FINAL PROJECT OF MATH 226A, 2009

We shall consider Newton's method for solving the nonlinear Poisson-Boltzmann equation for the potential u corresponding to a given charge density $\rho(x)$ reads

$$-\Delta u + \kappa^2 \sinh(u) = \rho(x) \quad x \in \Omega, \qquad u|_{\partial\Omega} = g. \tag{1}$$

For $\kappa = 1$ and $\rho = 0$, an exact solution in $1d$ is given by

$$\bar{u}(s) = \ln\left(\frac{1+\cos(s)}{1-\cos(s)}\right).$$

We consider a $2d$ problem on the unit square $\Omega = (0,1)^2$. Let $a = (1.0, 2.0)/\sqrt{5}$. We choose $\kappa = 1$, ρ, and g such that the exact solution of (1) is

$$u(x) = \bar{u}(1 + (x, a)).$$

Use standard Newton's method to compute finite element approximations of u on uniform grids.

(1) Mesh: construct a coarse grid of $(0,1)^2$ by hand and then apply uniformrefine.m several times to get a fine grid. Be careful on the orientation of the initial grid.

(2) Find the linearized Poisson Boltzmann equation and the residual equation in Newton method.

(3) Matrix: generate the stiffness matrix and mass matrix for the linearized Poisson Boltzmann equation.

  (a) For the computation of mass matrix, you can use three vertices quadrature rule i.e.

$$\int_\tau f(x)\,\mathrm{d}x = \frac{1}{3}\sum_{i=1}^{3} f(x_i)|\tau|.$$

  This will simplifies the computation a lot. In particular, the mass matrix becomes diagonal.

  (b) You can also use finite difference method to get the matrix equation since the grid is uniform.

  (c) The residual equation, including the matrix and the right hand side, should be updated every step in the Newton's method.

(4) Solver: use direct solver to solve the matrix equation.

(5) Convergence: compute the error in each Newton step and plot or display the error.