Initial Configurations

Random positions

- Simplest method of constructing the initial conf.
- Problems: atoms could end up overlapping each other
  - Unphysical for hard-core systems
  - Problematic for soft potentials: very large numbers

Initial Configurations

Positions in a lattice

- The more usual method
- Historically, the face-centered cubic lattice has been employed
- Lattice distance should correspond to liquid density
- Simulation kills the lattice, but to speed up the "melting" could add random small initial displacements to atoms

Initial Velocities

- Random, but conforming to the desired temperature
- Should be assigned also to conserve total P

$$\mathbf{P} = \sum_{i=1}^{N} m_i \mathbf{v}_i = 0$$

Initial Velocities

- Two usual possibilities:
  - Chosen from a uniform random distribution in the range ($-v_{max}$, $+v_{max}$)
  - Chosen from the Maxwell velocity distribution (ρ probability density for velocity component v_{ix})

$$\rho(v_{ix}) = \sqrt{\frac{m_i}{2\pi k_B T}} e^{(-\frac{1}{2} m_i v_{ix}^2 / k_B T)}$$

Note: choice is not important as uniform random will "Relax" into the Maxwell-Boltzmann after a few hundred steps.

Algorithms for Gaussian Distributions

Many times it is needed to generate random numbers drawn from a Gaussian distribution

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left[-\frac{(x - \langle x \rangle)^2}{2\sigma^2}\right]$$

with mean <x> and variance σ^2

But only have handy a function rand() that returns random from a uniformly distributed distribution [0,1]

Algorithms ...

Method 1:

- Generate two random numbers (from uniform distribution) ξ_1 and ξ_2
- Calculate two random nums. from Gaussian distribution by using

$$x_1 = \sqrt{-2 \ln \xi_1} cos(2\pi\xi_2)$$

$$x_2 = \sqrt{-2 \ln \xi_1} sin(2\pi\xi_2)$$

Algorithms ...

Problems with Method 1:

- Slow because of the calls to math library
- Has stability problems when ξ_1 is close to 0

Algorithms ...

Method 2:

- Calculate 12 uniform random numbers ξ_1, ..., ξ_{12}
- Obtain 1 Gaussian distributed random number by

$$x = \sum_{i=1}^{12} \xi_i - 6$$

Algorithms ...

Notes:

- Both methods generate random numbers (x) in the normal distribution with
  - Zero mean
  - Unit variance
- If need to generate (x') with mean <x'> and variance σ, use

$$x' = \langle x' \rangle + \sigma x$$

Equilibration

- After the start, a simulation needs to “find itself” away from the lattice or random initial conf.
- After an *equilibration time* the initial conf. should have been forgotten by the system
- Equilibration can be monitored using several quantities

Equilibration

- Potential and Kinetic energies: let them settle around an average value
- Pressure
- RMS displacement from orig positions:
  - let it exceed σ/2 and make sure that it is increasing for a “melted” system
- It is a problem close to phase transitions!