Interacting particle system with mobility and demographic dynamics (as biological models)

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Abstract

Our objective is to combine the Langevin equation which describes the motion and interaction with the Gillespie algorithm which describes the demographic events. In this way, we will be able to study system of particles which interact with each other and/or with the environment and move, and furthermore these particles can reproduce or die. These models can be a first approach to study biological systems such as bacteria colonies or in tissue cells. Therefore, in order to study some cases in the future, we also want to include active particles[1], since many of these systems are self-propelled.

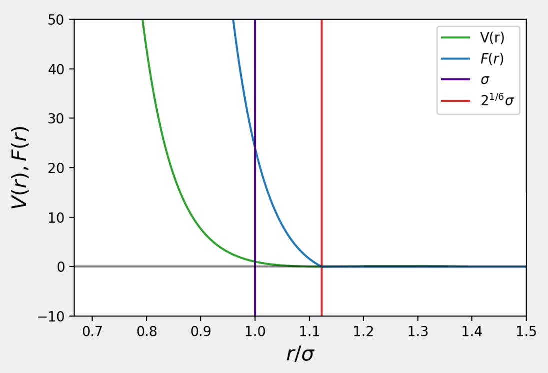
Langevin equation (Hard-core particles)

$$\dot{x}_i(t) = -\overbrace{\sum_{j\neq i}^{N} \nabla V(\boldsymbol{x}_i - \boldsymbol{x}_j)}^{Interaction} + \overbrace{\sqrt{2D}\,\boldsymbol{\xi}_i(t)}^{White\ Noise}$$

We will consider that the particles have a size, therefore, the interaction is via a hard-core potential, so that two particles cannot overlap. For this we will use the truncated **Lennard-Jones potential** which works quite well.

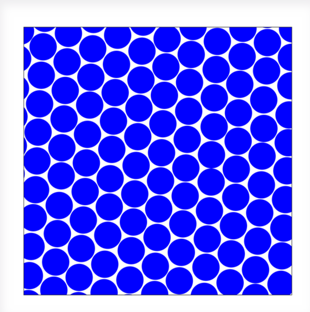
$$V(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \varepsilon & r \leq 2^{1/6}\sigma \\ 0 & r \geq 2^{1/6}\sigma \end{cases}$$

* σ *is the diameter of the particles*

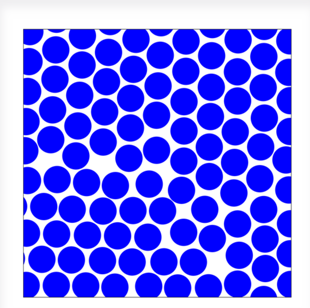


Phases

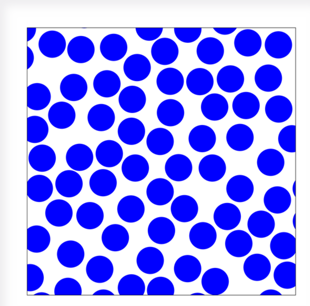
Solid phase



Hexatic phase



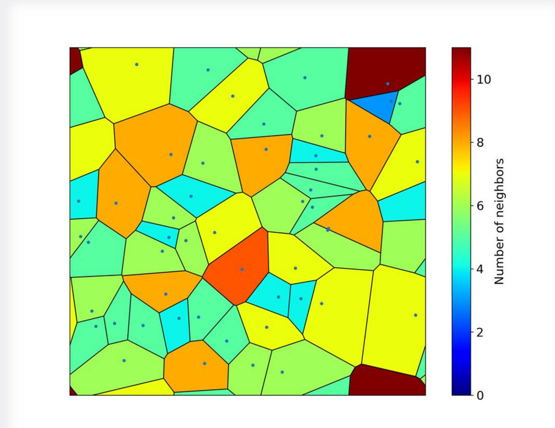
Liquid phase



We see that in the solid phase there are more defects than in the liquid phase. This is determined by the packing fraction[2], i.e. the density of the system.

