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Computational Physics I

Deadline: Oct 30, 2017

1.1 Numerical resolution

Determine the smallest number ε such that 1 and $1+\varepsilon$ can numerically be distinguished. Please note the processor and the program language with which you obtained your result.

Hint: pick $\varepsilon_0 = 1$ and reduce by factors of 2 until the difference vanishes.

1.2 Numerical derivatives

Derivatives can be approximated by finite differences in several ways, for instance

$$\frac{df}{dx} \approx \frac{f(x+h)-f(x)}{h} \approx \frac{f(x)-f(x-h)}{h} \approx \frac{f(x+h)-f(x-h)}{2h} \tag{1}$$

In the limit $h \to 0$, all three expressions are equivalent and exact, but for finite h there are differences. Moreover, for very small h the entries in the numerator are similar, causing cancellations and a loss of significant digits.

Calculate numerically the derivative of $f(x) = \cos(x)$ at $x = 1$ using the three expressions given above and step sizes $h = 2^{-n}$ for suitable n. Display the difference between the numerical results and the (analytically) exact value vs. h in a doubly logarithmic plot. How do you interpret the results?

1.3 Graphics

For the potential $V(x) = x^2 \exp(-x)$ plot the potential, the force, and the derivative of the force in the interval $x \in [-3, 3]$. Plot all three curves in one frame, or plot them in three frames next to each other, aligned in the horizontal or vertical direction.
Determine the equilibrium points where the force vanishes.