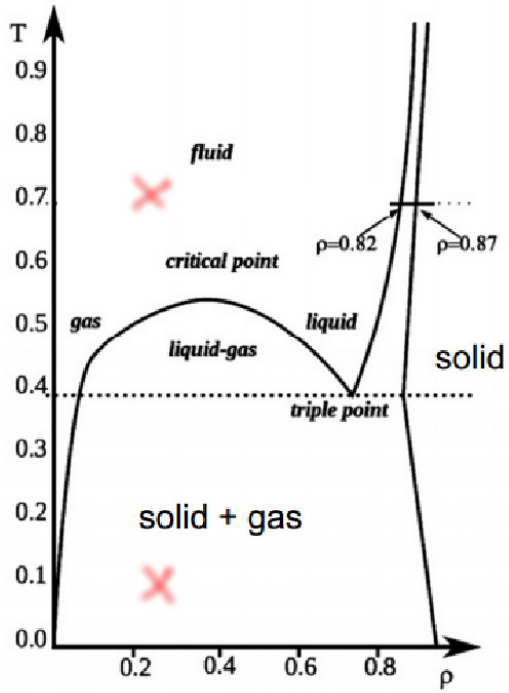
Wiecej gazu!

November 28, 2014

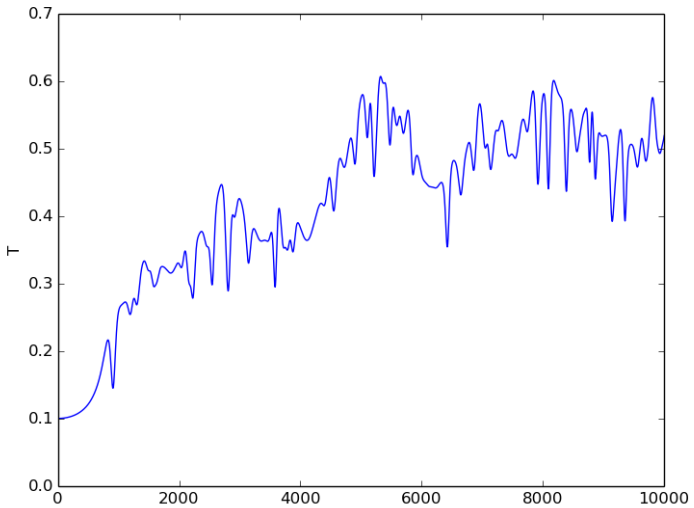
Diagram fazowy

- $T = const$
- $\rho = \frac{N}{S}\sigma^2$
- $T = 0.1,\ \rho = 0.25$ - solid
- $T = 0.7,\ \rho = 0.25$ - fluid

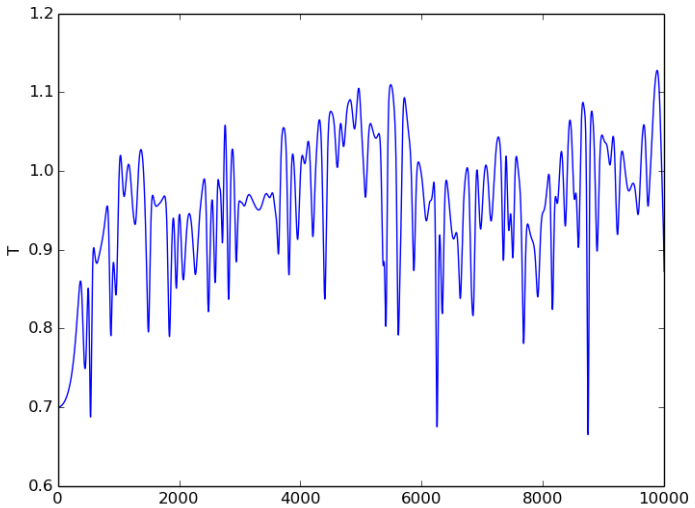


Bez termostatu :(

$T = 0.1,\ \rho = 0.25$



$T = 0.7,\ \rho = 0.25$



Potrzebujemy termostatu!

