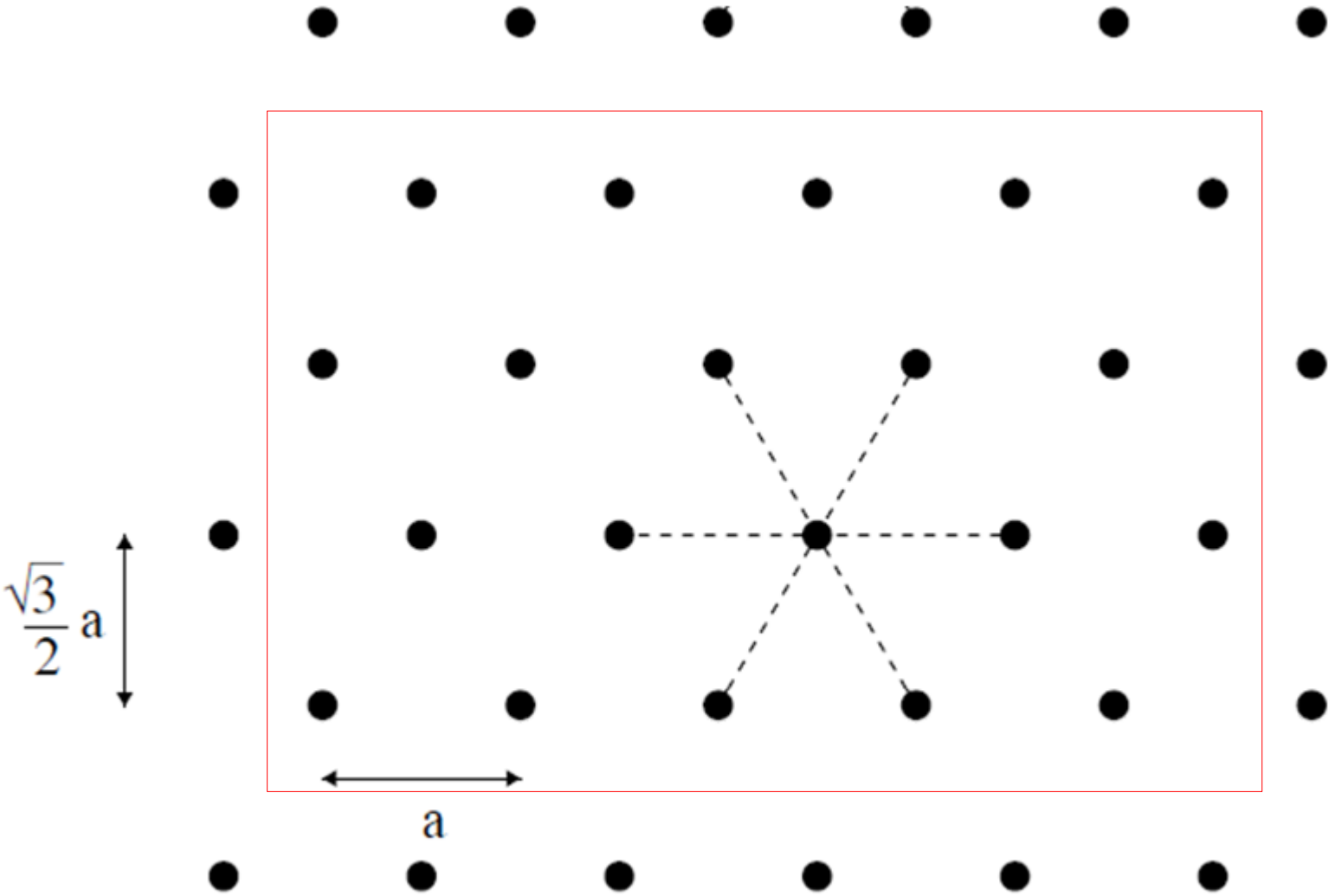
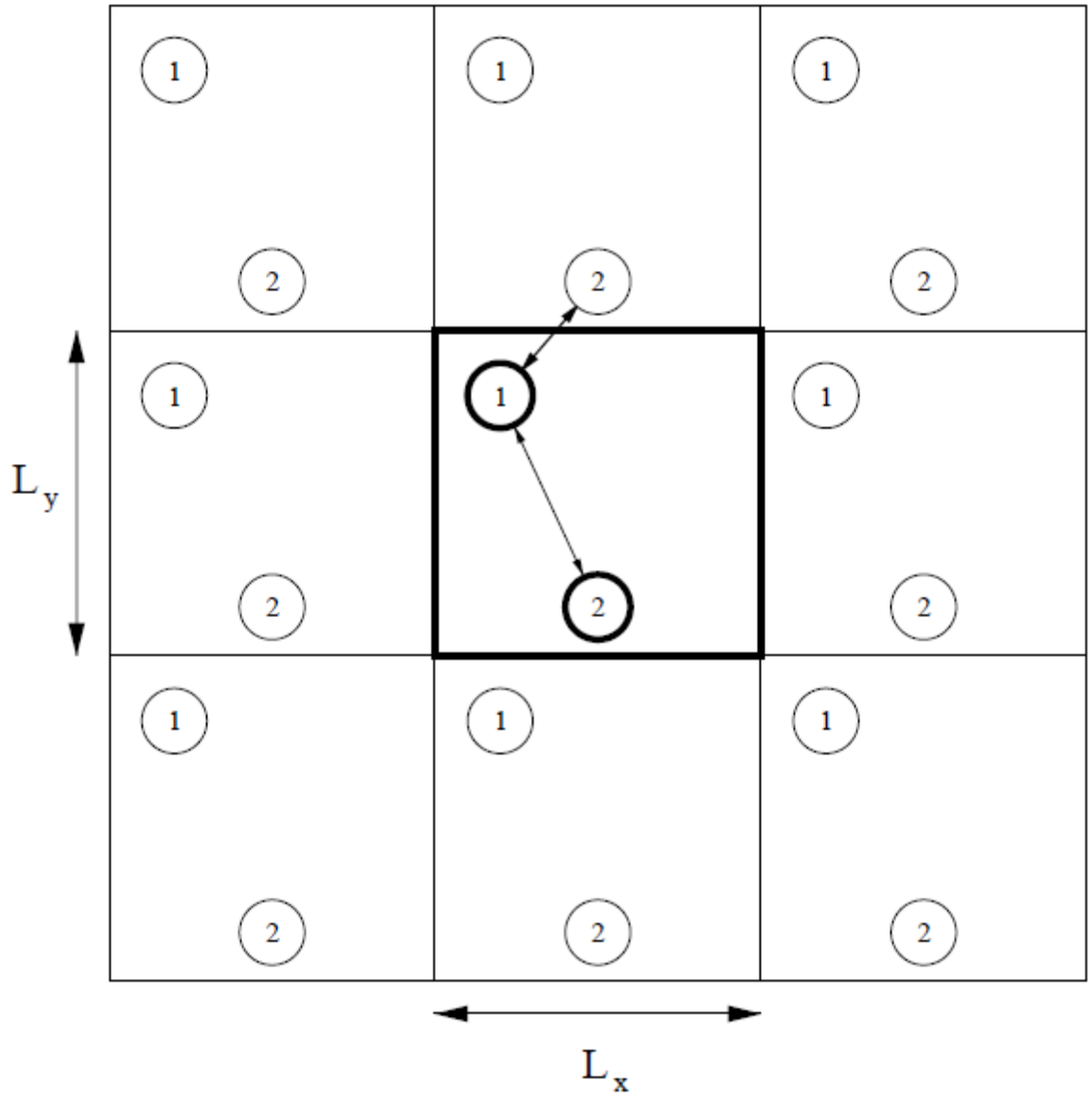
Rešetka u periodičnom području $L_x \times L_y$