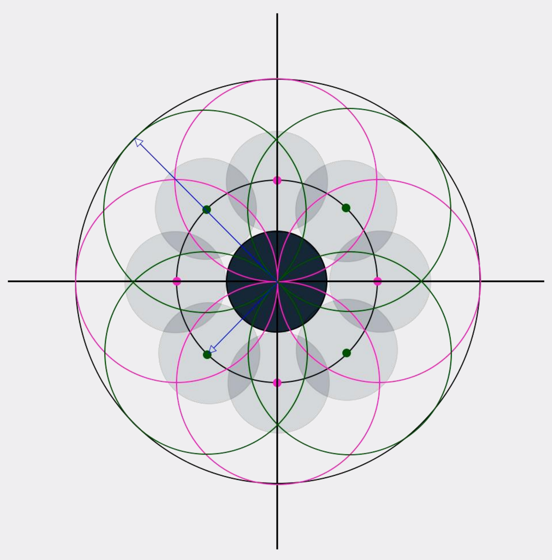
Nearest Neighbors

To compute the neighbors of each particle we have constructed the Voronoi tessellation. The nearest neighbors of each particle will be those particles whose cells are in contact.

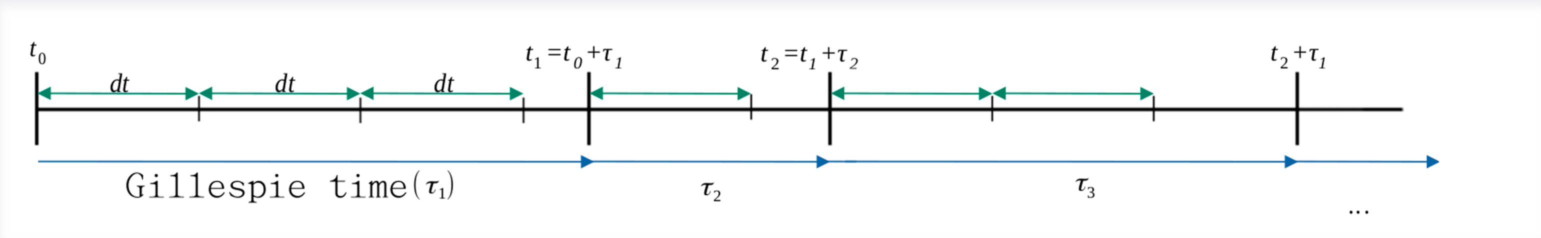


Langevin equation + Demographic events

The birth-death dynamics[3] (randomly) are implemented via a **Gillespie algorithm.**