Budujemy termostat z zabka

- Wykonaj pol kroku (bez sily oporu)

$$v^u(t) = v(t - \delta t/2) + (\frac{F(t)}{m})\frac{\delta t}{2}$$

- Oblicz chwilowa temperature

$$T(t) = \frac{2}{3Nk_b} < K^u >$$

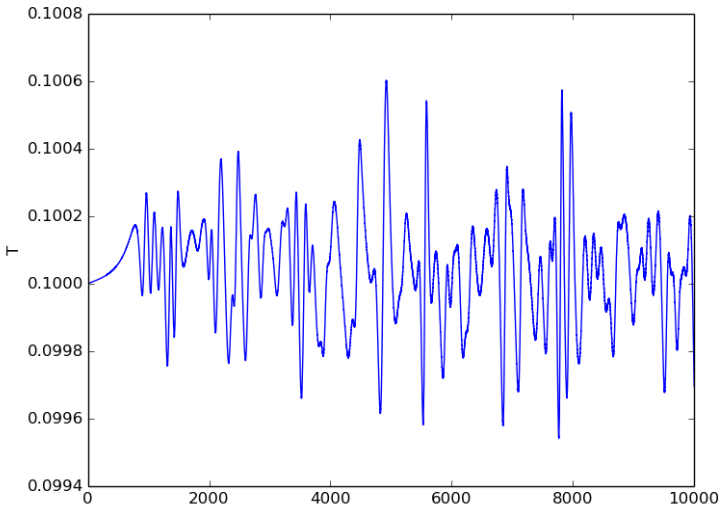
- Oblicz wspolczynnik $\eta = \sqrt{\frac{T_{ext}}{T}}$
- Dokoncz krok

$$v(t + \delta t/2) = (2\eta - 1)v(t - \delta t/2) + \eta(\frac{F(t)}{m})\Delta t$$

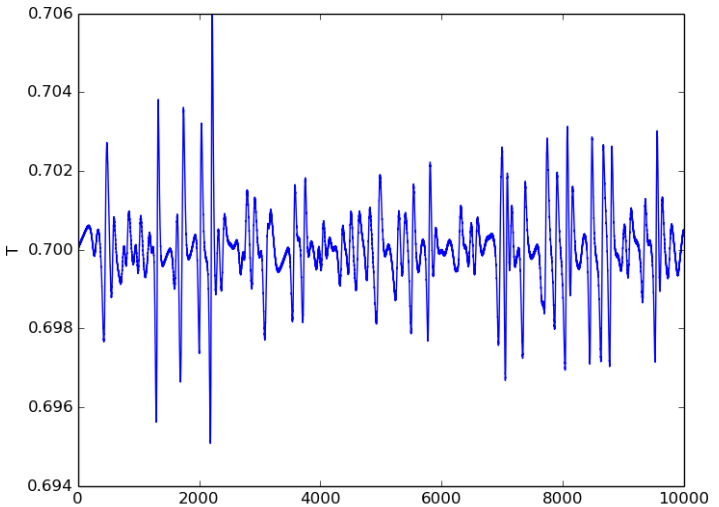
$$r(t + \delta t) = r(t) + v(t + \delta t/2)\Delta t$$

Z termostatem :)

