Exercise 06

Fixed time frame

1. **Compression of a Single Cell using the Subcellular Element Model in 2D.**
In the Subcellular Element model, a cell is represented by N computational Lagrangian particles. The particle-particle interaction is modelled by a Morse potential:

$$V(r) = u_0 \exp\left[2\rho\left(1 - \frac{r^2}{r_{\mathrm{eq}}^2}\right)\right] - 2u_0 \exp\left[\rho\left(1 - \frac{r^2}{r_{\mathrm{eq}}^2}\right)\right] \tag{1}$$

where r is the distance between two particles, r_{eq} the equilibrium distance, ρ a scaling factor, and u_0 an energy scale. The equilibrium distance r_{eq} is given as:

$$r_{\mathrm{eq}}(N) = 2R_{\mathrm{cell}}\left(\frac{p_2}{N}\right)^{1/2} \tag{2}$$

with $p_2 = \pi/(2\sqrt{3})$ being the packing density of disks in 2D, and R_{cell} being the radius of the cell to be simulated.

The equation of motion is given by:

Force : - the gradient of the potential.

Velocity

$$\eta\partial_t \boldsymbol{y}_\alpha = \xi_\alpha \boxed{- \nabla_\alpha \sum_{\beta \neq \alpha} V\left(\|\boldsymbol{y}_\alpha - \boldsymbol{y}_\beta\|\right)} \tag{3}$$

with $\eta = \eta_0/N$ being the scaled viscous damping constant, ξ_α Gaussian noise with zero mean and standard deviation $2\Delta\eta^2$ (where Δ is a noise amplitude) and $\boldsymbol{y}_\alpha$ the position vector of particle α.

For a detailed discussion of the equations and parameters, please read [1]. The goal of this exercise is to implement a 2D Subcellular Element Model in a programming or scripting language of your choice.

i) Plot the potential $v(r)$ given in Equation (1). Use the values from the appendix of [1] for the parameters η_0, u_0, Δ, ρ, R_{cell}. Can you spot the equilibrium distance r_{eq} in your plot?

ii) From the potential, derive the force acting between two particles. Plot it as a function of the distance r, analogous to i).

iii) Initialize $N = 36$ elements hexagonally at equilibrium distance, with $\sqrt{N}$ elements in each direction.

iv) Compute the forces acting on each particle. Do you have to compute the force between distant pairs of particles? Truncated
why not ? Too small to be included

v) Discretize Equation (3) with the explicit forward Euler scheme with a time step of 0.01 s. Simple time integration

vi) Repeat steps iv) and i) iteratively. Simulate a time period of 10 s in this way.

The core of the model is set up now, and we want to study the response of the cell when being compressed between two walls. Therefore:

vii) Define a stationary (not moving) bottom wall. Use a Hookean spring with force constant $k = 0.01\,\mathrm{N/m}$ to push back penetrating particles.

viii) Define a moving top wall. The wall is uniformly compressing the cell by one half of the cell radius during the first 1 s and then stops. Use the same force constant as in vii).

[1] Sandersius et al., Emergent cell and tissue dynamics from subcellular modeling of active biomechanical processes, Physical Biology 8, 045007 (2011)