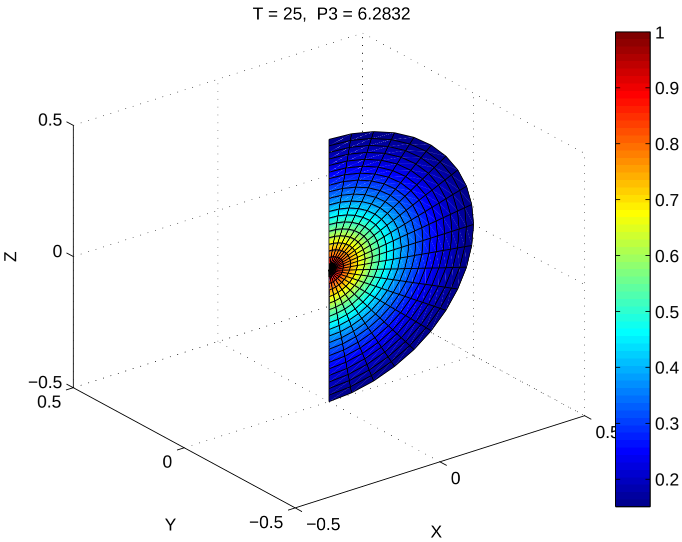
6. a. If we look for periodic solutions of the time-dependent Schrodinger equation 5.38 (p103), that is, solutions of the form $\psi(x,y,z,t) = \phi(x,y,z)e^{-i\omega t}$, we get the 3D "steady-state" Schrodinger equation 5.39, with $E \equiv \frac{h\omega}{2\pi}$. For the Hydrogen atom, the simplest possible case, the potential energy of the electron is given by $V(\rho) = -\frac{e^2}{4\pi\epsilon_0\rho}$, where ρ is the distance of the electron from the proton, which is considered fixed at the origin, e is the charge of an electron or proton, and ϵ_0 is the permittivity of free space. If the electron energy E is expressed in units of electron volts, and distance in Angstroms, equation 5.39 becomes:

$$\nabla^2\phi + \frac{3.7796}{\sqrt{x^2+y^2+z^2}}\phi = -0.26248\ E\phi$$

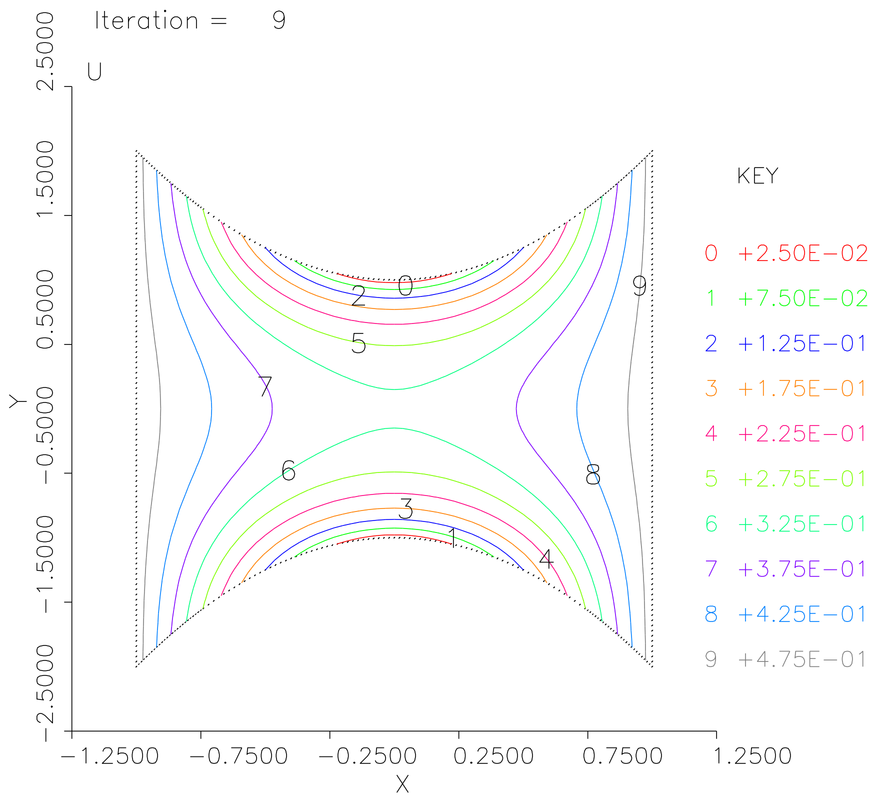
The boundary condition is that ϕ must be 0 at $\rho = \infty$, take ∞ to be $\rho = 10$. We are looking for energy values (E) for which there is a nonzero solution, so this is an eigenvalue problem. First solve this as a 3D eigenvalue problem, and look for the eigenvalue (E) closest to -15, which should be -13.60. Use spherical coordinates with a nonuniform grid, you need more gridlines near $\rho = 0$. (This problem is almost interactive driver example 11). Make MATLAB plots of the probability distribution function $|\phi|^2$ at constant longitude and constant latitude cross-sections. Note that there are parameters ICS1,ICS2,ICS3 in the pde2d.m code which determine which cross-sections are plotted by MATLAB. Since you turn in only your Fortran code, it is suggested that you set these correctly in the Fortran rather than reset them in pde2d.m everytime you run runpde2d. (Remember: to make MATLAB plots, remove all occurrences of "C!" with a single editor command, then when you run your program, files pde2d.m and pde2d.rdm will be created. Move these back to your PC and run pde2d.m using MATLAB, with pde2d.rdm in the same directory.)

