Final Exam in SIF4058 Computational Physics

Spring 2001

Use any aid and discuss the problems with whomever. However, you should of course write the programs and do the data analysis yourself. The solutions should be sent to me by email at 09:00 on Wednesday, June 13, in the form of a report written in any popular format: TeX, LaTeX, Word, PDF, Postscript... Good luck!

Problem 1 concerns the *travelling salesman problem.* It goes as follows: A travelling salesman based in — say Oslo — goes on a tour of European cities, $N = 15$ in all (including Oslo), visiting each once and returning to Oslo afterwards. Write an algorithm that finds the itinerary (i.e. order in which the cities are to be visited) which gives the shortest travel distance. What is this shortest distance in kilometers?

Here are the 15 cities and their positions given in degrees and minutes:

Athens	37 58 N	23 43 E
Barcelona	41 23 N	02 11 E
Bordeaux	44 50 N	00 34 W
Brno	49 13 N	16 40 E
Budapest	47 30 N	19 05 E
Cork	51 54 N	08 28 W
Glasgow	55 53 N	04 15 W
Hamburg	53 33 N	09 59 E
Madrid	40 24 N	03 41 W
Naples	40 51 N	14 17 E
Nice	43 42 N	07 15 E
Oslo	59 55 N	10 45 E
Paris	48 52 N	02 20 E
Reykjavik	64 09 N	21 51 W
Stockholm	59 20 N	18 03 E

Problem 2 In 1882 Heinrich Hertz calculated the force as a function of deformation of two elastic spheres that are pressed together [1]. The force F is that which is applied

along the axis passing through the two centers of the spheres, as they are pressed together. Assuming that the radii of the spheres are equal, the deformation D is the radius of the spheres (R) minus one half the actual distance between their centers. Hertz found the following law:

$$D = \left(6\,\frac{1-\sigma^2}{E}\right)^{2/3}\left(\frac{1}{R}\right)^{1/3} F^{2/3}\,, \tag{1}$$

where σ is the Poisson ratio and E the elastic constant. (See Ref. [2] for a detailed analytical derivation of this result.) This result forms the core of *Hertz contact theory,* and plays a fundamental rôle in many fields of physics, such as tribology (the study of friction) and granular media.

The task here is to *verify numerically the law*

$$D \propto F^{2/3}\,. \tag{2}$$

In order to do so, we start by simplifying the problem by noticing that the plane formed by the contact between the spheres is a symmetry plane. The problem is therefore equivalent to pressing a soft sphere into an infinitely rigid plane. Next simplification is to assume that it is the sphere that is infinitely rigid, and not the plane. (This change modifies the problem. However, Eq. (2) remains intact.) We assume that the plane forms the boundary of an inifinte elastic half space with elastic constant E (which you should set equal to 100) and Poisson ratio ($\sigma = 0.25$). We ignore all forces and deformations that are not prependicular to the symmetry plane. The reason for these assumptions is that we may now construct the Green function $G(x',y';x,y)$ that connects a point force f applied vertically at a point (x',y') in the plane with a deformation z at a point (x,y) (see Ref. [2], page 29),

$$z(x,y) = G(x,y;x',y')\; f(x',y')\,. \tag{3}$$

If $f(x,y)$ is a field (i.e. not just a point force), Eq. (3) becomes

$$z(x,y) = \int G(x,y;x',y')\; f(x',y')\; dx'\; dy'\,. \tag{4}$$

In order to implement this problem on the computer, we need to discretize the system. We represent the plane and the sphere by nodes (i,j) placed in a square network of size $L \times L$ (measured in units of the lattice constant a which we for convenience set equal to unity). The sphere makes first contact with the plane at $(L/2, L/2)$. After integrating Eq. (3) over the square with the four corners $(x-a/2, y-a/2)$, $(x-a/2, y+a/2)$, $(x+a/2, y+a/2)$, and $(x+a/2, y-a/2)$, and setting $(i,j)=(x,y)$ and $(i',j')=(x',y')$, we find

$$z(i,j) = \sum_{i',j'} G(i,j;i',j') f(i',j') \tag{5}$$

where $f(i,j)$ is the total force on the square of size $a \times a$ enclosing node (i,j). Let us define $u = i - i'$ and $v = j - j'$. The discretized Green function is then given by [3]

$$\begin{aligned} \frac{\pi E}{1-\sigma^2}\, G(u,v) \;&= (u+a/2)\;\ln\left[\frac{(v+a/2)+[(v+a/2)^2+(u+a/2)^2)]^{1/2}}{(v-a/2)+[(v-a/2)^2+(u+a/2)^2)]^{1/2}}\right] \\ &+ (v+a/2)\;\ln\left[\frac{(u+a/2)+[(v+a/2)^2+(u+a/2)^2)]^{1/2}}{(u-a/2)+[(v+a/2)^2+(u-a/2)^2)]^{1/2}}\right] \\ &+ (u-a/2)\;\ln\left[\frac{(v-a/2)+[(v-a/2)^2+(u-a/2)^2)]^{1/2}}{(v+a/2)+[(v+a/2)^2+(u-a/2)^2)]^{1/2}}\right] \\ &+ (v-a/2)\;\ln\left[\frac{(u-a/2)+[(v-a/2)^2+(u-a/2)^2)]^{1/2}}{(u+a/2)+[(v-a/2)^2+(u+a/2)^2)]^{1/2}}\right]\;. \end{aligned} \tag{6}$$

When the sphere is squeezed into the plane, there will be areas where there is direct contact between the sphere and the plane and areas where they are not in contact. Where there is no contact, the force f is zero, while where there is contact, the deformation of the plane is known (since the sphere is infinitely rigid and we control how deep it is indented into the plane).