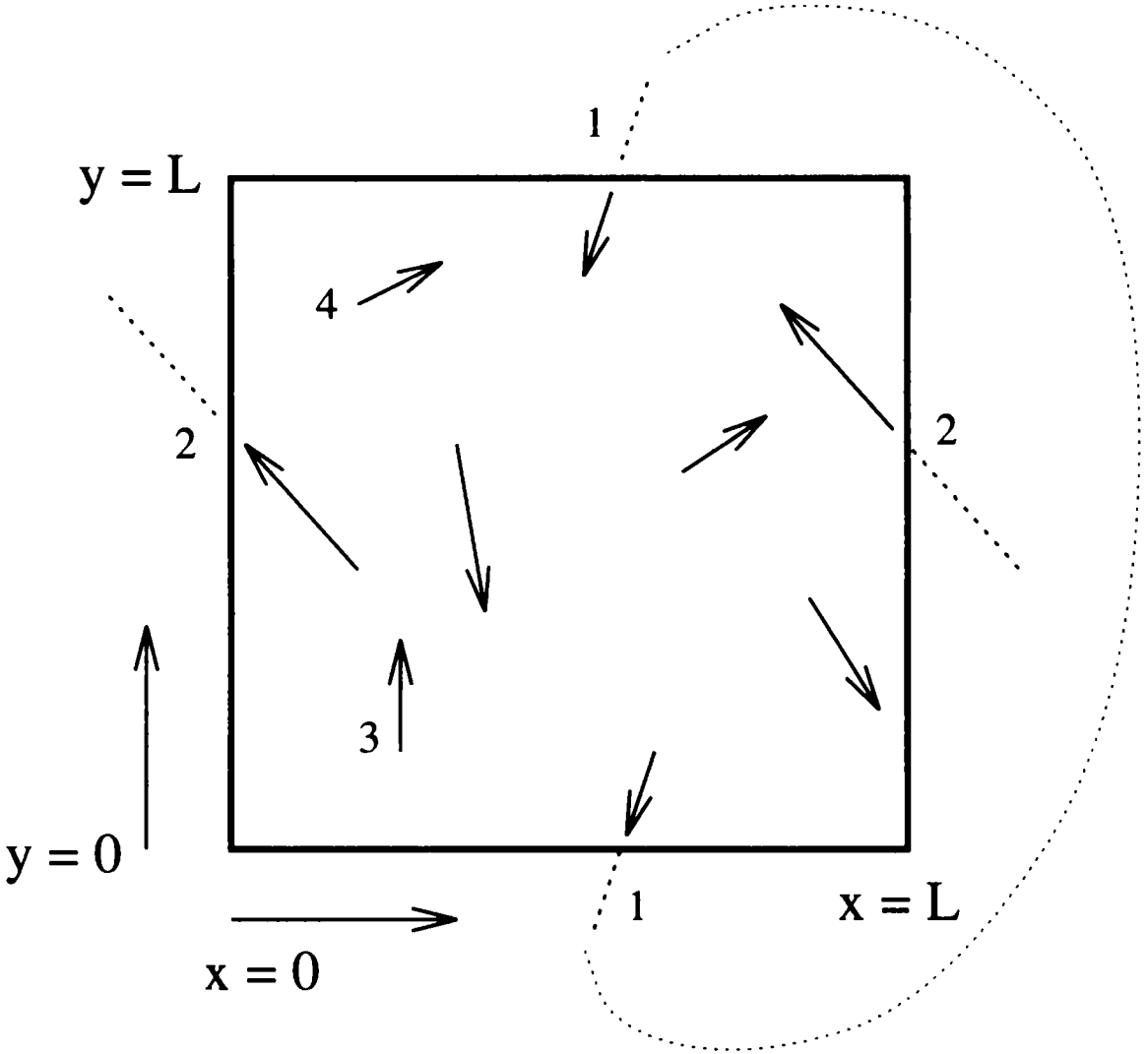
xy_trokutasta.c



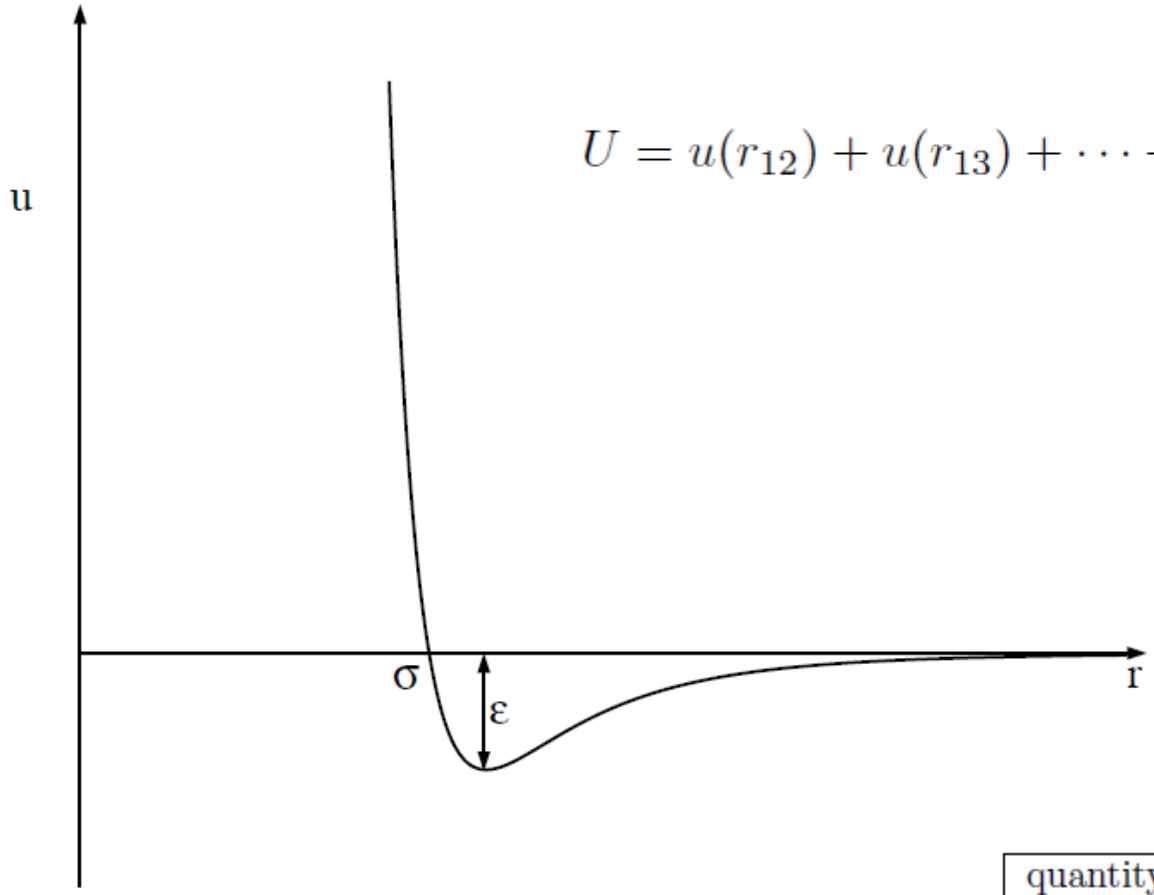
Lokalna gustoća – aproksimacija minimalnih slika



