Introduction to computational thinking and programming for CFD (13251)

Dr. rer. nat. Marten Klein

Chair of Numerical Fluid and Gas Dynamics, BTU Cottbus-Senftenberg

Sheet 4

Goals

- Finite difference method
- Numerical computation of 1st and 2nd derivative
- Numerical error
- Linear and semi-logarithmic plots

Tasks

1. We consider the Gaussian distribution ('bell curve')

$$g(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \quad \text{for} \quad \mu = 0.3, \quad \sigma = 1.2, \quad x \in [-5, 5],$$

where μ is the mean and σ the standard deviation ('width') of the unimodal distribution.

   (a) Calculate and plot $g(x)$ using N equispaced grid points $x_i = i \cdot h$ ($i = 0, 1, \ldots, N-1$) with uniform spacing $h = 10^{-2}$.

   (b) Calculate analytically and plot the first derivative $g'(x)$.

   (c) Numerically compute $g'(x)$ using the central difference approximation. *Hint:* Disregard the first and last grid point as these are now ghost points.

   (d) Calculate analytically and plot the second derivative $g''(x)$.

   (e) Numerically compute $g''(x)$ using the central difference approximation. Either discretize $g''(x)$ directly or apply the algorithm for the first derivative twice. *Hint:* In the latter case, disregard the first and last *two* grid points as these are now ghost points.

   (f) ($*$) Compute and plot the absolute error ε_1, ε_2 in linear and semi-log axes.

$$\varepsilon_1(x) = |g'_{\text{num}}(x) - g'_{\text{ref}}(x)|, \qquad \varepsilon_2(x) = |g''_{\text{num}}(x) - g''_{\text{ref}}(x)|,$$

   Hint: Plots with log-scaled y-axis are obtained with `pl.semilogy(x,y)`.

   (g) ($*$) How small must h be if the maximum error $\max(\varepsilon_1)$ is smaller than 10^{-3}?