

Exercise 02

Energy minimisation of force fields

Deadline: Please hand in your protocol in pdf format by Thursday, the 03rd of May 2018, 10 am to jan.joswig@fu-berlin.de or marco.manni@fu-berlin. The protocol should contain analytical solutions, short discussions, Python-code and plots.

2.1 Energy surface (100 points)

Consider a function given by:

$$U(x, y) = (x - y)^4 + 2x^2 + y^2 - x + 2y \quad (1)$$

1. Calculate the gradient and the hessian matrix of $U(x, y)$.
2. Write a Python-script that finds a local minimum of the function by the steepest decent method. Please use section 2.2.3 and equation 2.8 (page 45/46 in the script) as orientation. The algorithm should stop, when the energy correction (eps) is smaller than 10^{-10} or the number of iteration steps n reaches 1000. Show a table for the starting points $(1, 1)$, $(0, 0)$ and $(-0.3, 3)$, which holds the number of iterations n and the corresponding eps. Choose $\tau = 0.09$.
3. Create another table for the starting point $(1, 1)$ and choose three different values for τ .
4. Repeat task 2., but this time for the conjugate gradient method (page 47 in the script).
5. Draw for each of the starting points the sequence of iteration points into a contour diagram of the minimised function.