Periodični rubni uvjeti – probni pomaci



Lennard-Jones potencijalna energija (interakcija parova)



$$U = u(r_{12}) + u(r_{13}) + \cdots + u(r_{23}) + \cdots = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} u(r_{ij})$$

$$u(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

Sila

$$\mathbf{f}(r) = -\nabla u(r) = \frac{24\epsilon}{r} \left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \hat{\mathbf{r}}$$

Tlak

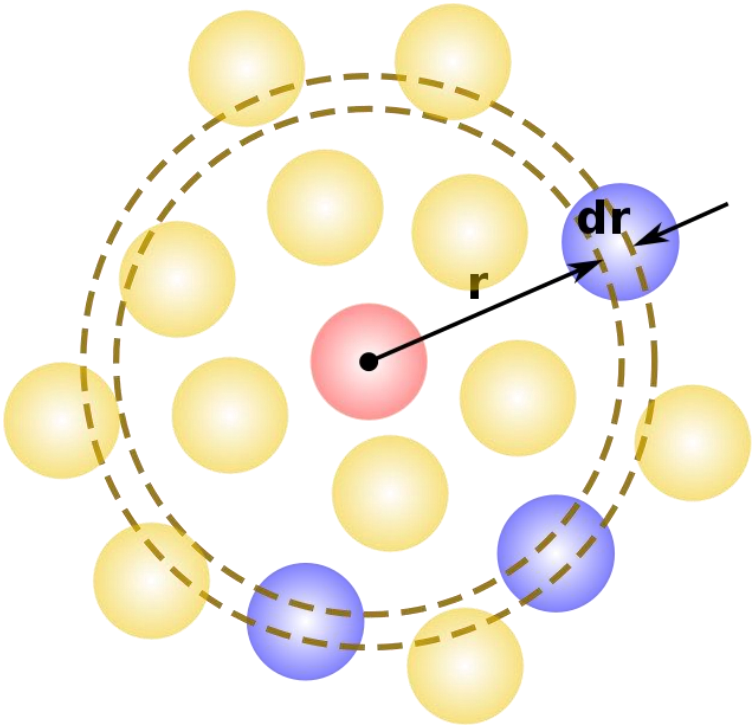
$$P(t) = \frac{N}{V} kT(t) + \frac{1}{dV} \sum_{i<j} \mathbf{r}_{ij}(t) \cdot \mathbf{F}_{ij}(t)$$

