PY 421 - Introduction to Computational Physics

Lecture notes.

1 Notes about the calculation of an electrostatic potential.

Let us consider a simplified problem, where we need to calculate a potential $\phi(x)$ in one dimension, assuming that it takes value V_0 at $x = 0$ and V_1 at $x = L$ and that there are no charges in between. ϕ will satisfy the equation

$$\frac{d^2\phi}{dx^2} = 0 \tag{1}$$

with boundary conditions

$$\phi(0) = V_0 \qquad \phi(L) = V_1 \tag{2}$$

The solution is

$$\phi(x) = V_0 + \frac{x}{L}\Big(V_1 - V_0\Big) \tag{3}$$

Let us approach the problem computationally. We discretize the interval $0 \leq x \leq L$ with $N = 5$ points uniformly separated by $a = L/(N-1)$. We denote by ϕ_n the value taken by ϕ at $x = na$. We discretize the second derivative by its central difference approximation, thus ϕ_n must satisfy

$$\phi_{n+1} + \phi_{n-1} - 2\phi_n = 0 \tag{4}$$

for $n = 1, 2, 3$. (We omitted the denominator a^2 in the approximation to the derivative, since the r.h.s. is 0.)

The only unknowns are ϕ_1, ϕ_2, ϕ_3. The three component array ϕ_n (with $n = 1, 2, 3$) will have to satisfy the system of equations 4. The equations are linear and *inhomogeneous*, because the equations for ϕ_1 and ϕ_3 contain $\phi_0 = V_0$ and, respectively, $\phi_4 = V_L$. The inhomogeneous nature of the equations can be put into evidence by defining a field $\phi^{(0)}_n$ with values $\phi^{(0)}_0 = V_0$, $\phi^{(0)}_4 = V_l$, and $\phi^{(0)}_n = 0$ for $n = 1, 2, 3$ and setting

$$\phi_n = \phi^{(0)}_n + \bar{\phi}_n \tag{5}$$

Equation 4 now gives

$$\bar{\phi}_{n+1} + \bar{\phi}_{n-1} - 2\bar{\phi}_n = -\rho_n \tag{6}$$

where ρ_n is given by

$$\phi^{(0)}_{n+1} + \phi^{(0)}_{n-1} - 2\phi^{(0)}_n = \rho_n \tag{7}$$

We see that $\bar{\phi}$ satisfies Dirichlet boundary conditions (vanishes at the boundaries) and an inhomogeneous system of equations. Of course, this is the same system of equations satisfied by ϕ_n for $n = 1, 2, 3$.