Massachusetts Institute of Technology

Mathematical Methods
for Materials Scientists and Engineers

3.016 Fall 2010

W. Craig Carter

Department of Materials Science and Engineering
Massachusetts Institute of Technology
77 Massachusetts Ave.
Cambridge, MA 02139

Problem Set 2: **Out: 13 Sept.** and **Due: 20 Sept.**

Individual assigments should be a combination of your hand-worked solutions and other printed material—they should be placed in the mailbox outside Prof. Carter's door. Email group assignments to 3016-psets(the symbol at)pruffle.mit.edu

For the individual problems indicated as "Handworked", you should work your solutions by hand and show your work. Print the results of software-worked solutions, and staple them to your hand-worked assignments before turning them in.

The following are this week's randomly assigned homework groups. The first member of the group is the "Jomework Jefe" who will be in charge of setting up work meetings and have responsibility for turning in the group's homework notebook. If some some reason, the first member in the list is incapacitated, recalcitrant, or otherwise unavailable, then the second member should take that position. *Attention slackers:* The Jefe should include a line at the top of your notebook listing the group members that participated in the notebook's production; only those listed will receive credit. Group names are boldfaced text.

Agaricales: *jschein, m_gibson, spuranam, yhelen*

Basidiomycota: *viviand, sltaylor, ernmart, llena*

Boletales: *jrm90, tsarathi, ronrose, msee, vtrevino*

Clavicipitales: *ezuniga, aypark, amelanie, chandrak*

Helotiales: *nsinatra, eperry4, changey, bwee, andy_c*

Pezizales: *chyan, dimitri_, ckopp, mcjasso, jchenlia*

Phallales: *eogorman, sojung, tsmickel, ssluo, pmelo*

Sphaeriales: *elizalde, aliciac, elomeli, hekopp*

Individual (Handworked) Exercise I2-1

Find the equation of line where the two planes: $z = 1 + 2x + 3y$ and $y = 3 - 2z - 4x$ intersect. Write the equation in parametric form. Write an equation representing the cylinder that co-axial with the intersection line you calculated above.

Individual Exercise I2-2

Display the previous problem graphically.

Individual Exercise I2-3

Define a symbol, *aDate*, in Mathematica that is set to the date (i.e., "Sun 12 Sept 2010 03:12:58") when it was defined, and then displays that fixed date whenever it is evaluated within that Mathematica session. Define another symbol, *theDate*, in Mathematica returns the correct date (i.e., "Sun 12 Sept 2010 03:15:12") *whenever* it is evaluated.

Individual Exercise I2-4

Construct a list of the first N Fibonacci numbers. Select and display those members of the list which are perfect squares (i.e., $4, 16, 36, 81, \ldots$).

Individual Exercise I2-5

Here are infinite products that converge to numbers that involve π:

Wallis' Product

$$\frac{\pi}{2} = \prod_{i=1}^{\infty} \left(\frac{2i}{2i - 1} \right) \left(\frac{2i}{2i + 1} \right) = \frac{2}{1} \times \frac{2}{3} \times \frac{4}{3} \times \frac{4}{5} \times \ldots$$

Viète's Formula

$$\frac{4}{\sqrt{2}\pi} = \prod_{i=1}^{\infty} \frac{\sqrt{R_f(i)}}{2}$$

$$R_f(i) = \frac{2 + 2\sqrt{R_f(i-1)}}{2}$$

and $R_f(1) = 1$. For example,

$$\frac{4}{\sqrt{2}\pi} = \frac{\sqrt{2 + \sqrt{2}}}{2} \times \frac{\sqrt{2 + \sqrt{2 + \sqrt{2}}}}{2} \times \frac{\sqrt{2 + \sqrt{2 + \sqrt{2 + \sqrt{2}}}}}{2} \times \ldots$$

First, find out if Mathematica knows that Wallis' product is related to π.

Next, find out how the two formulae converge to their asymptotic values as the product is carried out to infinity.

For each product, define a function that computes the product up to a specified iteration, (e.g., $P(N) = \prod_{i}^{N} f(i)$ or $P(N) = P(N-1)f(N)$).

Compute the respective $P(N)$ for $N = 1, 2, 3, \ldots$ and graphically explore the convergence (i.e., how the product converges to $\pi/2$ or $4/\sqrt{2}\pi$ with increasing N) of each product. Logarithms are useful for exploring the behavior of small differences.

Group Exercise G2-1

The purpose of this exercise is to explore data sets representing atomic positions and, using the data, infer something meaningful about their structures.

There are three data sets stored in files of several formats. In each file, each line has the x, y, z coordinates of an atomic center.

The files are located here:

Data Set A:

http://pruffle.mit.edu/3.016/Data/atomPositions_A.csv
http://pruffle.mit.edu/3.016/Data/atomPositions_A.tsv
http://pruffle.mit.edu/3.016/Data/atomPositions_A.xls

Data Set B:

http://pruffle.mit.edu/3.016/Data/atomPositions_B.csv
http://pruffle.mit.edu/3.016/Data/atomPositions_B.tsv
http://pruffle.mit.edu/3.016/Data/atomPositions_B.xls

Data Set C:

http://pruffle.mit.edu/3.016/Data/atomPositions_C.csv
http://pruffle.mit.edu/3.016/Data/atomPositions_C.tsv
http://pruffle.mit.edu/3.016/Data/atomPositions_C.xls

The data's centers of mass are near $x = 0, y = 0, z = 0$ and the atoms lie within a sphere of radius of approximately 8.

In addition to finding a discrete approximation to the radial distribution function, $g(|\vec{r}|)$, explore as many methods of discerning the structure from the data as you can create.

The radial distribution function is defined by: $\rho(|\vec{r}|) = \rho_{ave}g(|\vec{r}|)$, where ρ_{ave} is the average density, and $\rho(|\vec{r}|)$ is the density of atoms in the region $(|\vec{r}|, |\vec{r}|+\Delta|\vec{r}|)$ surrounding an atom located at $\vec{r} = \vec{0}$ (when averaging over a structure, the zero is translated to each atom being averaged). To get good statistics, it is a good idea to average the radial distribution functions for several atoms near the origin.

Each data set is "thermalized," (i.e., the atoms have been perturbed from their stable position as they would be at any instant at some finite temperaure). Some or all of the data sets are thermalized from a stable configuration with atoms decorating a Bravais lattice.

Can you decipher the characteristic structure of each data set?