In order to implement these mixed boundary conditions (force known where there is no contact, and deformation known where there is contact), one may follow the prescription given in Ref. [4]. We describe it in the following:

We define the *diagonal* $L^2 \times L^2$ matrix, $\mathbf{K}$, with elements equal to 1 on contact nodes and 0 on free (no-contact) nodes. Clearly the vector $\mathbf{K}\vec{z}$ is zero everywhere there is no contact. At contact points, $\mathbf{K}\vec{z}$ is equal to the imposed deformation given by the shape of the sphere. Eq. (5) can be rewritten as,

$$\mathbf{G}(\mathbf{I}-\mathbf{K})\vec{f} + \mathbf{G}\mathbf{K}\vec{f} = (\mathbf{I}-\mathbf{K})\vec{z} + \mathbf{K}\vec{z}\,, \tag{7}$$

where we use matrix-vector notation, and $\mathbf{I}$ is the identity. This form is convenient because as mentioned above, $\mathbf{K}\vec{z}$ is a known quantity (boundary condition). In addition, the vector $(\mathbf{I}-\mathbf{K})\vec{f}$ is always zero because the force $\vec{f}$ is nonzero only at contact points. Putting the unknowns on the left hand side and the boundary conditions on the right hand side of Eq. (7) we obtain,

$$\mathbf{GK}\vec{f} - (\mathbf{I} - \mathbf{K})\vec{z} = \mathbf{K}\vec{z}\,. \tag{8}$$

Now define the vector $\vec{x}$ representing all the unknown quantities. Clearly,

$$\vec{x} = \mathbf{K}\vec{f} + (\mathbf{I} - \mathbf{K})\vec{z}\,. \tag{9}$$

With this definition, and noting that $\mathbf{K}(\mathbf{I}-\mathbf{K}) = (\mathbf{I}-\mathbf{K})\mathbf{K} = 0$, $\mathbf{K}^2 = \mathbf{K}$, and $(\mathbf{I}-\mathbf{K})^2 = (\mathbf{I} - \mathbf{K})$ we can write Eq. (9) as

$$\mathbf{GK}\vec{x} - (\mathbf{I} - \mathbf{K})\vec{x} = \mathbf{K}\vec{z}\,, \tag{10}$$

and finally

$$\big(\mathbf{I} - (\mathbf{I} - \mathbf{G})\mathbf{K}\big)\vec{x} = \mathbf{K}\vec{z}\,. \tag{11}$$

Eq. (11) is of the familiar form, $\mathbf{A}\vec{x} = \vec{b}$ which can be solved using, for example, the Conjugate Gradient (CG) method. The difficulty is that the Green function $\mathbf{G}$, Eq. (6), is represented by a *full* $L^2 \times L^2$ matrix. This will lead to the number of operations per iteration scaling as L^4. The way to overcome this difficulty is by doing the matrix multiplications involving $\mathbf{G}$ in Fourier space by using FFTs. Why this is so, may be seen from the structure of the Green function. (If you have problems getting the FFTs to work, you can still work in real space using e.g. the CG algorithm.)

One more technical detail remains. The matrix $\mathbf{K}$, which indicates the contact points needs to be determined. The problem is that as we push the sphere into the elastic plane, the latter deforms. Therefore, the contact area is not equal to the area obtained by simply assuming that the plane will follow the contour of the sphere. We obtain the correct contact area as follows. Our initial assumption is that the contact area is equal to the area obtained from the plane following the shape of the sphere exactly. This determines the initial $\mathbf{K}$ which is then used in Eq. (11). The solution thus obtained gives the forces where there is contact and the deformations where there is none. Some of the forces thus obtained are negative since the elastic surface is trying to pull away from the rough surface. We therefore modify $\mathbf{K}$ by zeroing the the elements corresponding to nodes where the force is negative, and we solve again. We repeat this process until there are no nodes with negative forces. This algorithm always converges giving the correct contact area and forces.

Write a program that solves Eq. (11) for different indentations of the rigid sphere, and use the result to verify the Hertz contact law, Eq. (2). I used a 512×512 lattice and a sphere with radius $R = 6000$ when testing this out. This is a very large system, and it is not necessary for you to do so.

[1] H. Hertz, J. reine und angew. Mathematik, **92**, 156–171 (1882).

[2] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon Press, London, 1959).

[3] K. L. Johnson, *Contact Mechanics* (Cambridge University Press, Cambridge, 1985).

[4] G. G. Batrouni, A. Hansen and J. Schmittbuhl, Cond-Mat/0009426 (`http://xxx.lanl.gov/abs/cond-mat/0009462`).