Introduction to Computational Thinking and Programming for CFD

Module 13251

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5 Elementary numerical methods: Integration

5.1 Motivation

Spatial and temporal integration I

- Integrals appear in the integral form of the governing equations
  - **Volume integrals**, e.g. $\int_V \rho \, \mathrm{d}V$
  - **Surface integrals**, e.g. $\oint_A \rho \boldsymbol{u} \cdot \boldsymbol{n} \, \mathrm{d}A$
- The development of flow variables is described (predicted) by integrating the governing equations over time
  - **temporal integration**, e.g. mass density at point x_i

$$\rho_i(t) = \int \frac{\partial \rho}{\partial t}(\boldsymbol{x}_i, t) \, \mathrm{d}t$$

Spatial and temporal integration II

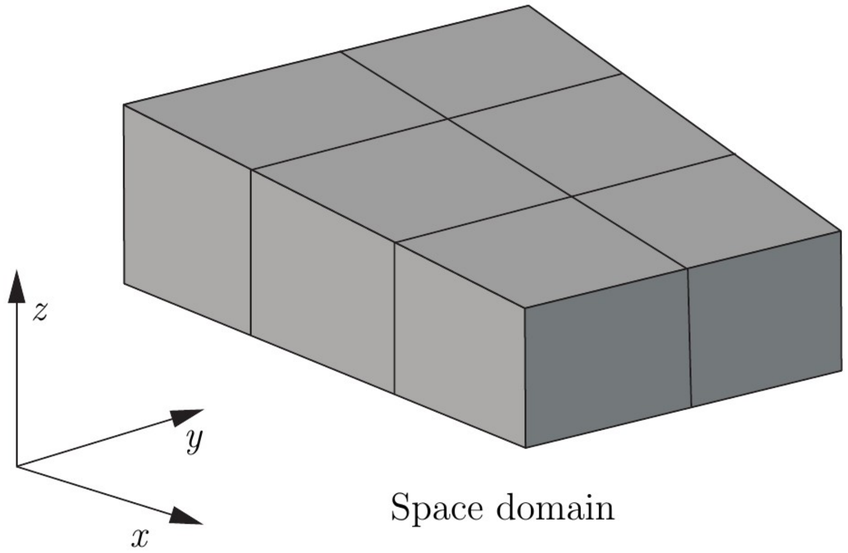

Figure 3.1: Discretisation of the solution domain

From: OpenFOAM Programmer's Guide, v2006, 2020. (www.openfoam.com/documentation)

Finite Volume Method (FVM)

- Discretization: Division of the computational domain into **finite volume cells**
- The grid cells are of simple geometry (e.g. polyhedra) in order to be able to approximate integral expressions numerically efficiently

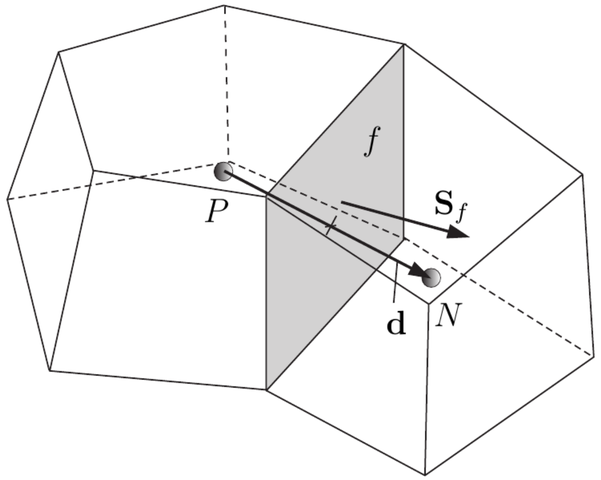

Figure 3.2: Parameters in finite volume discretisation

From: OpenFOAM Programmer's Guide, v2006, 2020. (www.openfoam.com/documentation)

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5.2 Simplification and Formulation

