# Building a Computational Model of Active Deformable Particles

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## Background

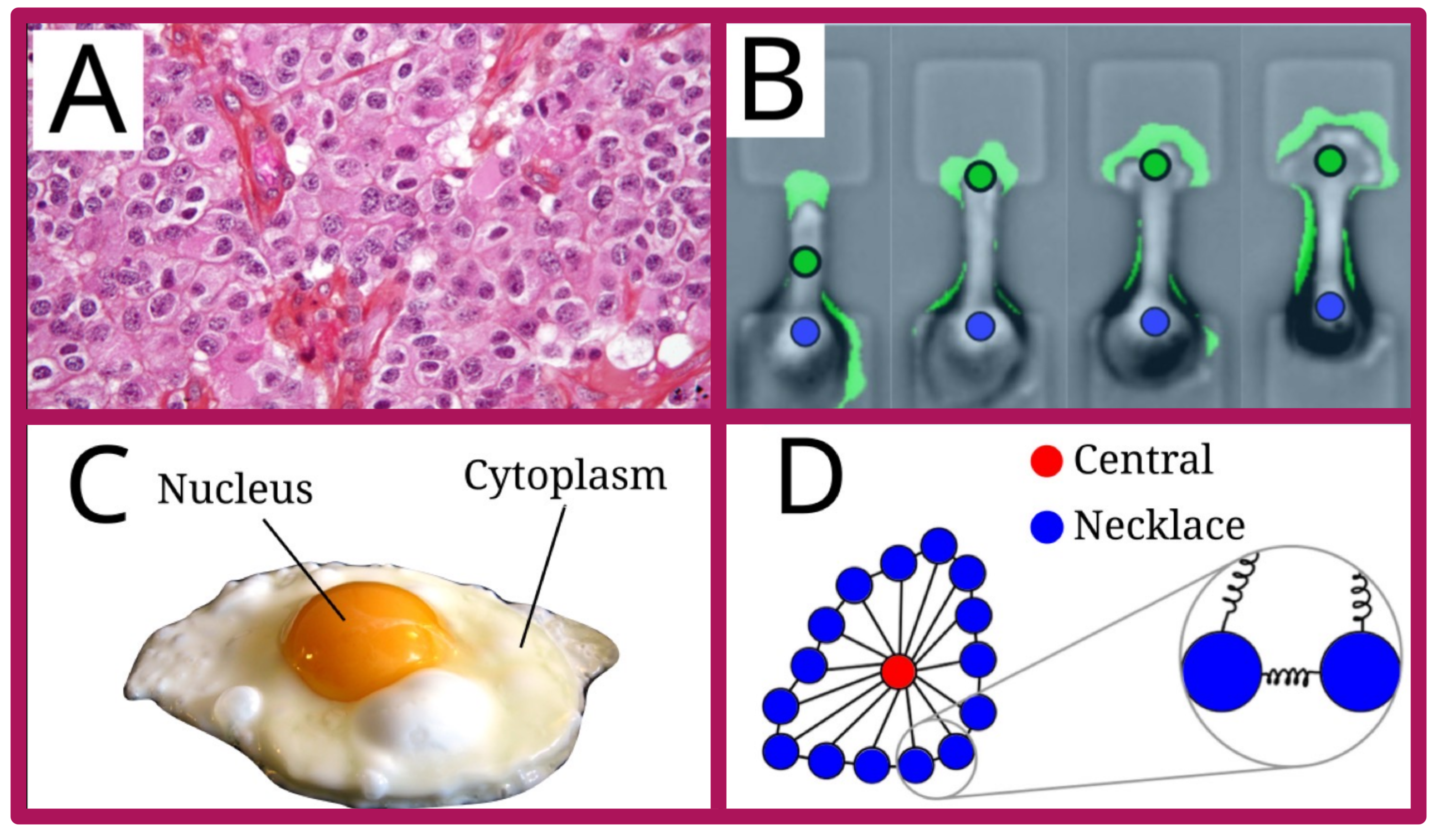


Fig 1. A) Micrograph of Oligodendroglioma – cc.by-SA3.owikipedia B) Cell migration in confined geometry, David B. Bruckner et al, Physical Review X 12 (2022), 10.1103/physrevx.12.031041. C) Fried egg with representations of nucleus and cytoplasm. D) 'Bead and Spring' schematic of our model.

