Solving the spherically symmetric Poisson's equation using B splines

Introduction

Poisson's equation is given by

$$\nabla^2\varphi = -\rho/\epsilon_0 \tag{1}$$

where φ is the electric potential, ρ is a charge distribution and ϵ_0 is the permittivity of free space. For a spherically symmetric problem, the equation simplifies to

$$\frac{\mathrm{d}^2\varphi}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}\varphi}{\mathrm{d}r} = -\rho(r)/\epsilon_0 \tag{2}$$

and by defining the function $u = r\varphi$, this becomes

$$\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + r\rho(r)/\epsilon_0 = 0. \tag{3}$$

A description will now be given on how this equation was solved numerically using B-splines for the following charge distributions:

1. A uniformily charged sphere,
$$\rho(r) = \begin{cases} 3q/(4\pi R^3), & r \le R \\ 0, & r > R \end{cases} \tag{4}$$
where q is the total charge and R is the radius of the sphere.

2. A uniformily charged shell,
$$\rho(r) = \begin{cases} 0, & r < R_1 \\ 3q/(4\pi(R_2^3 - R_1^3)), & R_1 \le r \le R_2 \\ 0, & r > R_2 \end{cases} \tag{5}$$
where R_1 and R_2 are the inner and outer radii, respectively.

3. The electron charge distribution in an hydrogen atom:
$$\rho(r) = \frac{q}{\pi a_0^3}e^{-2r/a_0} \tag{6}$$
where q is the charge of an electron and a_0 is the Bohr radius.

Method

Since $\varphi(r) = u(r)/r$ and we wish $\varphi(0)$ to be finite, we let $u(0) = 0$. For the first and second charge distributions, we know that $u(r) = q/4\pi\epsilon_0$ outside the enclosing volumes because of Gauss's law. Accordingly, we let $u(R) = q/4\pi\epsilon_0$ for the first distribution and $u(R_2) = q/4\pi\epsilon_0$ for the second distribution. For the third distribution, we introduce a cut-off so that $u(\alpha a_0) = q/4\pi\epsilon_0$ where α is some constant which will later be determined such that the error from this approximation becomes negliable. To facilitate the numerical caluclations, the following dimensionless variables were defined:

$$\begin{aligned} \xi &= r/r_0 \\ \lambda &= u/(q/4\pi\epsilon_0) \end{aligned} \tag{7}$$

where r_0 is equal to R for the first distribution, R_2 for the second distribution and αa_0 for the third distribution. Then equation (3) can be written as

$$\lambda''(\xi) + \xi\sigma(\xi) = 0 \tag{8}$$

where $\sigma = 4\pi r_0^3\rho/q$. The boundary conditions for λ are $\lambda(0) = 0$ and $\lambda(1) = 1$. Defining a new function, $g(\xi) = \lambda(\xi) - \xi$, we obtain the following boundary value problems:

$$\begin{aligned} &g''(\xi) + \xi\sigma(\xi) = 0 \\ &g(0) = g(1) = 0. \end{aligned} \tag{9}$$

These are the equations that were solved for the different charge distributions, σ.

To do so, a collocation method with B-splines as candidate solutions was used. The numerical solution to g was written as

$$\hat{g}(\xi) = \sum_{j=0}^{n-1} c_j B_{j,k}(\xi) \tag{10}$$

where $B_{j,k}$ are B-splines of order $k = 4$. Five knot points were placed at $\xi = 0$ and another five at $\xi = 1$ so that the only non-zero B-spline at $\xi = 0$ was $B_{1,k}$ and the only non-zero B-spline at $\xi = 1$ was $B_{n,k}$. The boundary conditions were thus satisfied by setting $c_1 = c_{n-1} = 0$. The collocation points were Chebyshev nodes,

$$\xi_k = \frac{1}{2} + \frac{1}{2}\cos\left(\frac{\pi(2k-1)}{2(n-2)}\right), \tag{11}$$

where $k = 1, 2, \dots n-2$. The coefficients were then obtained by solving the linear system of equations:

$$\begin{aligned} &c_0 = 0, \quad c_{n-1} = 0, \\ &\sum_{j=0}^{n-1} c_j B''_{j,k}(\xi_k) + \xi_k\sigma(\xi_k) = 0, \quad k = 1, 2\dots, n-2. \end{aligned} \tag{12}$$

Results