

Finite Differences Method: concepts of mass flow

Discretizations of advection and diffusion

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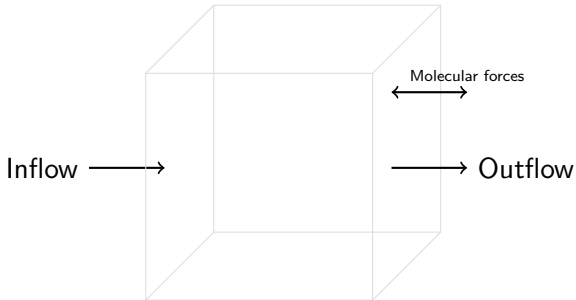


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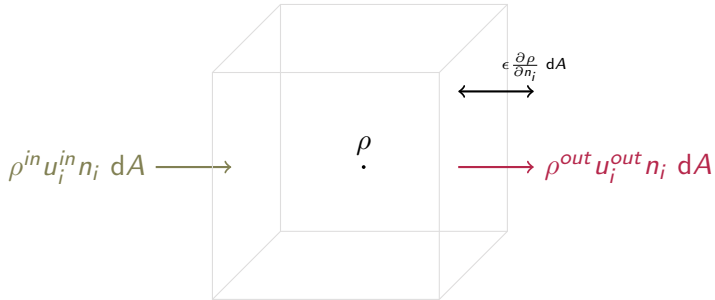
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Mass flow in a fixed control volume



Change over time = Inflow – Outflow + Molecular forces + External forces.

Mass flow in a fixed control volume



$$\int_V \frac{\partial \rho}{\partial t} dV = \int_A \rho^{in} u_i^{in} n_i dA - \int_A \rho^{out} u_i^{out} n_i dA + \int_A \epsilon \frac{\partial \rho^f}{\partial n_i} dA + \int_V F dV. \quad (1)$$

Mass flow in a fixed control volume

- We know ρ and u at the center, how do we get the values at the faces?

Mass flow in a fixed control volume

- We know ρ and u at the center, how do we get the values at the faces?
 - Using a Taylor expansion around the cell center

The Taylor approximation around a point x_0

When $f(x_0)$ is known, $f(x)$ can be found by

$$f(x) = f(x_0) + (x - x_0) \frac{\partial f}{\partial x} + \frac{1}{2} (x - x_0)^2 \frac{\partial^2 f}{\partial x^2} + \dots \quad (2)$$

The Taylor series

Theorem

Let f be an arbitrary function, and x_0 a point where f and all its derivatives are known

$$f(x) = \sum_{n=0}^{\infty} \frac{(x - x_0)^n}{n!} \frac{\partial^n f}{\partial x^n}. \quad (3)$$

Practical definition

When used in the context of modeling, and numerical analysis, the point at which f is known is x and the unknown is a point translated in relation to x , i.e., $x + \Delta x$. This leads to the practical definition

$$f(x + \Delta x) = f(x) + \Delta x \frac{\partial f}{\partial x} + \frac{1}{2} \Delta x^2 \frac{\partial^2 f}{\partial x^2} + \dots \quad (4)$$

Mass flow in a fixed control volume

- We know ρ and u at the center, how do we get the values at the faces?
 - Using a Taylor expansion around the cell center

The Taylor approximation around the point at the face

Let the control volume be defined with side length dx , and a point x as its center. The face where the inflow is coming from, for example, is at $x - \frac{1}{2}dx$. We can write the values at the faces as

$$\rho^{in} u^{in} = \rho u - \frac{1}{2} dx \frac{\partial \rho u}{\partial x} + \frac{1}{4} dx^2 \frac{\partial^2 \rho u}{\partial x^2} + \dots \quad (5)$$

$$\rho^{out} u^{out} = \rho u + \frac{1}{2} dx \frac{\partial \rho u}{\partial x} + \frac{1}{4} dx^2 \frac{\partial^2 \rho u}{\partial x^2} + \dots \quad (6)$$