$T = 0.1,\ \rho = 0.25$

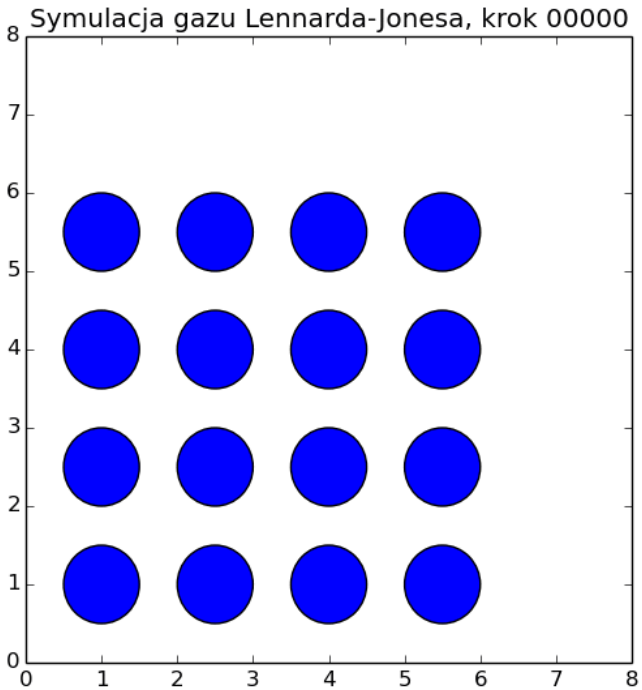


$T = 0.7,\ \rho = 0.25$

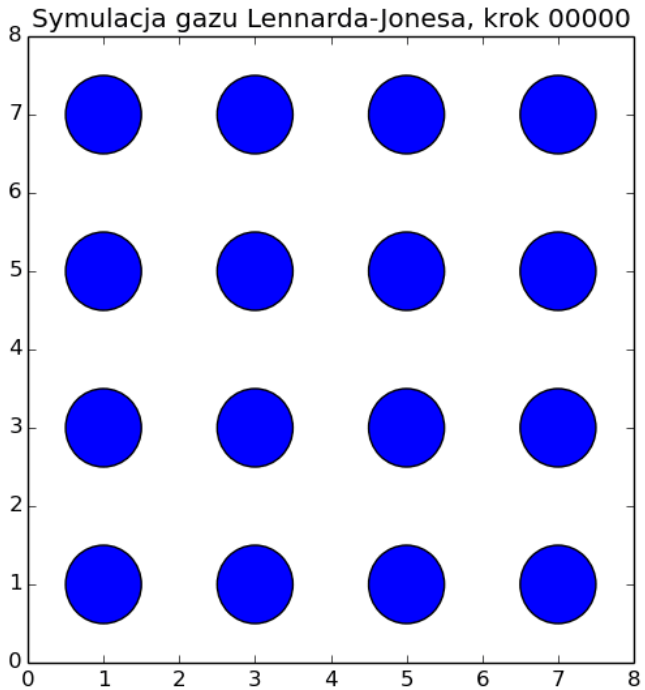


Z termostatem :)

