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Algorithms of Scientific Computing II

Exercise 1

1) Orders of Magnitude

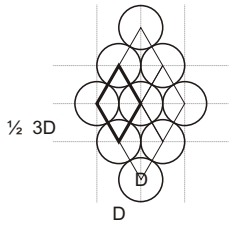
In this exercise, we want to gain some understanding, systems of which size can still be simulated in a reasonable time. As practical example we want to do a molecular simulation of 1 liter of beer for 1 second. Try to find a generous estimate for the lower bound of the computation time. We make the following assumptions:

- A time step of our simulation should be 10^{-15} s.
- A liter of beer has the same molar mass as water ($18\frac{g}{mol}$).
- We apply a perfectly linear algorithm, which needs only one calculation per molecule per time step.
- We have unlimeted cpu time on the fastest supercomputer with approximatelly 1 petaflops.
- We are perfect programmers, so our implementation always reaches peak performance.

What can we conclude? Assuming, Moore's Law continues to be valid, when does it make sense to start the simulation?

2) Hardsphere-Model in 3d

In 2D, the dense packing of the spheres standing for the molecules of an examined substance is given as shown here:



Determine a dense packing of spherical molecules in 3D and compute the resulting relative density given by the relation between the volume filled by molecules and the total volume of a surrounding box.