- Cells are the workhorses of biology, as they perform many functions in various environmental conditions.
- Many cells (E.g., mammalian cells) exist in dense environments (Fig.1.A) and have a central nucleus surrounded by a cytoplasm.
- Also, experiments are being done to prove how such cells move in geometries (Fig.1.B).
- Currently there is a lack of unification between observations of deformable cells which a minimal modelling approach can provide.

## Deformable 'Fried-Egg' Particle Model

- Particles in this model do not overlap due to interaction potential.
- Central bead can be enlarged to more accurately represent a nucleus.
- Parameters of this model include internal bond strength (k), necklace bond strength ($k_n$), internal bond length (l), necklace bond length ($l_n$)

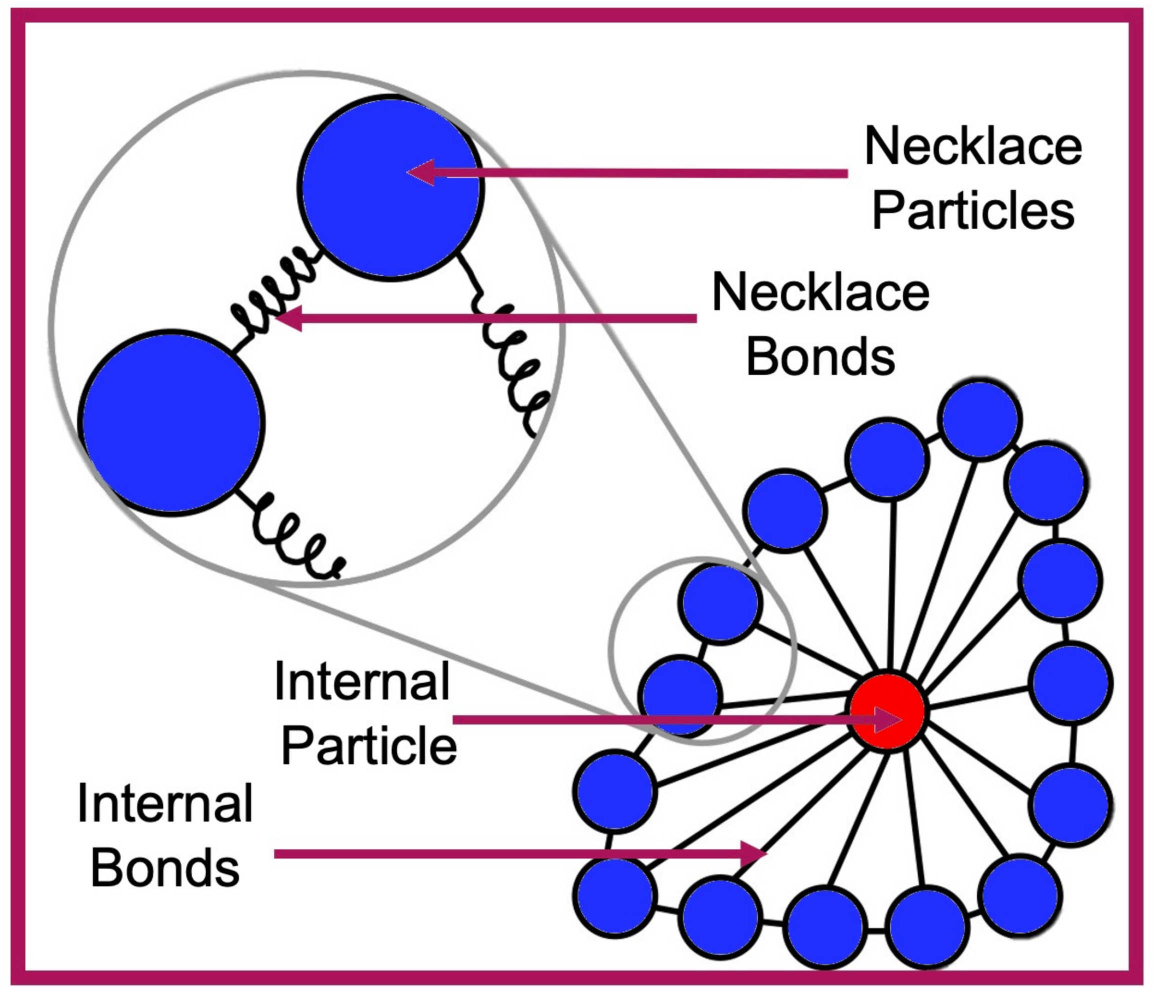


Fig 2. Labelled schematic of deformable particle.

