An agent-based model for cell collective dynamics

L. NAVORET [1] R. SUBLET [1] M. SZOPOS[2]

[1]IRMA, Université de Strasbourg

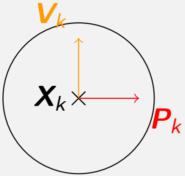
[2]MAP5, Université Paris Cité

From Cells to Tissues Lake Como School:
Monday, June 10, 2024

Model

There are N cells that evolve in a $2D$ space Ω. Each cell has a position $\boldsymbol{X}_k \in \mathbb{R}^2$, a velocity $\boldsymbol{V}_k \in \mathbb{R}^2$, a polarity $\boldsymbol{P}_k \in \mathbb{S}^1$, which describes the preferred direction.

- Positions: $\boldsymbol{X} = (\boldsymbol{X}_k)_k \in \mathbb{R}^{2N}$
- Velocities: $\boldsymbol{V} = (\boldsymbol{V}_k)_k \in \mathbb{R}^{2N}$
- Polarities: $\boldsymbol{P} = (\boldsymbol{P}_k)_k \in (\mathbb{S}^1)^N$



Model ingredient:

- Vicsek-type interaction [Vicsek et al. 1995]
- Contact forces (hard sphere) [Maury and Venel 2011]
- Soft attraction-repulsion forces [Beatrici et al. 2023]

Adapted from a model validated against experimental data [Vecchio et al. 2024].

Equations on $\boldsymbol{X}$, $\boldsymbol{V}$ and $\boldsymbol{P}$

Position dynamics

$$\frac{d\boldsymbol{X}_k}{dt} = \boldsymbol{V}_k.$$

Velocities dynamics

$$\boldsymbol{V} = \mathrm{Proj}_{\mathcal{C}_{\boldsymbol{X}}}(c\boldsymbol{P} + \gamma \boldsymbol{F}(\boldsymbol{X}))$$

- Hard sphere repulsion: projection onto the set of admissible velocities $\mathcal{C}_{\boldsymbol{X}}$
- Soft attraction-repulsion force $\boldsymbol{F}$ of stiffness κ

Polarity dynamics

$$d\boldsymbol{P}_k = \mathrm{Proj}_{\boldsymbol{P}_k^{\perp}}\left(\mu(\overline{\boldsymbol{P}}_k - \boldsymbol{P}_k)dt + \delta\left(\frac{\boldsymbol{V}_k}{\|\boldsymbol{V}_k\|} - \boldsymbol{P}_k\right)dt + \sqrt{2D}(dB_t)_k\right)$$

Equations on $\boldsymbol{X}$, $\boldsymbol{V}$ and $\boldsymbol{P}$

Position dynamics

$$\frac{d\boldsymbol{X}_k}{dt} = \boldsymbol{V}_k.$$

Velocities dynamics

$$\boldsymbol{V} = \mathrm{Proj}_{\mathcal{C}_{\boldsymbol{X}}}(c\boldsymbol{P} + \gamma \boldsymbol{F}(\boldsymbol{X}))$$

Polarity dynamics

$$d\boldsymbol{P}_k = \mathrm{Proj}_{\boldsymbol{P}_k^{\perp}} \left(\mu(\overline{\boldsymbol{P}}_k - \boldsymbol{P}_k)dt + \delta \left(\frac{\boldsymbol{V}_k}{\|\boldsymbol{V}_k\|} - \boldsymbol{P}_k \right) dt + \sqrt{2D}(dB_t)_k \right)$$

- Alignment to the local averaged polarity $\overline{\boldsymbol{P}}_k$ (Viscek-type interaction)
- Relaxation to the velocity direction $\frac{\boldsymbol{V}_k}{\|\boldsymbol{V}_k\|}$
- Gaussian white noise: $(dB_t)_k$
- Projection to keep the polarity of norm 1

