Exercise sheet 6

To be discussed on 15 and 18 June

Exercise 1

Consider a non moving electrically charged particle with negative charge $Q = -q$ in d-dimensional space, which is positioned in the centre of a grounded *cubic box*. It is known that, by introducing a d-dimensional lattice, the Poisson equation

$$\hat{\Delta}\,\hat{\phi}(\hat{\mathbf{r}}) = \hat{\delta}(\hat{\mathbf{r}})$$

(written in terms of dimensionless quantities) can be mapped into a system of linear equations $A_{ij}\hat{\phi}_j = b_i$.

(i) Argue that the matrix A is sparse, symmetric and negative definite.

(ii) Implement the conjugate gradient (CG) iterative method, which has been discussed in the lecture, and use it to solve the discretized Poisson equation in 1 dimension. Test your code by comparing results to the solutions obtained previously with direct methods (cf. with the previous sheet; for $d = 1$ there is no difference between a sphere and a cube).

(iii) Consider $d = 2$, i.e. a square of side $2R$. Calculate the electrostatic potential $\hat{\phi}$ on a lattice with few hundreds points in each direction, using the CG method with a precision $|A \cdot \hat{\phi} - \mathbf{b}| \leqslant 10^{-10}$. Repeat the same calculation doubling the number of lattice points in each direction.

(iv) How many iterations and how much time does your algorithm take to converge to the solution? Estimate roughly how much memory your program would need in both cases using a direct method to solve the system of linear equation. How much memory did you use instead? How close to the continuum limit can you get on your PC? How would you estimate it?

Exercise 2 [*Volume of the unit sphere in d dimensions*]

For any natural number $n = d - 1$, a n-sphere of radius r is defined as the set of points in d-dimensional Euclidean space that are at distance r from some fixed point called centre. A unit n-sphere is a n-sphere of radius 1.

Consider the unit n-sphere in 2-, 3- and 10-dimensional Euclidean spaces and calculate its volume using the Monte-Carlo integration method discussed in the lecture. Said differently, consider the integral

$$V_d \equiv \int_{-1}^{+1} \mathrm{d}x_1 \int_{-1}^{+1} \mathrm{d}x_2 \cdots \int_{-1}^{+1} \mathrm{d}x_d \, \Theta(1 - x_1^2 - x_2^2 - \ldots - x_d^2) \quad ,$$

with $d \in \{2, 3, 10\}$. For each value of d, use $N_1 = 10^6$ and $N_2 = 10^8$ random points to evaluate the integral and estimate the statistical error of your result. Compare what you obtained with the expected analytical result and try to explain how and why the statistical error varies as function of N_i and of d.