Mass flow in a fixed control volume

Inserting the computed values into the conservation equation

$$\begin{aligned}
 \int_V \frac{\partial \rho}{\partial t} dV &= \int_A \rho u_i n_i - \frac{1}{2} dx \frac{\partial \rho u_i}{\partial x_i} n_i + \frac{1}{4} dx^2 \frac{\partial^2 \rho u_i}{\partial x_i^2} n_i + \dots dA \\
 &\quad - \int_A \rho u_i n_i + \frac{1}{2} dx \frac{\partial \rho u_i}{\partial x_i} n_i + \frac{1}{4} dx^2 \frac{\partial^2 \rho u_i}{\partial x_i^2} n_i + \dots dA \\
 &\quad + \int_A \epsilon \frac{\partial \rho^f}{\partial n_i} dA + \int_V F dV. \tag{7} \\
 &= - \int_A \frac{\partial \rho u_i}{\partial x_i} n_i dx_i dA + \int_A \epsilon \frac{\partial \rho^f}{\partial n_i} dA + \int_V F dV. \\
 &= - \int_V \frac{\partial \rho u_i}{\partial x_i} dV + \int_A \epsilon \frac{\partial \rho^f}{\partial n_i} dA + \int_V F dV.
 \end{aligned}$$

Note

The values $\dots$ do not cancel, however, they are small enough to be neglected, and consistently go to zero when $dV \rightarrow 0$.

Mass flow in a fixed control volume

- We know ρ and u at the center, how do we get the values at the faces?
 - Using a Taylor expansion around the cell center
- The same derivation is valid for molecular forces on opposite faces, considering the function $\epsilon \frac{\partial \rho^f}{\partial x_i}$.

The mass flow equation

Taking the limit $dV \rightarrow 0$ leads to the following general mass flow equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\epsilon \frac{\partial \rho}{\partial x_i} \right) + F. \quad (8)$$

The advection equation

Considering a constant speed, u_i , and taking $\epsilon = F = 0$ leads to the advection equation

$$\frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x_i} = 0. \quad (9)$$

This equation is hyperbolic of the first-order (referring to the order of the derivatives).

Hyperbolic partial differential equations (PDEs)

Hyperbolic PDEs

Any PDE of the form

$$\frac{\partial^2 \psi}{\partial t^2} - w^2 \frac{\partial^2 \psi}{\partial x^2} = 0 \quad (10)$$

is hyperbolic since $(0) - (1)(-w^2) = w^2 > 0$.

- How is that consistent when the derivatives are first-order?

The advection equation

The advection equation

By setting $\phi = \frac{\partial \psi}{\partial t}$ and $\rho = \frac{\partial \psi}{\partial x}$, we can rewrite the second-order hyperbolic form as

$$\frac{\partial \phi}{\partial t} - w^2 \frac{\partial \rho}{\partial x} = 0. \quad (11)$$

Taking the x derivative of ϕ leads to

$$\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial x} \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial t} \frac{\partial \psi}{\partial x} = \frac{\partial \rho}{\partial t}. \quad (12)$$

We can show by choosing $u_i = -w^2$, if $u_i < 0$, and $u_i = w^2$, if $u_i > 0$,

$$\frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x} = 0. \quad (13)$$

The finite difference concept

- How do we approximate the derivative?

The finite difference concept

- How do we approximate the derivative?
 - Utilize the definition of the derivative!

Definition of the derivative

for a continuous and differentiable function f its derivative with respect to x is defined as

$$\frac{\partial f}{\partial x} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}. \quad (14)$$

Basic approximation

Thinking of the limit $h \rightarrow 0$ as a sequence of values converging to the limit, we can consider an instance of these values Δx as an approximation

$$\frac{\partial f}{\partial x} \simeq \frac{f(x + \Delta x) - f(x)}{\Delta x}. \quad (15)$$

The finite difference concept

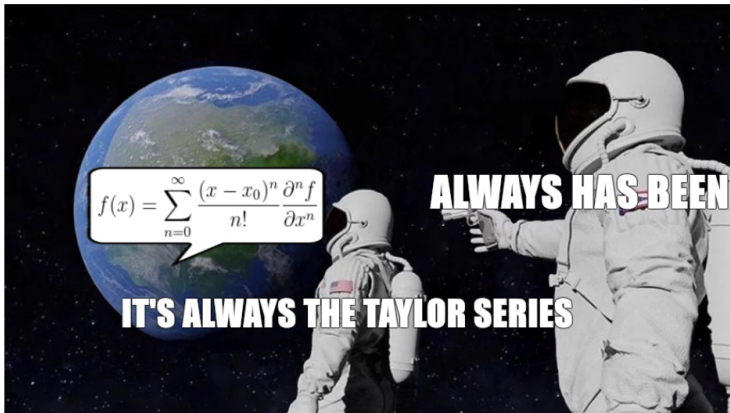
- What tool can we use to measure how good is the approximation?

