Computational Science 1

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Seminar Exercises

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Exercise 10 (23.1.2018): **Electrostatic shielding**

from ***An Introduction to Computer Simulation Methods***,
Chapter 10, Problem 10.8

We know that the (static) electric field is zero inside a conductor, all excess charges reside on the surface of the conductor, and the surface charge density is greatest at the points of greatest curvature. Although these properties are plausible, it is instructive to do a simulation to see how these properties follow from Coulomb's law. For simplicity, consider the conductor to be twodimensional so that the potential energy is proportional to $\ln r$ rather than $1/r$. It also is convenient to choose the surface of the conductor to be an ellipse.

a) If we are interested only in the final distribution of the charges and not in the dynamics of the system, we can use a Monte Carlo method. Our goal is to find the minimum energy configuration beginning with the N charges randomly placed within a conducting ellipse. One method is to choose a charge i at random, and make a trial change in the position of the charge. The trial position should be no more than δ from the old position and still be within the ellipse. Choose $\delta \approx b/10$, where b is the semiminor axis of the ellipse. Compute the change in the total potential energy given by (in arbitrary units)

$$\Delta U = -\sum_j \left(\ln r_{ij}^{(\mathrm{new})} - \ln r_{ij}^{(\mathrm{old})} \right) \quad . \tag{1}$$

The sum is over all charges in the system not including i. If $\Delta U > 0$, then reject the trial move, otherwise accept it. Repeat this procedure many times until very few trial moves are accepted. Write a program to implement this Monte Carlo algorithm. Run the simulation for $N \geq 20$ charges inside a circle and then repeat the simulation for an ellipse. How are the charges distributed in the (approximately) minimum energy distribution? Which parts of the ellipse have a higher charge density?

b) Repeat part (a) with the added condition that there is a fixed positive charge of magnitude $N/2$ located outside the ellipse. How does this fixed charge effect the charge distribution? Are the excess free charges still at the surface? Try different positions for the fixed charge.