$T = 0.1,\ \rho = 0.25$

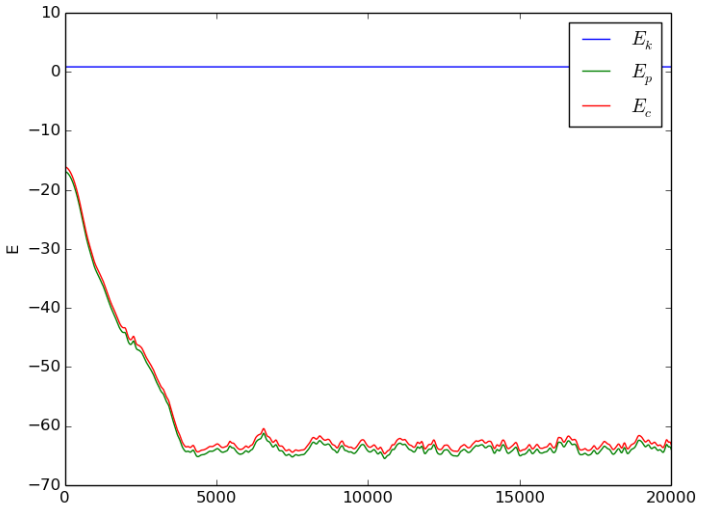


$T = 0.7,\ \rho = 0.25$



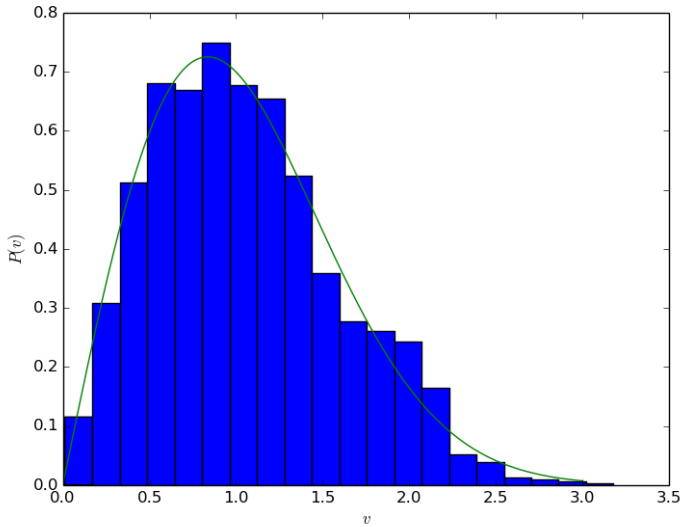
Dochodzenie do rownowagi

- Obliczamy $E_k(t)$ na podstawie predkosci czastek
- Obliczamy $E_p(t)$ na podstawie potencjalu Lennarda-Jonesa
- $E_c(t) = E_p(t) + E_k(t)$
- Szukamy takiego t gdzie E_c jest z grubsza stale - krok 5000



Rozklad predkosci

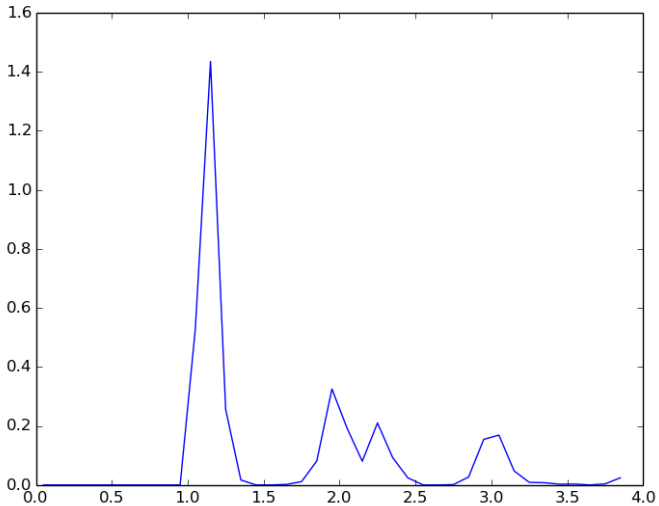
- Bierzemy wszystkie v i tworzymy znormalizowany histogram
- Im wicej probek tym lepiej (tutaj 3000 klatek)
- Nanosimy dwuwymiarowy rozklad Maxwella $P(v) = \frac{mv}{kT} e^{-\frac{mv^2}{2kT}}$



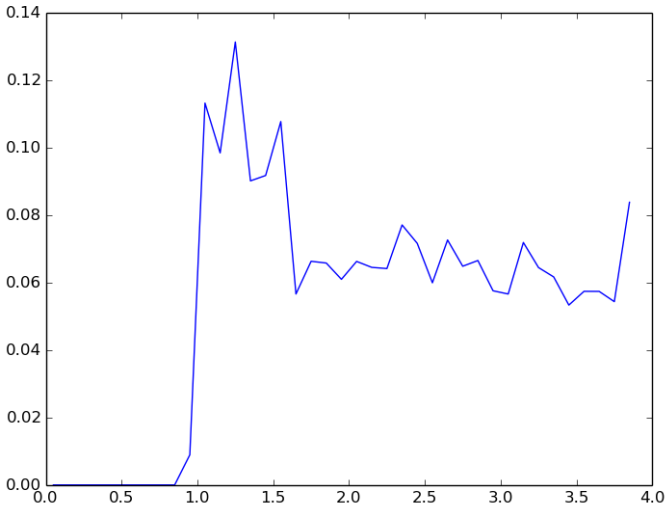
Radialna funkcja rozkladu

- Bierzemy wszystkie r_{ij} i tworzymy znormalizowany histogram
- Im wiecej probek tym lepiej (tutaj 3000 klatek) - u mnie dla wyroznionej czastki
- Zamiast tradycyjnego histogramu - odpowiadajace mu linie

$T = 0.1,\ \rho = 0.25$



$T = 0.7,\ \rho = 0.25$



End of file :)

Dziekuje za uwage