Definition of reciprocal lattices:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_1 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}.$$

Homework:

1. Prove that that reciprocal lattice primitive vectors defined above satisfy

$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}.$$

Hint: Write $\vec{b}_1$ (but not $\vec{b}_2$ or $\vec{b}_3$) in terms of the $\vec{a}_i$, and use the orthogonality relations of $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$.

2. Show that the reciprocal vectors of $\vec{b}_i$ are just the original direct lattice primitive vectors of $\vec{a}_i$, i.e., show at

$$2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)} = \vec{a}_1, \text{ etc.}$$

Hint: Write $\vec{b}_3$ in the numerator (but not $\vec{b}_2$) in terms of the $\vec{a}_i$, and use the vector identity $A \times (B \times C) = B(A \cdot C) - C(A \cdot B)$, and appeal to the orthogonality relations and the results from problem 1.

3, Show the packing fraction in the following crystal structures: bcc = ( √ 3/8)pi, fcc = ( √ 2/6)pi, and Diamond=( √ 3/16)pi.

4, write a small program to integrate f(x) = $x^6$ from [-1, +1] using trapezoidal rule and random sampling. Calculate the squared deviation from the true value as a function of M sample points or N slices and compare the difference of these two algorithms.

Submit your HW solution, code, and a brief report of problem 4 to our TA. Due in two weeks.