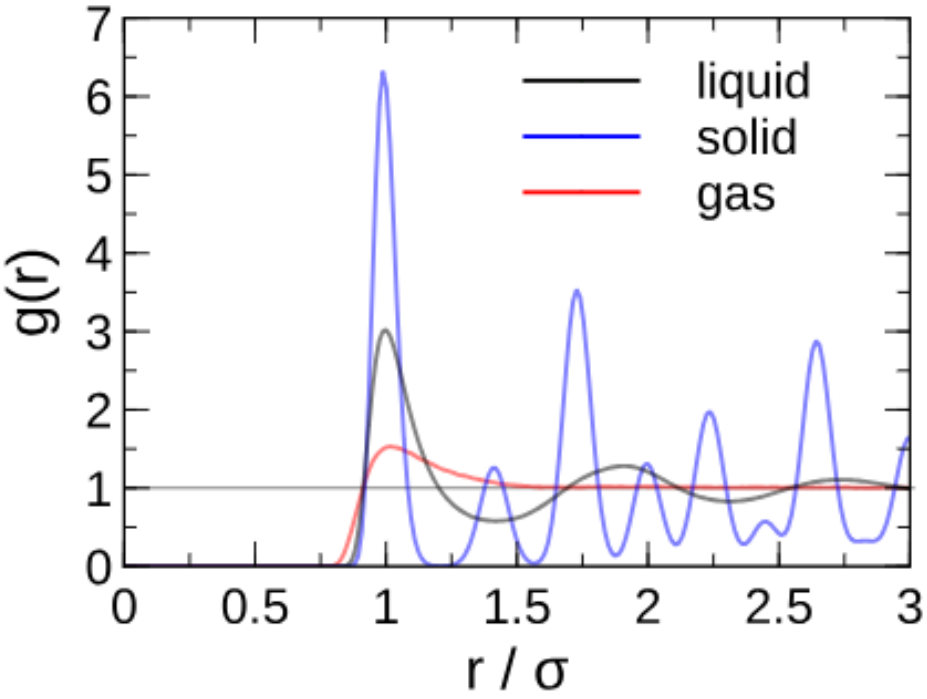
quantity	unit	value for argon
length	σ	$3.4 \times 10^{-10}\,\mathrm{m}$
energy	ϵ	$1.65 \times 10^{-21}\,\mathrm{J}$
mass	m	$6.69 \times 10^{-26}\,\mathrm{kg}$
time	$\sigma(m/\epsilon)^{1/2}$	$2.17 \times 10^{-12}\,\mathrm{s}$
velocity	$(\epsilon/m)^{1/2}$	$1.57 \times 10^{2}\,\mathrm{m/s}$
force	ϵ/σ	$4.85 \times 10^{-12}\,\mathrm{N}$
pressure	ϵ/σ^2	$1.43 \times 10^{-2}\,\mathrm{N \cdot m^{-1}}$
temperature	ϵ/k	$120\,\mathrm{K}$

Radijalna distribucijska funkcija (za *bulk*)

$$\rho(r) = \rho^{bulk} g(r)$$

$$g(\mathbf{r}) = \frac{1}{\rho}\left\langle \sum_{i \neq 0} \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle = V \frac{N-1}{N} \left\langle \delta(\mathbf{r} - \mathbf{r}_1) \right\rangle$$