Discretization: let Δt be our time step

The update of $\boldsymbol{X}^n$ is:

$$\boldsymbol{X}_k^{n+1} = \boldsymbol{X}_k^n + \boldsymbol{V}_k^{n+1}\Delta t$$

The update of $\boldsymbol{V}^n$ is made by resolving the following optimization problem with an Uzawa algorithm, [Maury and Venel 2011]

$$\boldsymbol{V}^{n+1} = \underset{\boldsymbol{V}\in\mathcal{C}^{\Delta t}_{\boldsymbol{X}^n}}{\operatorname{argmin}} \frac{1}{2}\left\|\boldsymbol{V} - c\boldsymbol{P}^{n+1} - \gamma \mathrm{F}(\boldsymbol{X}^n)\right\|^2$$

The update of $\boldsymbol{P}^n$ is made by discretization of the angle of $\boldsymbol{P}_k^{n+1} = (\cos(\theta_k^{n+1}), \sin(\theta_k^{n+1}))$ [Motsch and Navoret 2011]:

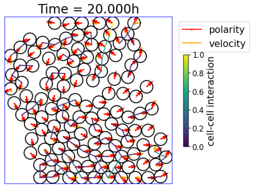
$$\theta_k^{n+1} = \theta_k^n + 2\left(\theta[\boldsymbol{Q}_k^n] - \theta_k^n\right) + \sqrt{2D\Delta t}\,\xi_k^n$$

- $\boldsymbol{Q}_k^n = \boldsymbol{P}_k^n + \frac{\Delta t}{2}\left(\mu\left(\overline{\boldsymbol{P}}_k^n - \boldsymbol{P}_k^n\right) + \delta\left(\frac{\boldsymbol{V}_k^n}{\left\|\boldsymbol{V}_k^n\right\|} - \boldsymbol{P}_k^n\right)\right)$

Influence of the attraction-repulsion force

Default parameters:

$R_c = 9.5\mu\text{m}$
$\kappa = 10^4 \text{pN}\,\mu\text{m}^{-1}$
$\gamma = 10^{-5}\text{pN}^{-1}\text{h}^{-1}\mu\text{m}$

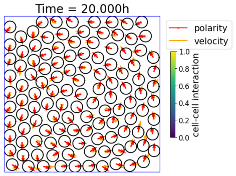


Observation:

- Rotating movement
- Lot of contacts

Strong attraction-repulsion:

$R_c = 9.5\mu\text{m}$
$\boxed{\kappa = 16.10^4 \text{pN}\,\mu\text{m}^{-1}}$
$\boxed{\gamma = 10^{-4}\text{pN}^{-1}\text{h}^{-1}\mu\text{m}}$

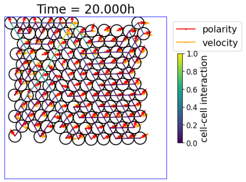


Observation:

- Better rotating movement
- Few contact

Strong attraction:

$\boxed{R_c = 7.5\mu\text{m}(= R_0)}$
$\boxed{\kappa = 16.10^4 \text{pN}\,\mu\text{m}^{-1}}$
$\boxed{\gamma = 10^{-4}\text{pN}^{-1}\text{h}^{-1}\mu\text{m}}$



Observation:

- Movement up-down
- Cells glued together

Thanks for your attention!

- Beatrici, C. et al. (2023). "Comparing individual-based models of collective cell motion in a benchmark flow geometry". In: *Soft Matter* 19.29, pp. 5583–5601.
- Maury, B. and J. Venel (2011). "A discrete contact model for crowd motion". In: *ESAIM Math. Model. Numer. Anal.* 45.1, pp. 145–168.
- Motsch, S. and L. Navoret (2011). "Numerical simulations of a nonconservative hyperbolic system with geometric constraints describing swarming behavior". In: *Multiscale Model. Simul.* 9.3, pp. 1253–1275.
- Vecchio, S. Lo et al. (2024). "Spontaneous rotations in epithelia as an interplay between cell polarity and boundaries". In: *Nature Physics*.
- Vicsek, T. et al. (1995). "Novel type of phase transition in a system of self-driven particles". In: *Phys. Rev. Lett.* 75.6, p. 1226.