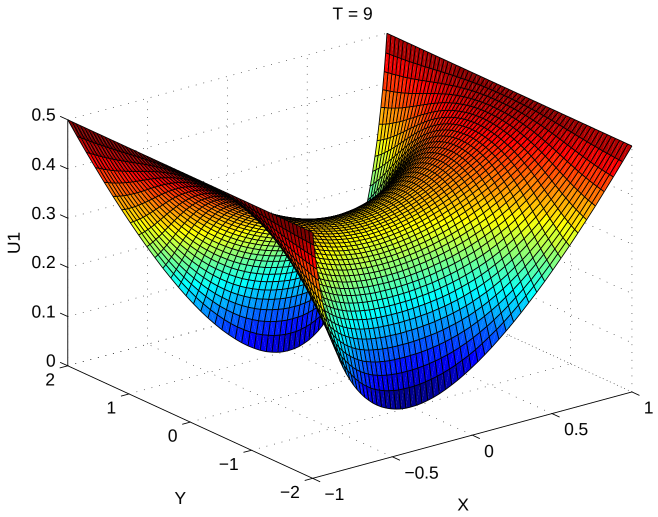


b. Next, solve this as a 1D problem, assuming ϕ is a function of ρ only, by writing $\nabla^2\phi$ as $\frac{\partial^2\phi}{\partial\rho^2} + \frac{2}{\rho}\frac{\partial\phi}{\partial\rho}$ (5.24c). This time compute all eigenvalues (ITYPE=4 and set p8z=-20 so the eigenvalues closest to -20 will be printed first). These will include only the energy levels whose probability distributions are functions of ρ only, the first two should be $E_1 = -13.60$ and $E_2 = -3.40$.

7. a. Now we will solve the 2D nonlinear minimal surface problem 7.18 (p134). The region will be the "hour-glass" figure, $-1 < x < 1, -(1 + x^2) < y < (1 + x^2)$, and on the boundary of this figure, the surface has a height $u = x^2/2$. Solve using the Galerkin method (recommended that you use the INTRI=2 initial triangulation generation option), and make a PDE2D surface or contour plot of $u(x, y)$. Compute the integral of u over the region. This is a highly nonlinear problem, so a reasonable initial guess is important, otherwise Newton's method may not converge.

b. Re-solve the problem using the collocation method. This will require expanding out the indicated divergence and simplifying the equation. Make a PDE2D contour plot and a MATLAB surface plot of the minimal surface.





c. (**Extra Credit**) To derive the minimal surface equation (7.18a), suppose $u(x, y)$ is the surface with $u = g(x, y)$ on the boundary of Ω

which minimizes the surface area $SA(u) \equiv \int\int_\Omega \sqrt{1+u_x^2+u_y^2}\ dA$ (7.17). Then if $e(x,y)$ is any smooth function with $e = 0$ on the boundary, $SA(u+\alpha e) \geq SA(u)$ for any α, thus $f(\alpha) \equiv SA(u+\alpha e)$ should have a minimum at $\alpha = 0$ and so $\frac{df}{d\alpha}(0)$ should be zero. Show that

$$\frac{df}{d\alpha}(0) = -\int\int_\Omega e\nabla \bullet \left[\frac{\nabla u}{\sqrt{1+u_x^2+u_y^2}}\right]\ dA$$

You will need to do a (multivariate) integration by parts and use the divergence theorem, see the "Review of Multivariate Calculus" link near the bottom of the class web page.

Since e is an arbitrary smooth function in the interior of Ω, we conclude that the factor multiplying e must be zero everywhere, which is (7.18a).