Composite Trapezoidal Rule: Formulas, Geometric Schemes, and Numerical Application

1 Class Introduction Script

In this session, we will focus on three key objectives:

1. Understanding the geometric formulation of the composite trapezoidal rule and how summing elementary subintervals leads to the general quadrature formula.
2. Analyzing the global numerical error, and how to bound the error using function derivatives.
3. Applying this numerical method to a real thermodynamic problem: calculating the expansion work performed by an ideal gas during an isothermal process.

Let's begin by reviewing the fundamental mathematical formulas and their physical interpretation.

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2 Summary of Formulas and Structural Explanations

2.1 Basic Trapezoidal Rule (Single Subinterval)

For a single interval $[x_i, x_{i+1}]$ of width $h = x_{i+1} - x_i$, the definite integral is approximated by the area of a linear trapezoid:

$$I_i = \int_{x_i}^{x_{i+1}} f(x)\,dx \approx T_i = \frac{h}{2}\left[f(x_i) + f(x_{i+1})\right] \tag{1}$$

Local Error Formula:

$$E_{\text{loc},i} = -\frac{h^3}{12} f''(\xi_i), \quad \xi_i \in [x_i, x_{i+1}] \tag{2}$$

The local error depends on the cube of the step size h^3 and the second derivative f'', representing the local curvature of the function.

2.2 Composite Trapezoidal Rule (Summation over N Subintervals)

To integrate over $[a, b]$, the domain is divided into N equal subintervals of width $h = \frac{b-a}{N}$. Summing the individual trapezoidal areas yields:

$$\begin{aligned} I_{\text{trap}} &= \sum_{i=1}^{N} T_i = T_1 + T_2 + \cdots + T_N \\ &= \frac{h}{2}\left[f(x_1) + f(x_2)\right] + \frac{h}{2}\left[f(x_2) + f(x_3)\right] + \cdots + \frac{h}{2}\left[f(x_N) + f(x_{N+1})\right] \end{aligned} \tag{3}$$

Factoring out $\frac{h}{2}$ gives the **General Composite Formula**:

$$I_{\text{trap}} = \frac{h}{2}\left[f(x_1) + 2\sum_{i=2}^{N} f(x_i) + f(x_{N+1})\right] \tag{4}$$

Boundary points $x_1 = a$ and $x_{N+1} = b$ belong to only one trapezoid each (weight 1), whereas interior nodes $x_2, \ldots, x_N$ are shared between adjacent trapezoids (weight 2).

2.3 Global Error and Upper Bound Formulas

Exact Global Error Expression:

$$E_{\text{glob}} = -\frac{(b-a)}{12}h^2 f''(\xi), \quad \xi \in [a, b] \tag{5}$$

Theoretical Error Upper Bound (E_{max}):

$$|E_{\text{glob}}| \leq E_{\text{max}} = \frac{(b-a)^3}{12N^2}M_2, \quad \text{where } M_2 = \max_{x\in[a,b]} |f''(x)| \tag{6}$$

The composite method is second-order accurate $\mathcal{O}(h^2)$. Halving the step size h (or doubling N) reduces the global error bound by a factor of 4.

3 Geometric Schematics of the Method

3.1 Summation of Composite Trapezoids

The diagram below illustrates how summing the individual trapezoids over $N = 4$ subdivisions yields the complete composite approximation.

