Projeto 6 - Dinâmica molecular

Jefter Santiago (12559016)

Entrega: 01/06/2024

1 Introdução

Potencial de Lennard-Jonnes

$$\mathcal{U}(\vec{r}) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^1 2 - \left(\frac{\sigma}{r}\right)^6 \right] \tag{1}$$

Com $m = 1$:

$$a_j^x = \sum_{j=1}^{N} \sum_{\ell \neq j}^{N} F_{j,\ell} \cos(\theta_{j,\ell})$$

$$a_j^y = \sum_{j=1}^{N} \sum_{\ell \neq j}^{N} F_{j,\ell} \sin(\theta_{j,\ell})$$

- Cálculo das componentes de aceleração
assim temos uma forma para calcular os senos e cossenos de $\theta_{j,\ell}$

$$\sin(\theta_{j,\ell}) = \frac{dy_{j,\ell}}{d_{j,\ell}}$$

$$\cos(\theta_{j,\ell}) = \frac{dx_{j,\ell}}{d_{j,\ell}}$$

1.1 Detalhes de implementação

2 Tarefa A

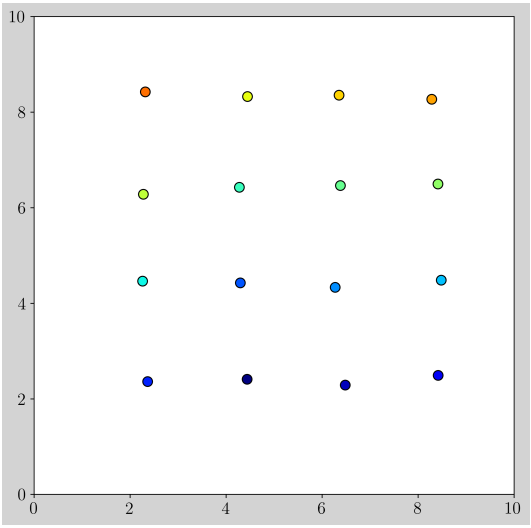

Figura 1: Posições iniciais das partículas.

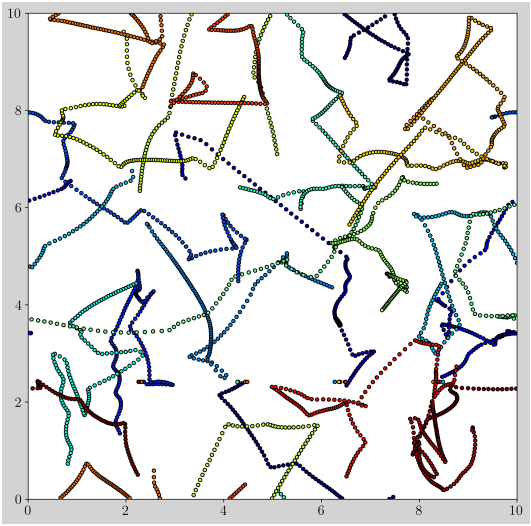

Figura 2: Coordenadas das partículas projetadas à cada $3\Delta t$.

3 Tarefa B

4 Tarefa C

5 Tarefa D

6 Tarefa E

7 Tarefa F

Referências

[1] N.J. Giordano. *Computational Physics*. Prentice Hall, 2006. ISBN: 9780133677232.

[2] Wikipedia contributors. *Periodic boundary conditions — Wikipedia, The Free Encyclopedia*. [Online; accessed 20-June-2024]. 2024. URL: https://en.wikipedia.org/w/index.php?title=Periodic_boundary_conditions&oldid=1229053854.