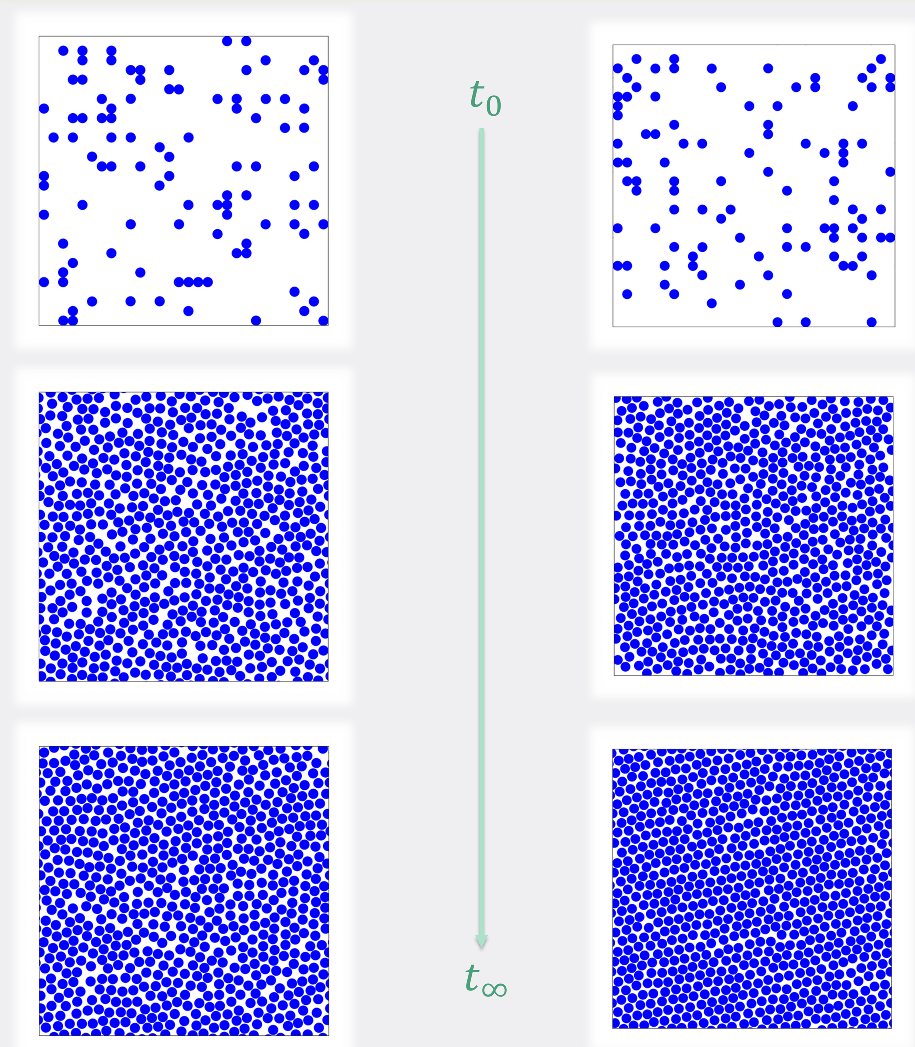


When a particle is chosen to give birth, the position is also chosen randomly among the different points of the circumference with distance 2σ from the parent. (In the figure above there are 8 possible sites).

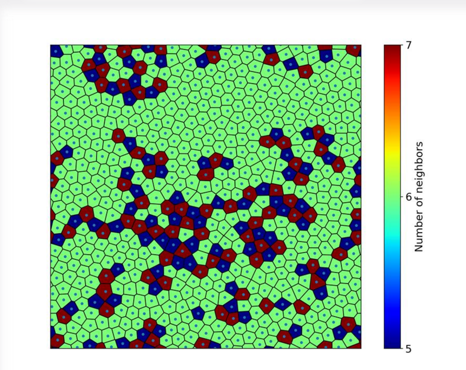


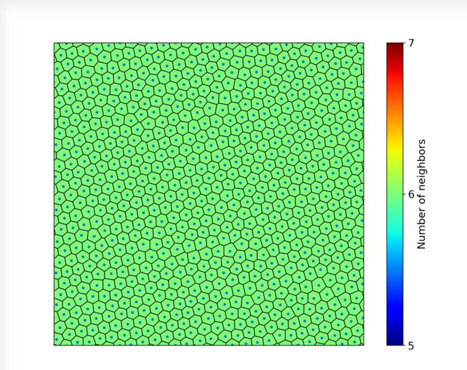
Our model has two parts: the integration of the Langevin equation using a numerical method (Euler's method) and the second part, the demographic events simulated using Gillespie's algorithm.

- Using Gillespie's method we obtain: which event occurs (birth or death), in which particle, and the time until the next event. This depends on two parameters, the birth and death rate. When a particle dies, it is removed, but when it reproduces, it must have enough space available to fit another particle of the same size attached to it.
- To integrate the Langevin equation, we divide the Gillespie time into chunks of size "*dt*" and integrate the equation until this time is reached.



➢ Using different sets of parameters (birth (r_λ) and death (r_β) rate) we can obtain different results. As we can see in the figures on the right, for different sets of parameters we can obtain results with more or less defects. (Left: $\mu = r_\lambda - r_\beta = 0.0980 - 0.0020 = 0.096$, Right: $\mu = 0{,}0999 - 0{,}0001 = 0{,}0998$)





Conclusions

As preliminary results we see that due to this succession of events (birth and death) the system has to be reconfigured each time an event occurs. This leads to a higher number of defects than if it there were no demographic events. Furthermore, we have seen that by increasing the number of available sites for a particle to be born, the total number of particles is higher, resulting in a lower number of defects.

Acknowledgments

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References

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