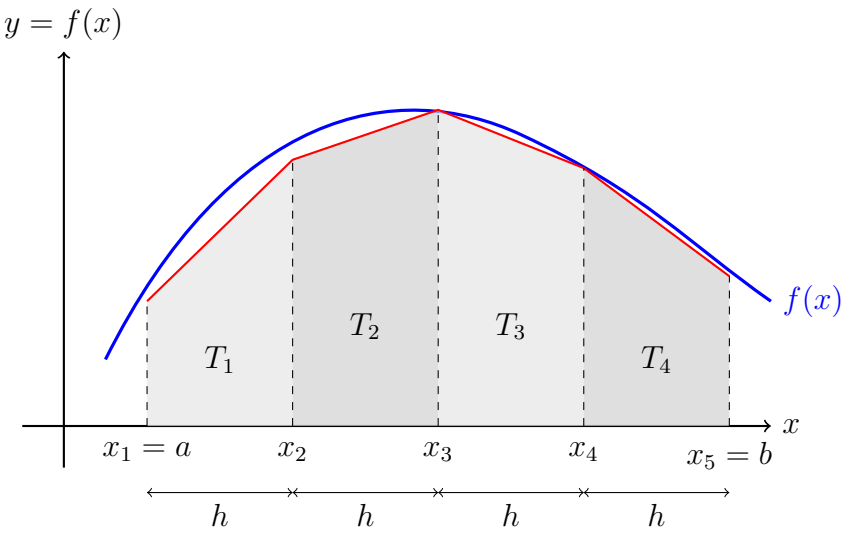


Figure 1: Composite trapezoidal integration over 4 subintervals: $I_{\text{trap}} = T_1 + T_2 + T_3 + T_4$.

4 Thermodynamic Numerical Example

4.1 Problem Statement

Calculate the thermodynamic work done during the reversible isothermal expansion of $n = 2.0$ mol of an ideal gas at $T = 300.0$ K from $V_1 = 0.005$ m^3 to $V_2 = 0.025$ m^3 using $N = 4$ subintervals:

$$W = -\int_{V_1}^{V_2} P(V)\,dV = -\int_{V_1}^{V_2} \frac{nRT}{V}\,dV \tag{7}$$

Constants: $C = nRT = (2.0)(8.314)(300.0) = 4988.4$ J, $h = \frac{0.025-0.005}{4} = 0.005$ m^3.

4.2 Numerical Integration Results

Node i	Volume V_i (m^3)	Pressure $P(V_i)$ (Pa)	Quadrature Weight w_i
1	0.005	997 680.0	1
2	0.010	498 840.0	2
3	0.015	332 560.0	2
4	0.020	249 420.0	2
5	0.025	199 536.0	1

Table 1: Discretization grid and trapezoidal weights for $P(V) = \frac{4988.4}{V}$.

Calculated Values:

- **Exact Work:** $W_{\text{exact}} = -4988.4 \ln(5) = \mathbf{-8028.53}$ J
- **Trapezoidal Work:** $W_{\text{trap}} = -\frac{0.005}{2}\,[997680 + 2(498840) + 2(332560) + 2(249420) + 199536] = \mathbf{-8397.14}$ J
- **Actual Error:** $E_{\text{actual}} = |-8397.14 - (-8028.53)| = \mathbf{368.61}$ J (Relative error: 4.59%)

4.3 Variation Table for Second Derivative and Error Bounding

To determine the maximum upper bound $M_2 = \max_{V\in[V_1,V_2]} |P''(V)|$, consider $P(V) = \frac{C}{V}$ and its higher derivatives:

$$P'(V) = -\frac{C}{V^2} < 0, \quad P''(V) = \frac{2C}{V^3} > 0, \quad P'''(V) = -\frac{6C}{V^4} < 0 \tag{8}$$

Since $P'''(V) < 0$ on $[0.005, 0.025]$, the second derivative $P''(V)$ is strictly decreasing across the domain.

Theoretical Error Bound Calculation:

$$M_2 = P''(0.005) = \frac{2 \times 4988.4}{(0.005)^3} = 7.98144 \times 10^{10}\ \text{Pa} \cdot \text{m}^{-6} \tag{9}$$

$$E_{\max} = \frac{(0.025 - 0.005)^3}{12 \times 4^2} \times (7.98144 \times 10^{10}) = \mathbf{3325.60}\ \text{J} \tag{10}$$

Conclusion: $E_{\text{actual}}(368.61\ \text{J}) \leq E_{\max}(3325.60\ \text{J})$, confirming the error bound.

V	0.005		0.025
$P'''(V)$		$-$	
$P''(V)$	7.98144×10^{10} **(Maximum M_2)**	$\searrow$	6.38515×10^{8}

Table 2: Variation table of $P''(V)$ showing its strictly monotonic decrease.