Problem statement and further simplification

- The **basic problem** can be formulated as follows:
  - We consider a given function *f(x)*.
  - For this, we seek the definite integral $I(a,b)$ on the interval $x \in [a,b]$.
- The **fundamental theorem of analysis** allows the evaluation of the integral over the antiderivative *F(x)*

$$I(a,b) = \int_a^b f(x)\,\mathrm{d}x = F(b) - F(a)$$

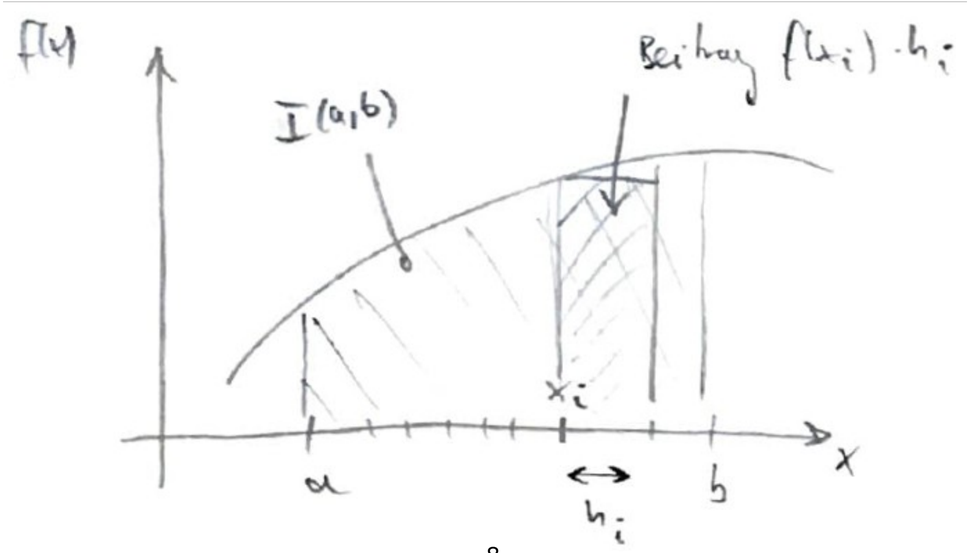
- But that doesn't help us in CFD, because we neither have a closed expression for $f(x)$, let alone know $F(x)$.

Definition of the integral

- We use the definition of the **Riemann integral**

$$I(a,b) = \underbrace{\lim_{\substack{N\to\infty \\ \max_i(h_i)\to 0}}}_{\text{Limit}} \underbrace{\sum_{i=1}^{N}}_{\text{Sum}} \underbrace{f(x_i)}_{\text{Nodal Value}} \cdot \underbrace{h_i}_{\text{Weight}}$$

- **Note**: A definite integral is a *number* that gives the *area* between the *x-axis* and the graph $y = f(x)$ over a selected interval $[a, b]$.

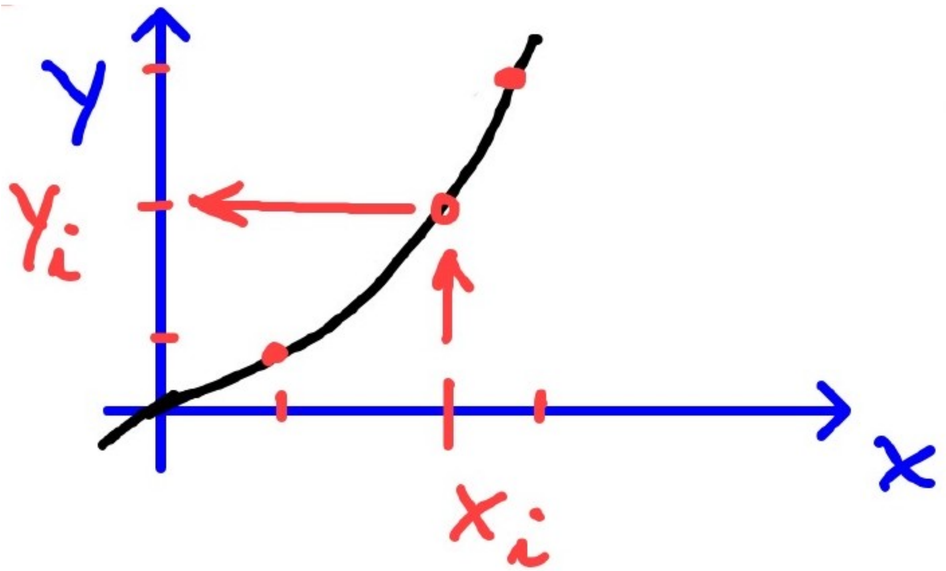


Grid vertices and nodal values

To remember…

$$y_i = f(x_i)$$

- Grid point (vertex) x_i
- Nodal value y_i



Approximation: Quadrature rules

- **Riemann sum**: $\lim_{N \to \infty}$

Stop the limit process of the Riemann integral at finite N!

