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 Degree of exactness

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

3 Area under exponential function

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 :

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

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

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

1. In your *main* file, vary N between 10 and 10^5 using *logspace(1, 5, 100)*.

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

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

4. 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.

5. Provide the output in an appropriate format in the command window using *fprintf*.

6. Provide the output using an output file: open it in the form *outputfile=fopen('outputfile.txt','w')*; then use *fprintf* to write information into it and then *fclose* to close the file