
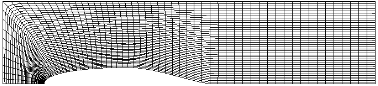
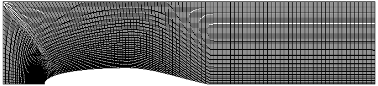
Mach number



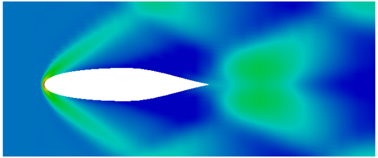
Grid Resolution: Axi-symmetric Slender Body

G3DFLOW

coarse mesh	medium mesh	fine mesh
31 × 21	61 × 41	121 × 81

density



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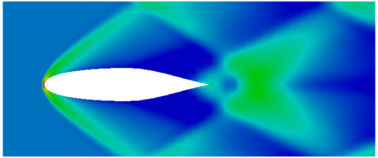

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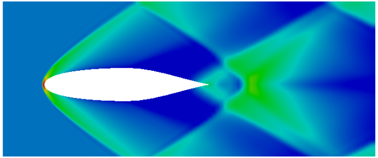

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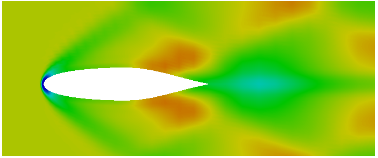

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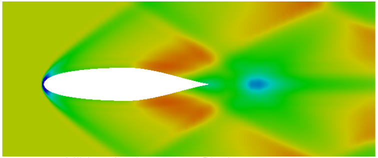

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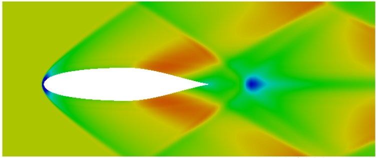
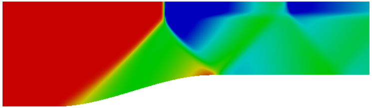


Numerical Scheme: Compression Ramp

first-order upwind

density

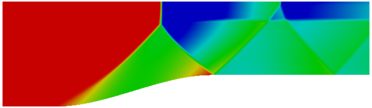
Mach number



second-order upwind

density

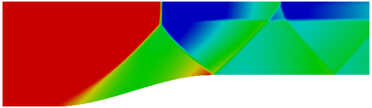
Mach number



third-order upwind

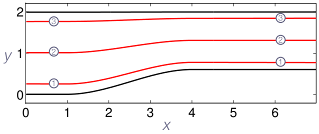
density

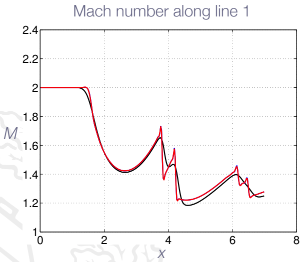
Mach number

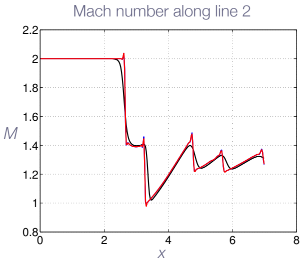


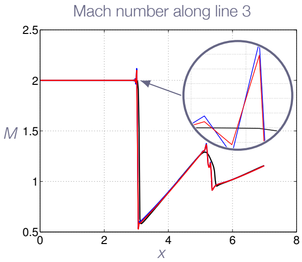
Artificial Numerical Damping: Compression Ramp

Low artificial numerical damping





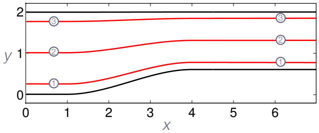


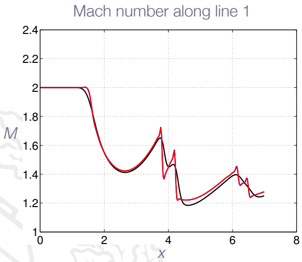


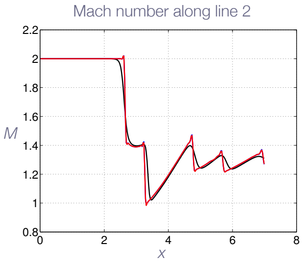
first-order upwind scheme
second-order upwind scheme
third-order upwind scheme

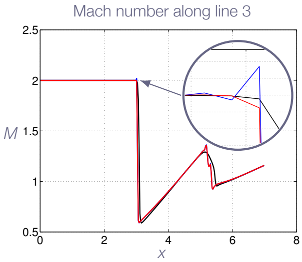
Artificial Numerical Damping: Compression Ramp

