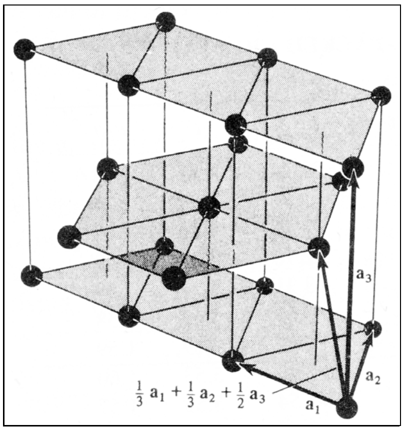
Molecular dynamics 2015

Exercise 2 to chapter 2: Random numbers etc.

1. (6 p) Modify your program of exercise 1 to construct a hexagonal close-packed (HCP) structure (using an orthorhombic unit cell; i.e. cell that has all three lattice vectors orthogonal with each other[1]). Using a visualization program demonstrate the (small) difference between the face centered cubic (FCC) and HCP structures: the different stacking order of (111) crystal planes. *Hint: the primitive unit cell depicted on the right contains two atoms, while the non-primitive orthorhombic cell contains four atoms.*



HCP

unit cell (non-orthorhombic)

$\mathbf{a}_1 = a\mathbf{i}$

$\mathbf{a}_2 = a/2\mathbf{i} + \sqrt{3}a/2\mathbf{j}$

$\mathbf{a}_3 = \sqrt{8/3}a\mathbf{k}$

basis
(atoms in the unit cell)

$\mathbf{b}_1 = 0$

$\mathbf{b}_2 = \frac{1}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$

2. (7 p) Write subroutines which generate random numbers with an even and a Gaussian distribution. Generate 1 million Gaussian-distributed random numbers (with the standard deviation $\sigma = 1$ and mean $\mu = 0$), make a histogram of their distribution with a bin width of e.g. 0.01 and the *area* normalized to unity and make a plot. Also generate the same Gaussian distribution

$$f(x) = [2\pi]^{-1/2}e^{-x^2/2}$$

analytically and plot in the same figure as the random plot.

Return the code and the figure as pdf, postscript or png, jpeg, or the like.

3. (7 p) Equipartition theorem states that[2]: *Every degree of freedom of a body that contributes a square term of a coordinate or momentum to the total energy has a mean energy of $k_B T/2$ in that degree of freedom.* Based on this explain why the temperature drops by a factor 2 in the beginning of the simulation[3]. Would you expect the factor be 2 also at very high temperatures?

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1. Lecture notes, chapter 2, page 15.
2. G. W. Wannier: *Statistical Physics* (Dover, New York, 1966), ch. 4-5.
3. Lecture notes, chapter 2, page 17.