Computational Science 1

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Seminar
Exercises

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Exercise 8 (19.1.2017):

The structure of $g(r)$ for a dense liquid and a solid

from ***An Introduction to Computer Simulation Methods***,
Chapter 8, Problem 8.13

a) Use the example `LJParticleApp` and incorporate methods which compute the radial distribution function $g(r)$ for a system of $N = 64$ particles that are fixed on a triangular lattice with $L_x = 8$ and $L_y = \sqrt{3}L_x/2$. The normalization condition for $g(r)$ is

$$\rho \int g(r) d\mathbf{r} = N - 1 \approx N \tag{1}$$

where the volume element $d\mathbf{r} = 2\pi r dr$ in two dimensions. What is the density of the system? What is the nearest neighbor distance between sites? At what value of r does the first maximum of $g(r)$ occur? What is the next nearest distance between sites? Does your calculated $g(r)$ have any other peaks? If so, relate these peaks to the structure of the triangular lattice.

b) Modify your molecular dynamics program and compute $g(r)$ for a dense fluid ($\rho > 0.6$, $T \approx 1.0$) with $N \geq 64$. How many peaks in $g(r)$ can you observe? In what ways do they change as you decrease and as you increase the density? Take care that the velocities are rescaled such that the temperature stays at $T \approx 1.0$. How does the behavior of $g(r)$ for a dense liquid compare to that of a dilute gas and a solid?