- Various **quadrature formulas** can approximate $I(a,b)$. The general form is: $$I(a,b) \approx \sum_{i=1}^{N} f_i \cdot h_i$$
- The simple case of an *equidistant grid* yields $$h_i = \Delta x = \frac{b-a}{N} = \text{const} \quad \Rightarrow \quad x_i = a + i \cdot \Delta x$$
- $f_i = f(x_i)$ are the nodal values at locations x_i with $i = 0,1,\ldots,N$
- **Note**: f_i only has to be in the interval h_i, but it doesn't necessarily have to be right at the location x_i. Instead, one can also take intermediate positions, e.g. $i = \frac{1}{2}, \frac{3}{2}, \ldots$

5 Elementary numerical methods: Integration

5.3 Standard quadrature formulas

Newton-Cotes formulas

- The numerical integration on *equidistant grids* is described by the **Newton-Cotes rules**

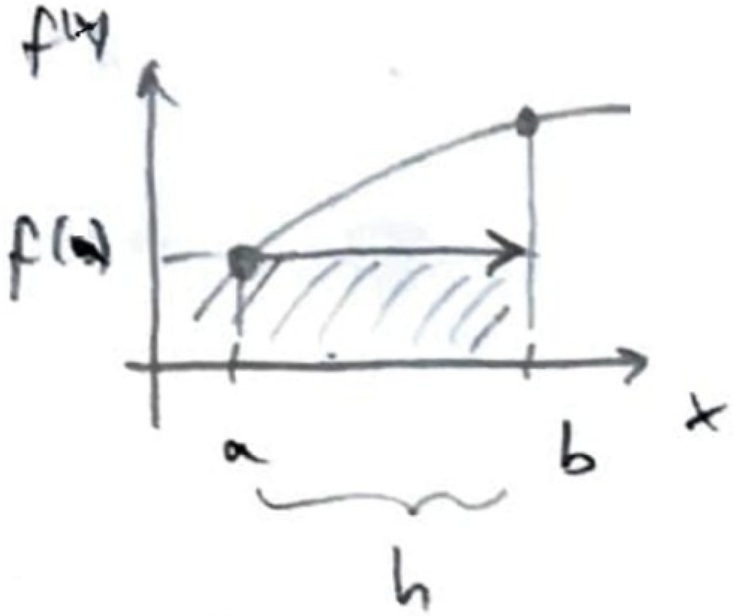
  1. Consider N intervals of length $h = \Delta x = \text{const}$.
  2. Approximate the function in these intervals using polynomials.
  3. Derive the formula for any "*small*" interval h.
  4. Sum the results for all N subintervals to approximate $I(a,b)$.

- There are two types of formulas:
  - *closed formulas*: boundary values *f(a)* and *f(b)* are included
  - *open formulas*: boundary points are not included