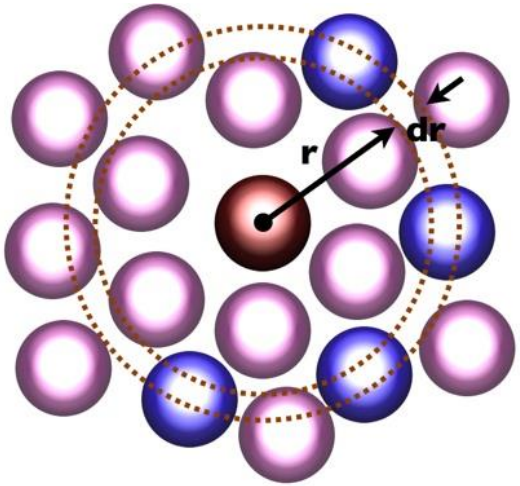


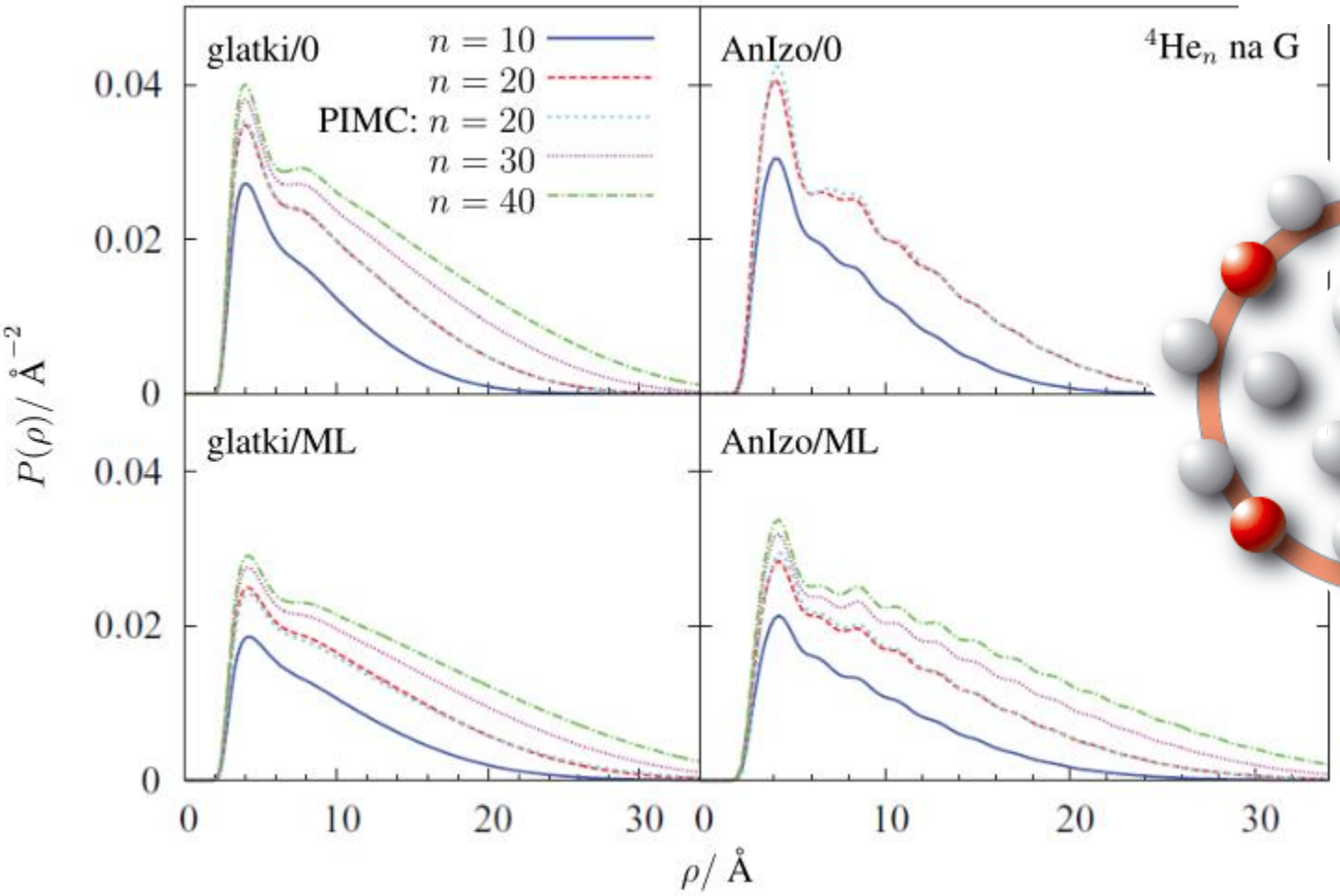


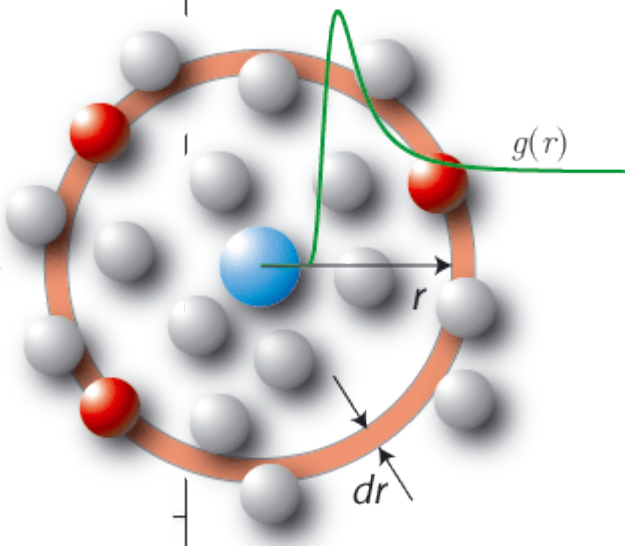
https://commons.wikimedia.org/wiki/File:Simulated_Radial_Distribution_Functions_for_Solid,_Liquid,_and_Gaseous_Argon.svg