## Passive Case

- Passive equation of motion:

$$\frac{d\vec{r}_i}{dt} = \underbrace{-\mu\vec{\nabla}_i U(\{\vec{r}\})}_{\text{The Potential}} + \underbrace{\sqrt{2D}\vec{\eta}_i}_{\text{Thermal Noise}}$$

- Here, the thermal noise component is the 'randomness' responsible for Brownian motion, the potential refers to the interaction energy.
- As we are building a new model, we first explore the passive (non-active) case.
- In Fig.3, you can see how parameters k and $k_n$ impact the cell membrane.

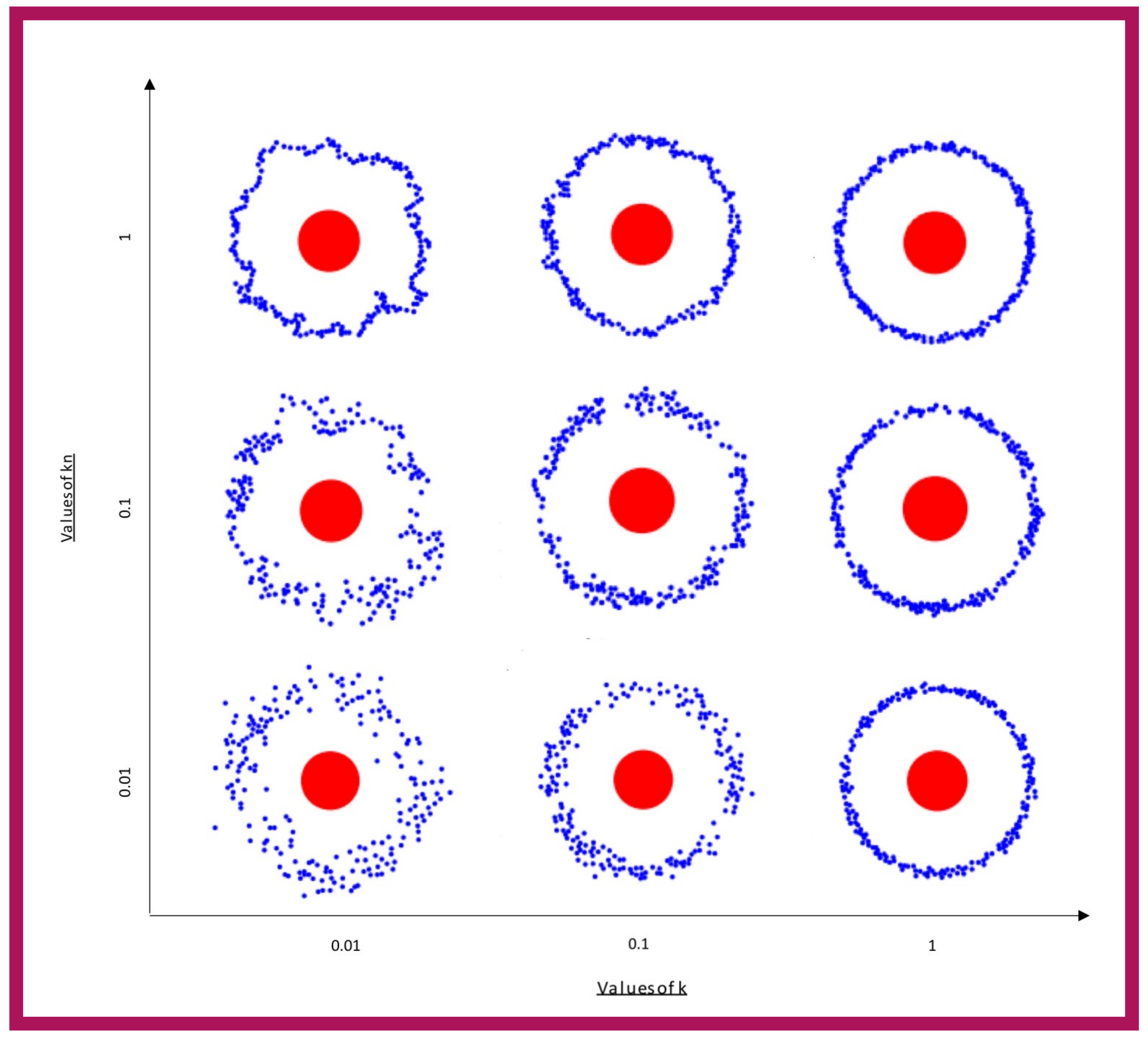


Fig 3. Phase diagram of $k_n$ by k.