Lower Sum

$$I_U(a,b) = f(a) \cdot h \qquad \textbf{Error :} \quad O(f' \cdot h^2)$$

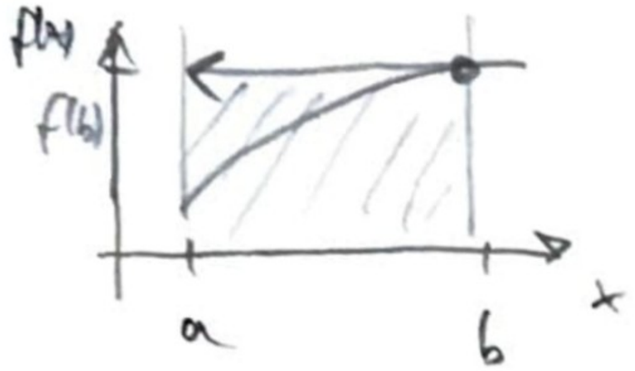
- 1 point, 1 weight -



Upper sum

$I_O(a,b) = f(b) \cdot h$ **Error :** $O(f' \cdot h^2)$

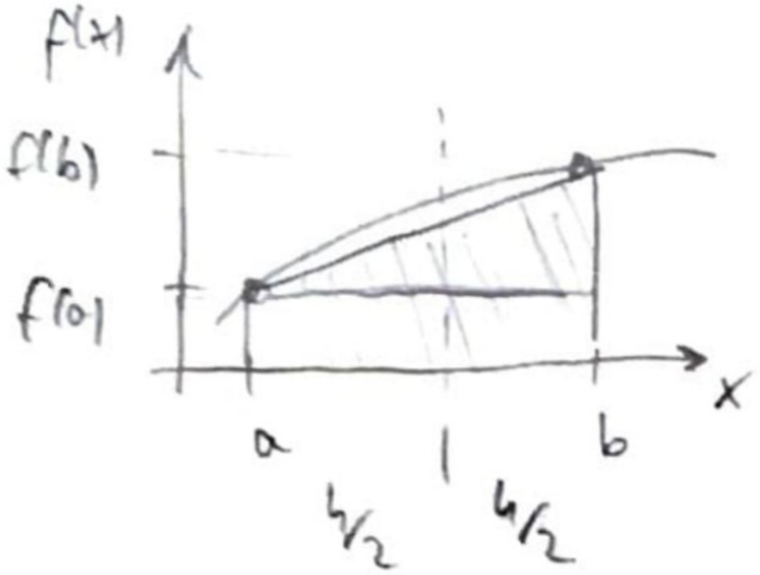
- 1 point, 1 weight -



Trapezoidal rule

$$I_T(a,b) = \left[f(a) + f(b)\right] \cdot \frac{h}{2} \qquad \textbf{Error :} \quad O(f'' \cdot h^3)$$

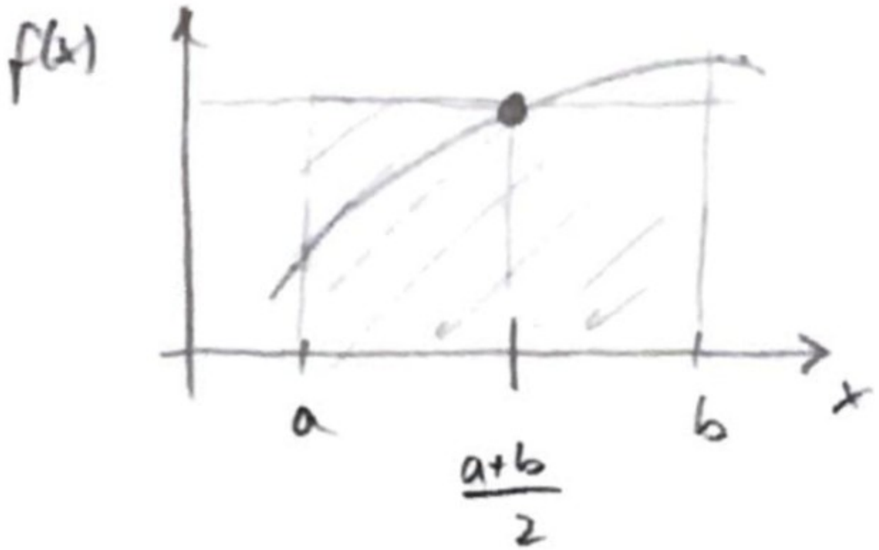
- 2 points, 2 weights -



Midpoint rule

$$I_M(a,b) = f\left(\tfrac{a+b}{2}\right) \cdot h \qquad \textbf{Error :} \quad O(f'' \cdot h^3)$$

- 1 point, 1 weight -



Higher-order integration methods

- Higher-order Newton-Cotes formulas:
  - **Simpson's rule** - 3 points, 3 weights $I_S(h) = \left[f(a) + 4 \cdot f\left(\frac{a+b}{2}\right) + f(b)\right] \cdot \frac{h}{6}$ Error : $O(f^{(4)} \cdot h^5)$
  - **3/8 rule** with $O(f^{(4)} \cdot h^5)$ - 3 points, 3 weights
  - **Milne's rule** with $O(f^{(6)} \cdot h^7)$ - 4 points, 4 weights
  - **Weddie's rule** with $O(f^{(8)} \cdot h^9)$ - 6 points, 6 weights
- **Romberg method** extrapolates from h, $h/2$, $h/4$, ... to h → 0
- **Gauss-Lobatto quadrature** selects interpolation points adapted to the problem
- Interpretation as an initial value problem of **differential calculus**

$$I(a,b) = \int_a^b f(x)\,\mathrm{d}x \quad \Rightarrow \quad \frac{\mathrm{d}I}{\mathrm{d}b} = f(b) \quad \text{with} \quad I(a,a) = 0$$