High artificial numerical damping



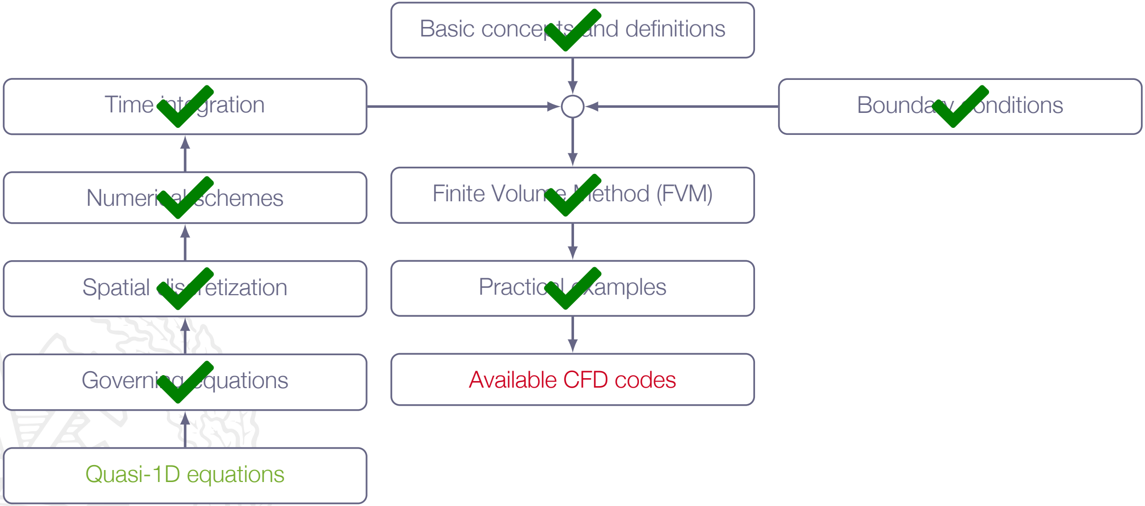






first-order upwind scheme
second-order upwind scheme
third-order upwind scheme

Roadmap - The Time-Marching Technique



Available CFD Codes

CFD Codes

List of free and commercial CFD codes:

http://www.cfd-online.com/Wiki/Codes

Free codes are in general unsupported and poorly documented

Commercial codes are often claimed to be suitable for all types of flows
The reality is that the user must make sure of this!

CFD Codes - General Guidlines

Simulation of high-speed and/or unsteady compressible flows:

Use correct solver options

otherwise you may obtain completely wrong solution!

1. coupled solver
2. equation of state
3. energy equation included

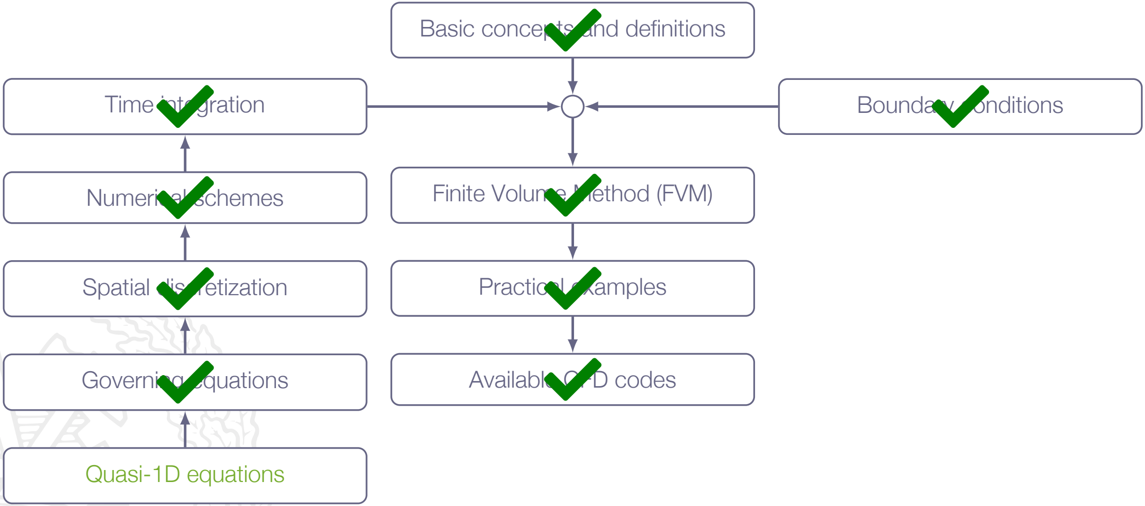
Use a high-quality grid

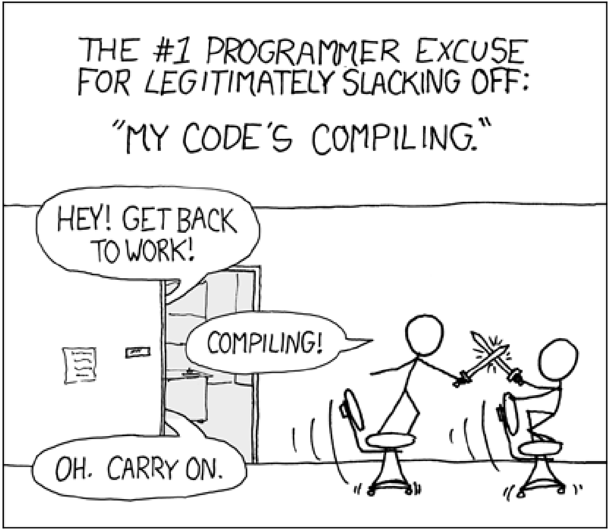
a poor grid will either not give you any solution at all (no convergence) or at best a very inaccurate solution!

ANSYS-FLUENT®/STAR-CCM+® - Typical Experiences

1. Very robust solvers - will almost always give you a solution
2. Accuracy of solution depends a lot on **grid quality**
3. **Shocks** are generally **smeared** more than in specialized codes
4. Solver is generally very **efficient** for **steady-state** problems
5. Solver is less efficient for truly unsteady problems, where both flow and acoustics must be resolved accurately

Roadmap - The Time-Marching Technique




THE #1 PROGRAMMER EXCUSE FOR LEGITIMATELY SLACKING OFF:
"MY CODE'S COMPILING."
HEY! GET BACK TO WORK!
COMPILING!
OH. CARRY ON.