Rzdioba međučestičnih udaljenosti

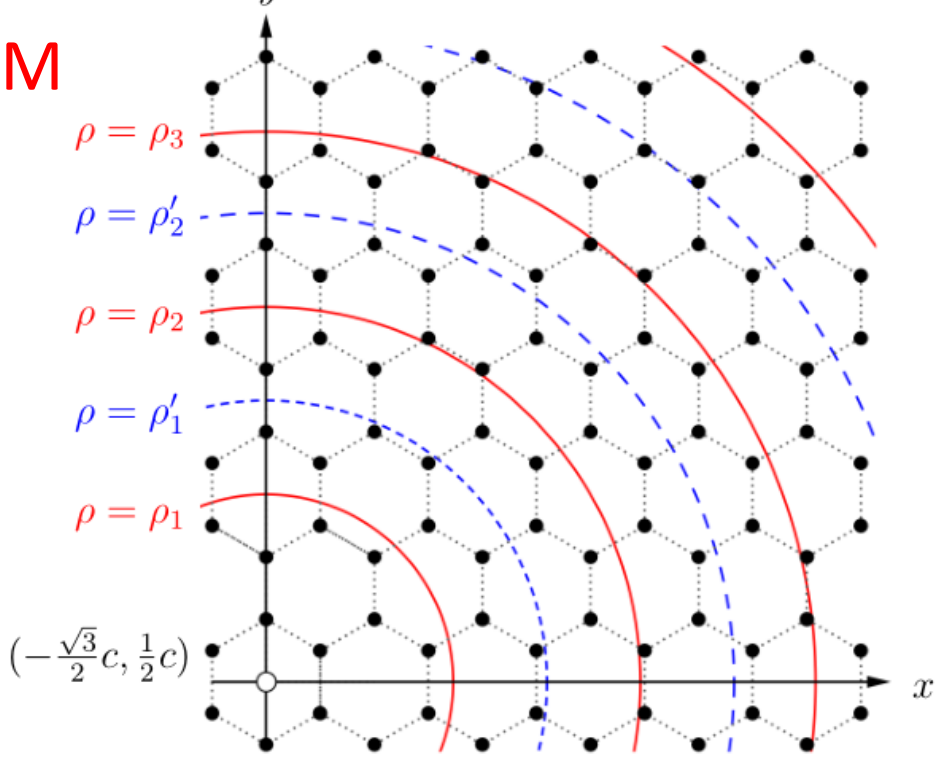
Primjeri za konačni sustav
- normu obično postavljamo na 1 ili N