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5.4 Numerical errors

How do we get the (local) error? I

- **Idea:** Taylor expansion of the function $f(x)$ over a small interval $[a,b]$ of length h
- **Lower Sum** (upper sum analogous)
  - Constant contribution exact. Consider: $f(x) = f(a)$

$$I(a,b) = \int_a^b f(a)\,\mathrm{d}x = f(a) \cdot \underbrace{(b-a)}_{h} \stackrel{!}{=} I_U(a,b)$$

  - Leading-order error occurs in the linear term. Consider: $f(x) = f' \cdot x$

$$I(a,b) = \int_a^b f' \cdot x\,\mathrm{d}x = \frac{f'}{2} \cdot \left(b^2 - a^2\right) = f' \cdot \frac{b+a}{2} \cdot h$$

$$I_U(a,b) = f' \cdot a \cdot h$$

$$\Rightarrow \quad \varepsilon_U = I_U(a,b) - I(a,b) = -f' \cdot \frac{b-a}{2} \cdot h = -\frac{f'}{2} \cdot h^2 = O(f' \cdot h^2)$$

  - Note: f' is the constant derivative applicable at any point in $[a,b]$.

How do we get the (local) error? II

Trapezoidal rule

- The approximation can integrate constant and linear functions $f(x)$ *exactly*.
- The error associated with the Taylor expansion must disappear at the support points (boundary points a and b).
- The leading error must therefore come from the quadratic term of the Taylor series, i.e., from the curvature or second derivative f''.

$$\varepsilon_T = I_T(a,b) - I(a,b) \approx \int_0^h -\frac{f''}{2} \cdot x \cdot (x-h)\,\mathrm{d}x$$

$$= \frac{f''}{2} \int_0^h \left(-x^2 + x \cdot h\right)\,\mathrm{d}x = \frac{f''}{12} \cdot h^3 = O(f'' \cdot h^3)$$

How do we get the (local) error? III

Midpoint rule

- For linear functions $f(x) = A \cdot x$, the midpoint rule, and the trapezoidal rule lead to the same formula:

$$f\left(\tfrac{a+b}{2}\right) = A \cdot \tfrac{a+b}{2} = \tfrac{1}{2} \cdot A \cdot a + \tfrac{1}{2} \cdot A \cdot b = \tfrac{1}{2} \cdot \left[f(a) + f(b)\right]$$

- Due to the Taylor expansion, the error must disappear at the support point, that is, for the midpoint $x = (a + b)/2$.

- However, as with the trapezoidal rule, the leading error can only come from the quadratic term of the Taylor series, i.e. from the second derivative f''.

$$\varepsilon_{\mathrm{M}} = I_{\mathrm{M}}(a,b) - I(a,b) \approx \int_0^h -\frac{f''}{2} \cdot \left(x - \tfrac{h}{2}\right)^2 \,\mathrm{d}x$$

$$= -\frac{f''}{2} \int_{-h/2}^{h/2} x^2 \,\mathrm{d}x = \frac{f''}{24} \cdot h^3 = O(f'' \cdot h^3)$$

Global error and optimal step size

- The above local errors $\varepsilon = O(h^p)$ apply per grid cell of size h.
- The global error ε_{tot} results from the sum over N local contributions for the given grid.
- **How do the errors add up?**
  - In the *worst case*, the the leading-order errors are all the same. The total error increases linearly with N.