The finite difference concept

- What tool can we use to measure how good is the approximation?
 - The Taylor series...

The finite difference concept

- What tool can we use to measure how good is the approximation?
 - The Taylor series...



The approximation error

Truncation error

By taking the difference between the derivative and its approximation, we can obtain the truncation error τ

$$\tau = \left| \frac{\partial f}{\partial x} - \frac{f(x + \Delta x) - f(x)}{\Delta x} \right|. \quad (16)$$

From Eq. (4), we get the Taylor expansion of $f(x + \Delta x)$ around x . Inserting it into the truncation error yields

$$\begin{aligned} \tau &= \left| \frac{\partial f}{\partial x} - \frac{\partial f}{\partial x} - \left(\frac{1}{2} \frac{\partial^2 f}{\partial x^2} \right) \Delta x + \dots \right| \\ &= \left(\frac{1}{2} \frac{\partial^2 f}{\partial x^2} \right) \Delta x + \dots = \mathcal{O}(\Delta x). \end{aligned} \quad (17)$$

The terms in $\dots$ are dominated by Δx , allowing us to utilize the Big-O notation $\mathcal{O}(\cdot)$.

The Big-O notation

Definition of Big-O

For functions f and g , such that $f \leq Cg$,

$$f \in \mathcal{O}(g). \quad (18)$$

Conventional use

When $f \leq Cg$, the relation can be written as $f = \mathcal{O}(g)$. For the truncation error above,

$$\tau \leq \left(\sum_{n=2}^{\infty} \frac{\Delta x^{n-2}}{n!} \frac{\partial^n f}{\partial x^n} \right) \Delta x \leq C \Delta x. \quad (19)$$

The tail of the series (term in parenthesis) is bounded by a constant, which can be understood given the fact that truncated tail goes to 0 in the limit.

The approximation error

The order of approximation

The concept of order comes from the idea that the more terms of the Taylor series are represented, the more accurate is the approximation. Each term of the series represents an “order”, starting with 0

$$f(x + \Delta x) = \underbrace{f(x)}_{\text{order zero}} + \underbrace{\Delta x \frac{\partial f(x)}{\partial x}}_{\text{order one}} + \cdots + \underbrace{\frac{\Delta x^n}{n!} \frac{\partial^n f(x)}{\partial x^n}}_{\text{order } n} + \cdots \quad (20)$$

The approximation error

Identifying the order of approximation

For an approximation

$$\frac{\partial^m f(x_0)}{\partial x^m} = \frac{f(x_0) + \sum_{i=1}^n f(x_i)}{(n+m-1)! \Delta x^m} + \mathcal{O}(\Delta x^n) \quad (21)$$

with m as the order of the derivative. We can define the order as n from:

- $\mathcal{O}(\Delta x^n)$, the power in the truncation error
- $(n+m-1)!$, the coefficient multiplying the Δx
- $\sum_{i=1}^n$, the number of additional points used

The approximation error

Arbitrary order design

We can utilize the idea that the number of additional points dictates the order to derive a scheme of arbitrary order n by solving the linear system

$$\frac{\partial^m f(x_0)}{\partial x^m} - c_0 f(x_0) + \sum_{i=1}^n c_i f(x_i) = 0 \quad (22)$$

for the coefficients c_i .

Literature

- Masatsuka, Katate. "I do like CFD, VOL. 1, version 2.6." (2018). pp. 45-46
- LeVeque, R. "Finite Difference Methods for Ordinary and Partial Differential Equations, Society for Industrial and Applied Mathematics, Philadelphia, 2007." . pp. 3-9

Summary of Concepts

Equations of motion

Equation	Form	Examples
Mass flow	$\frac{\partial \psi}{\partial t} + \frac{\partial f(\psi)}{\partial x} = 0$	Advection, Burgers, Continuity
Momentum		
Energy		

Summary of concepts

Types of PDEs

Type	Form	Examples
Hyperbolic	$\frac{\partial^2 \psi}{\partial t^2} - w^2 \frac{\partial^2 \psi}{\partial x^2} = 0$	Advection, Burgers
Parabolic	$\frac{\partial \psi}{\partial t} + \frac{\partial f(\psi)}{\partial x} = \epsilon \frac{\partial^2 \psi}{\partial x^2}$	Heat
Elliptic	$\epsilon \frac{\partial^2 \psi}{\partial x^2} = 0$	Heat (at $t \rightarrow \infty$), Pressure term (in NS)

Thanks for your attention!

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