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 3: **Out: 20 Sept.** and **Due: 27 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.

Bau: *eperry4, jschein, amelanie, ronrose*

Bho: *hekopp, aliciac, mcjasso*

Gav: *ezuniga, jrm90, tsarathi*

Guau-Guau: *llena, vtrevino, spuranam*

Meong: *nsinatra, dimitri_, chandrak*

Vogh: *eogorman, changey, jchenlia*

Wan: *msee, chyan, ssluo*

Wang: *tsmickel, yhelen, sojung*

Waouh: *andy_c, ckopp, m_gibson*

Woof: *pmelo, aypark, ernmart*

Zaunk: *bwee, viviand, elomeli*

Individual (Handworked) Exercise I3-1

Solve the following sets of equations for p, q, and r (find exact solutions).

$$
\begin{aligned}
p + \frac{-3}{2} q - r &= 99 \\
\frac{1}{3} p + \frac{-1}{3} q + r &= 33 \\
-2p - q + 2r &= 99
\end{aligned}
$$

$$
\begin{aligned}
p + \frac{-3}{2} q - r &= 0 \\
\frac{1}{3} p + \frac{-1}{3} q + r &= 0 \\
7p - 9q + 5r &= 0
\end{aligned}
$$

Individual Exercise I3-2

Invert the following matrix $\underline{M}$ given below and multiply it by the column vector $\vec{b}$ given below.

$$
\underline{M} = \begin{pmatrix} 1 & -\frac{3}{2} & -1 \\ \frac{1}{3} & -\frac{1}{3} & 1 \\ -2 & -1 & 3 \end{pmatrix} \qquad \vec{b} = 33 \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix}
$$

By plotting the three planes associated with the rows of $\underline{M}$ and $\vec{b}$, produce a graphical illustration of the solution.

Individual Exercise I3-3

Invert the following matrix $\underline{Q}$ given below and multiply it by the column vector $\vec{\zeta}$ given below.

$$
\underline{Q} = \begin{pmatrix} 1 & -\frac{3}{2} & -1 \\ \frac{1}{3} & -\frac{1}{3} & 1 \\ 7 & -9 & 5 \end{pmatrix} \qquad \vec{\zeta} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
$$

By plotting the three planes associated with the rows of $\underline{Q}$ and $\vec{\zeta}$, produce a graphical illustration of the solution.

Individual Exercise I3-4

Many physical models are constructed in terms of a few model parameters (for example, the Lennard-Jones potential $V(r) = A/r^{12} - B/r^6$ which is a simple and frequently used model for the potential energy between to atoms). One difficulty with exploring the physical nature of such models is picking the "appropriate" parameters to visualize the behavior graphically and analytically. In such cases, it is very instructive to introduce non-dimensionalized physical units. For background on non-dimensionalization see the notes here:
`http://pruffle.mit.edu/3.016/Appendices/`

One such "universal model" is the van der Waals model for gasses which is a modification of the ideal gas law that accounts for the finite size of molecules and their interactions. The van der

Waals equation of state for one mole of gas is:

$$(P + \frac{a}{V^2})(V - b) = RT$$

The goal is to examine the behavior of this model for *any generic gas.*

1. The temperature and pressure must always be positive real quantities. What restrictions do these restrictions place on the van der Waals parameters a and b? (the function `Reduce` may be useful).

2. The van der Waal's model is usually investigated by looking at the behavior of P and V for isotherms (i.e., T = Constant for different values of the constant.) For water vapor, the van der Waal's constants are $a = 558$ pascal/meter^6, $b = 3.05 \times 10^{-5}$ meter^3, and $R = 8.03$ joule/mole Explore the behavior of water by plotting isotherms of $T = 700,\ 647,\ 600$K. Compare your behavior with the critical point of water on its single-component P-T phase diagram (the critical point is where the phase boundary between liquid and vapor disappears). What is your predicted molar volume at the critical point?

3. It is more instructive to treat all gasses on the same footing. This is done by introducing a dimensionless pressure (Π), dimensionless volume (Ω), and dimensionless temperature (Θ). These quantities are constructed by referring to the critical point: $\Pi = P/P_{\text{crit}}$, $\Omega = V/V_{\text{crit}}$, and $\Theta = T/T_{\text{crit}}$. You should observe from your plot for water that the critical point occurs when
$$\left(\frac{\partial P}{\partial V}\right)_T = 0 \quad \text{and} \quad \left(\frac{\partial^2 P}{\partial V^2}\right)_T = 0$$
Compute a and b in terms of the the critical point values, back substitute, and use the definitions for the non-dimensional quantities to write the van der Waals equation of state in terms of Π, Ω, and Θ.

4. Visualize the behavior of the van der Waals equation of state for a generic gas.

5. The bulk modulus of a material is given by $\beta = -V\left(\frac{\partial P}{\partial V}\right)_T$, what are the units of β? Find a non-dimensional form of β. How does this non-dimensional form behave near the critical point?

6. The coefficient of thermal expansion of a material is given by $\alpha = (1/V)\left(\frac{\partial V}{\partial T}\right)_P$, what are the units of α? Find a non-dimensional form of α? How does this non-dimensional form behave near the critical point?

7. The difference between the heat capacity at constant pressure and at constant volume $c_P - c_V$ can be shown to be equal to $TV\alpha^2\beta$. A material cannot be thermodynamically stable unless $c_p > c_v$. When is a van der Waals gas thermodynamically stable?

Group Exercise G3-1

The purpose of this problem is to explore the relationship between lattices, point-group symmetry, and their combinations that create space-group symmetry.

To do this exploration, your group will place polyhedra with faces that are colored to produce symmetry and then place identical polyhedra onto primitive Bravais lattices.

In this file `http://pruffle.mit.edu/3.016/Homeworks/cube-transformations-setup.nb`, you will find examples and functions for creating, coloring faces, distorting, and translating polyhedra. After you have studied how these examples and functions work, you should use them to do—*at least*—the following:

1. Show that the face-normals computed for the tetrahedron in the supplied notebook are correct.

2. By placing tetrahedra on a primitive cubic lattice, create a structure with no additional symmetry (i.e., no rotational, mirror, inversion, rotoinversion, rotoreflection or glide symmetry).

3. By placing appropriately colored and/or rotated cubes onto the primitive cubic lattice, produce a structure with a three-fold rotation axis. The cubes must have at least two differently colored faces. In addition to displaying the structure, make sure you describe the result.

4. By placing appropriately colored and/or rotated tetahedra onto the primitive cubic lattice, produce a structure with a mirror plane. The tetrahedra must have at least two differently colored faces.

5. By placing appropriately colored and/or rotated cubes onto the primitive cubic lattice, produce a structure with a four-fold axis. The cubes must have at least two differently colored faces. Describe any other symmetries that arise from your structure.

6. By placing appropriately colored and/or rotated cubes onto the primitive cubic lattice, produce a structure with a three-fold rotoinversion axis. The cubes must have at least two differently colored faces. Describe any other symmetries that arise from your structure.