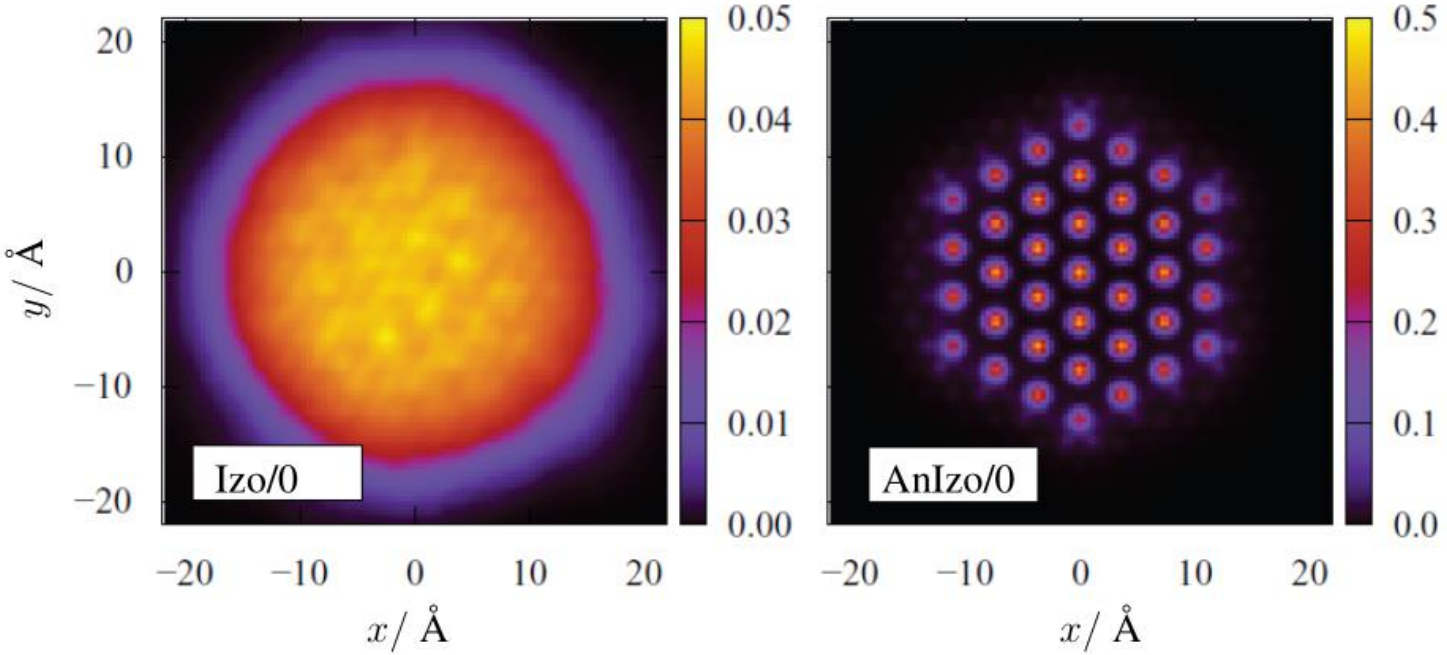




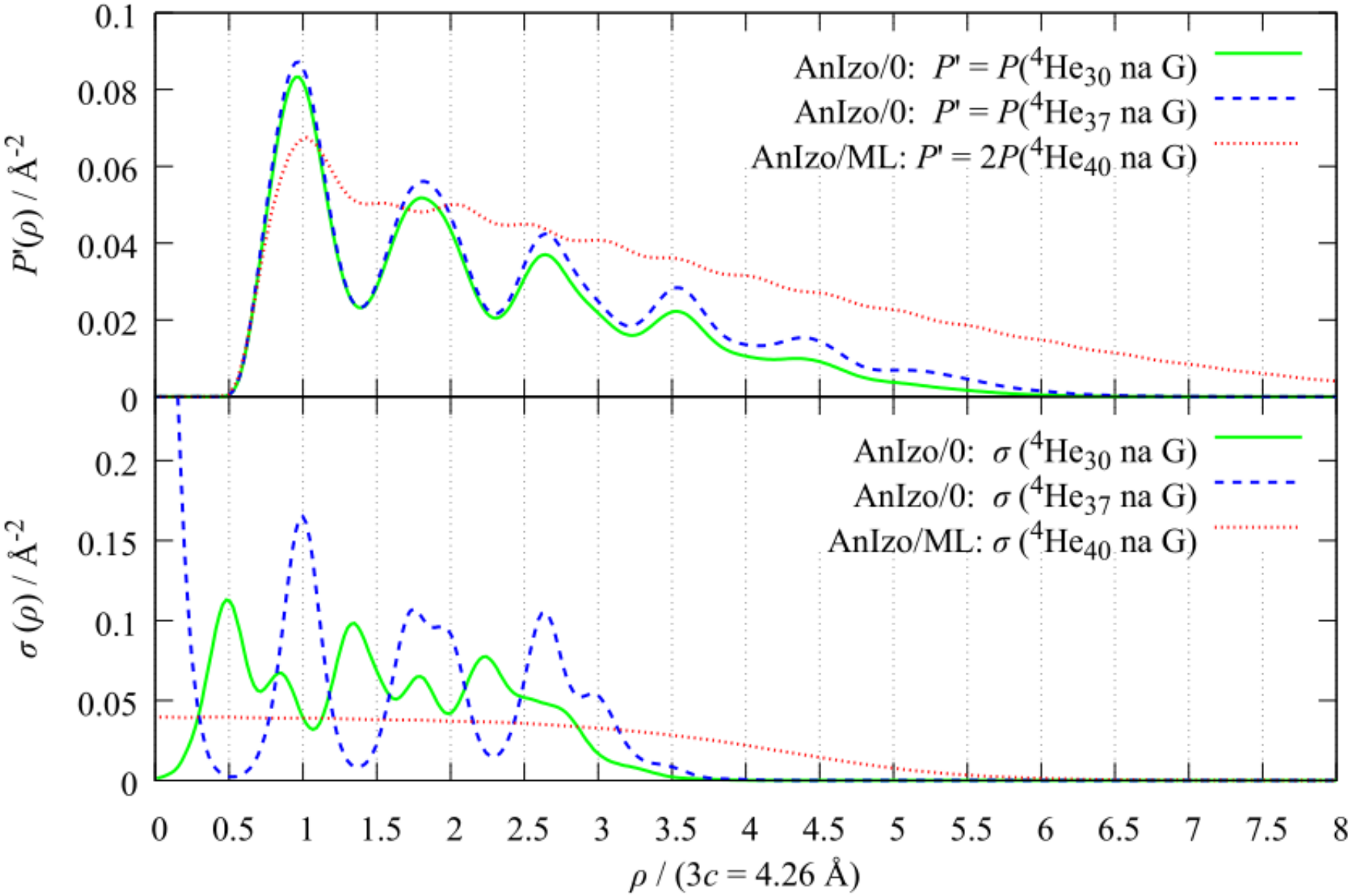
Primjeri gustoće u odnosu na CM



$^4He_{37}$



Primjeri razdioba međučestičnih udaljenosti i gustoće u odnosu na CM



Z11:

Unutar mape 11 Klasicni sustavi priložen je klasicni_sustav.c kojeg treba dovršiti prema uputama – zadacima (ZAD). Simulirajte sustav koji nalikuje krutini (podesite parametre da bude takav). Uzmite šire područje od trenutno postavljenoga…

- Pokrenite i prilagodite xy_trokutasta.c za slaganje početnih položaja u trokutastu rešetku.
- Testirajte duljinu simulacija promatrajući kako se ukupna srednja energija i njen prosjek bloka ponašaju tijekom simulacije (priložite graf).
- Grafički prikažite g(r).
- Priložite kodove skripte i graf.