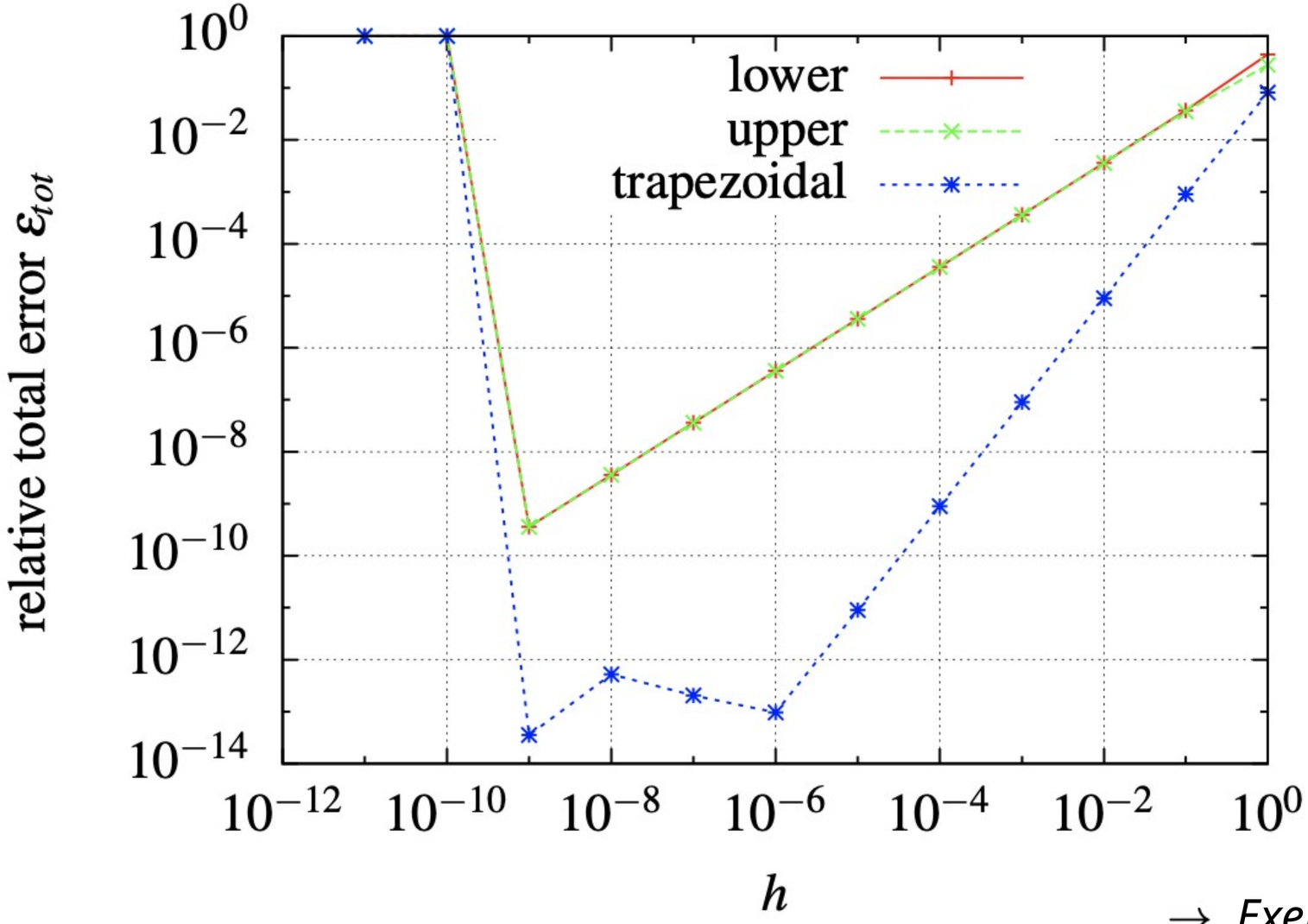
$$\varepsilon_{\text{tot}} = N \cdot \varepsilon = \frac{b-a}{h} \cdot O(h^p) = O(h^{p-1})$$

  - In a *better case*, the signs of the N local errors of maximum size ε change in an unpredictable way.

$$\varepsilon_{\text{tot}} \simeq \sqrt{N} \cdot \varepsilon = \sqrt{\frac{b-a}{h}} \cdot O(h^p) = O(h^{p-1/2})$$

- The **optimal (minimal) error** or the **minimum step** size can be estimated using the same considerations and formulas as for the derivation. That is, by round-off and discretization errors.

Convergence



← error of the integral $I(1,2)$ for $f(x) = 1/x$

→ *Exercise!*

Keywords

- Riemann integral
- Approximation of the integral, finite volume method (FVM)
- Quadrature formulas (upper & lower sum, midpoint & trapezoidal rule)
- Convergence and behavior of numerical errors

Thank you