## Active Case

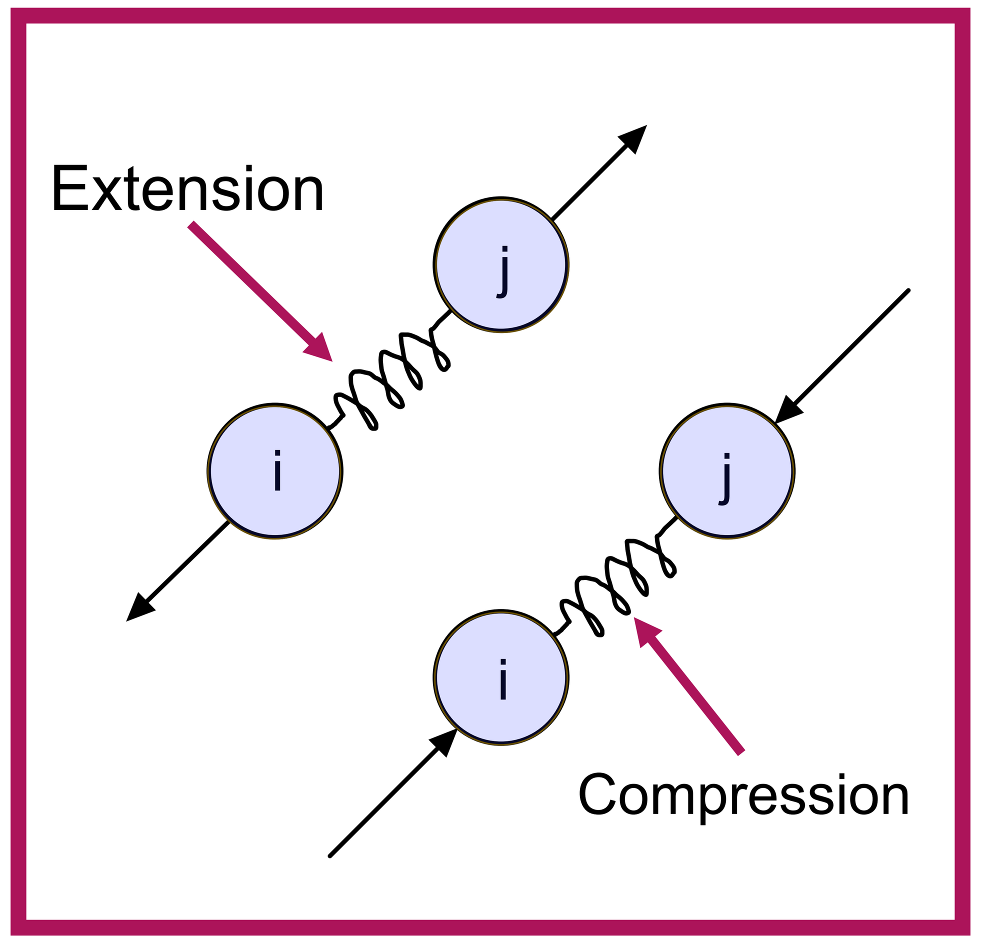


Fig 4. Active bonds

- To activate passive model, we considered adding self propulsion term to the dynamics of the necklace particles. Active equation of motion:

$$\frac{d\vec{r}_i}{dt} = \underbrace{-\mu\vec{\nabla}_i U(\{\vec{r}\})}_{\text{The Potential}} + \underbrace{\sqrt{2D}\vec{\eta}_i}_{\text{Thermal Noise}} + \underbrace{\vec{v}_i}_{\text{Self Propulsion}}$$

- We also developed the theory to a new way of implementing active bonds. Forces are calculated along the direction of the bonds (Fig.4):

$$\vec{f}_i = f(-1)^{\gamma_{ij}}$$

$$\vec{f}_j = -\hat{f}_i$$

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