

Computational Science 2

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Seminar Exercises

Exercise 1 (9.4.2015):

Numerical solution of the Laplace equation

from *An Introduction to Computer Simulation Methods*,

Chapter 10, Problems 10.11-12

- Modify `LaplaceApp` to compute the potential for the configuration in Figure 1a).
- Change `LaplaceApp` to evaluate the potential $V(x, y)$ using the *Gauß-Seidel relaxation*. First check that the potential at each site is updated immediately. This way a new potential of a site is computed using the most recent values of its nearest neighbor potentials. Then imagine the grid resembles a checkerboard consisting of red and black sites. Modify the program so that all the red sites are updated first, and then all the black sites are updated. This ordering is repeated for each iteration. Do your results converge more quickly than using the original `LaplaceApp`? Now improve the *Gauss-Seidel* method by using an overrelaxation method that updates the new potential as $V_{new}(x, y) = wV_{ave}(x, y) + (1 - w)V(x, y)$, where $V_{ave}(x, y)$ is the average of the potential of the four neighbors of (x, y) and the overrelaxation parameter $w \in (1, 2)$. Explore the w -dependence of the convergence.
- Compute $V(x, y)$ between the two concentric square cylinders shown in Figure 1b).
- A system of two conductors with charge Q and $-Q$ respectively has a capacitance C that is defined as the ratio of Q to the potential difference ΔV between the two conductors. Determine the capacitance per unit length of the configuration from part (c). The charge Q can be determined from the fact that near a conducting surface, the surface charge density is $\rho = E_n/4\pi$, where $E_n = -\delta V/\delta r$ is the magnitude of the electric field normal to the surface. δV is the potential difference between a boundary site and an adjacent interior site a distance δr away. Are the charges equal and opposite in sign? Compare your numerical result to the capacitance per unit length, $1/(2\ln(r_{out}/r_{in}))$, of a system of two concentric circular cylinders of radii r_{out} and r_{in} . Assume that the circumference of each cylinder equals the perimeter of the corresponding square, that is, $2\pi r = 4L$.
- Move the inner square 2 sites off center and repeat the calculations of parts (c) and (d). How do the potential surfaces change? Is there any qualitative difference if we set the inner conductor potential equal to -5 .

