1 Numerical Integration

The analytical solution for the concentration profile in a semi-infinite slab at time `t` and position `z` reads

$$\begin{aligned} \frac{c - c_0}{c_\infty - c_0} &= \frac{2}{\sqrt{\pi}} \int_0^\zeta \exp(-s^2)\mathrm{d}s \\ \zeta &= \frac{z}{\sqrt{4Dt}} \end{aligned} \tag{1}$$

1. Write a Matlab program to calculate and plot the concentration profile in the slab, using the following values:
   - $c_\infty = 0$, $c_0 = 1$, $D = 10$
   - To do this, create a vector `zeta = linspace(1e-6, 3)`, calculate the value of `c` for each `zeta`, then plot `c` vs. `zeta`.
   - Use `integral` or `quadl` for the integration.
2. Create a function which calculates an integral using the trapezoidal rule

$$\int_a^b f(x)\mathrm{d}x \approx h\left(\sum_{k=1}^{n-1} f(x_k) + \frac{f(x_n) + f(x_0)}{2}\right)$$

   - Your function file header should read something like function `IntValue = trapInt(f, n, a, b)` where `f` is the function that has to be integrated, `n` is the number of nodes and a and b denote the interval boundaries.
   - Use for the step size `h = (b-a) / (n-1)`
   - Provide the mean error of the two methods (1. and 2.) using `fprintf`

2 Area under exponential function (Core)

1. Determine the degree of exactness of the **midpoint**, **trapezoidal** and **Simpson** rules on paper.

   The area A under the exponential function in the range from -2 to 2 shall be evaluated with three different composite quadrature rules.

$$\begin{aligned} f(x) &= e^x \\ A &= \int_{-2}^{2} e^x dx \end{aligned} \tag{2}$$

   Using a discretization $x_k = a + hk$ with $h = (b-a)/N$ and $k = 0, 1, ..., N$, those are given by :

$$\text{Midpoint: } Q_0^N[f] = h \sum_{k=1}^{N} f\left(\frac{x_{k-1} + x_k}{2}\right) \tag{3}$$

$$\text{Trapezoïdal: } Q_1^N[f] = h\left(\frac{1}{2}f(a) + \sum_{k=1}^{N-1} f(x_k) + \frac{1}{2}f(b)\right) \tag{4}$$

$$\text{Simpson: } Q_2^N[f] = \frac{h}{6}\left(f(a) + 2\sum_{k=1}^{N-1} f(x_k) + 4\sum_{k=1}^{N} f\left(\frac{x_{k-1} + x_k}{2}\right) + f(b)\right) \tag{5}$$

2. In your *main* file, vary N between 10 and 10^5 using *round(logspace(1, 5, 100))*, where *round()* rounds the values to the nearest integer.

3. Calculate the relative absolute error of the three approximations compared to the analytical solution of (4) for each h.

4. Plot h vs. the relative errors using *loglog* for the three methods.

5. The order of accuracy can be determined as the slope of the double-logarithmic plot. Use *polyfit* to obtain the corresponding slope for each of the methods.

   a. In the case of non-linear behavior reduce the fitting to the linear area. Why can the non-linear behavior at very small relative errors be neglected?

   b. Compare your results with the rules from the lecture.