## Molecular dynamics model on cell motion

To use molecular dynamics to simulate 2D cell motion, each cell is simulated as a list of connected atoms on the membrane. A timer ticks every 100ms and the atoms on the membrane move by a certain distance each time the timer ticks. The movement of these atoms on the membrane is governed by the Newton’s equation of motion. The forces applied to the atoms are from several sources and listed below.

### Cell membrane forces

There are three mechanisms regarding cell membrane forces.

The first membrane forces are elastic forces. The adjacent atoms on the membrane have an equilibrium distance and there is a restoring force when the distance deviates from the equilibrium. We can regard the atoms as being connected by springs.

Here denotes the elastic force between atom and . is the elastic constant. represents the distance between atom and whereas is the equilibrium length.

The second forces are damping forces. The adjacent atoms can have resistance forces according to their relative velocity. We can take it as a dashpot connecting adjacent atoms.

In the equation, denotes the damping force between atom and . is the damping constant. is the relative velocity between atom and .

The third mechanism is osmosis pressure. There is an equilibrium area (volume) for each cell and there will be forces on the atoms pointing inward or outward when the actual area is larger or smaller than the equilibrium area. This is the way we keep the area of the cell close to the equilibrium area.

The osmosis force is related to the difference of cell area and equilibrium area . is the osmosis constant.

### Cell interaction forces

The interaction between cells is caused by van der Waals force. We use Leonard-Jones potential to approximate this interaction. The Leonard-Jones forces keep the cells from overlapping with each other.

The Leonard Jones potential is related to the distance between an atom and an edge connecting two other atoms, . is a normalizing parameter on distance while is a constant on Leonard Jones potential.

### Active forces

Other than the passive responsive forces mentioned above, we also have active forces which drives the deformation of cells. These active forces are applied through adding additional springs to the membrane and are similar to the elastic forces. The first active force is the apical constriction of ventral mesodermal cells, which we simulate by adding springs with a shorter equilibrium length to the apical side of mesodermal cells. Such springs can have a compressive force to the apical edges, which simulates apical constriction of cells.

Here the apical constriction force is related to a shorter equilibrium length . is the elastic constant.

The second active force is the lateral compression, which we achieve by adding shorter springs to the lateral edges of ectoderm cells. The mechanism resembles the apical constriction force.

### Temporal distribution

In the model we can also change the time profile of the force to align with the actual case in real embryo. The constants can be tuned with respect to time. For example, the lateral compression happens after the apical constriction, so we modify with respect to time so that it becomes significant after a certain time point.

### Spatial distribution

The spatial distribution of forces can also be tuned along the edges of cells. The apical membrane of mesodermal cells has non-uniform constriction. Therefore, when applying apical constriction in the model, we add springs with different elastic constant to every edge of the cells.