Technische Universität Dresden • Faculty of Mathematics

Diffusitivity of deformable cells

Master's thesis

to obtain the second degree

Master of Science
(M.Sc.)

written by

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Day of submission: April 18, 2025

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Contents

1 Cell model

This section is a recap of the DF cell model and its dynamics that were introduced in my Bachelor's thesis [**?**].
We are considering cells in the two dimensional space $\mathbb{R}^2$.

Definition 1.1. Polygon
A polygon is a closed geometric figure in the two dimensional space $\mathbb{R}^2$, formed by connecting a finite number of straight line segments. It can be represented be a sequence $(\vec{x}_1, \dots, \vec{x}_N)$ of its vertices.
The following characteristic can be attributed to a polygon.

1. A **simple** polygon is a polygon where no two line segments cross each other.

2. A polygon has a **positive orientation** if the vertices are ordered counter-clockwise.

3. A polygon has a **negative orientation** if the vertices are ordered clockwise.

The cell model introduced in [**?**] uses polygons as cells.
Thereby, each cell has a fixed number of N_v vertices.

Definition 1.2. Discrete form (DF)
An ordered sequence of points $C = (\vec{x}_1, \dots, \vec{x}_N)$ is considered to be a cell in its discrete form (DF) if the polygon that results when connecting every point with its neighbours and $\vec{x}_1$ with $\vec{x}_N$ is simple and positively orientated.
Cells in the DF model are sometimes just called discrete cells.

2 Sanity check

Having introduced our cell dynamics, we now want to take a look at the simulation results. Therefore, we aim to compare our simulation results to results from an established cell model from [Bruna and Chapman, 2012]. In [Bruna and Chapman, 2012] the diffusion dynamics of first a point particle model and second a hard sphere model is studied. Thereby, the two density distributions:

- the joint probability density function $P(\vec{X}, t)$ of the system of all cell centres $\vec{X}$ at time t,

- the marginal distribution function of the first particle $p(\vec{x}_1, t)$

play an important roll.
The joint probability density function $P(\vec{X}, t)$ is a function describing the positions of all particles in the system, while the marginal distribution function $p(\vec{x}_1, t)$ is a function describing only the position of the first particle.
It is sufficient to consider only the marginal distribution function of first particle, because all particle act similarly.
Gaining $p(\vec{x}_1, t)$ from $P(\vec{X}, t)$ is a big reduction of complexity, since we reduce from a high-dimensional PDE for P to a low-dimensional PDE for p.
The most simple model that gets considered for the diffusion dynamics of cell systems is the point particle model. Here the cells get modeled with sizeless points that perform a Brownian motion on the domain.
Since the cells do not have a real size, no interaction between the cells can occur, since they will never hit upon each other.
The paper [Bruna and Chapman, 2012] analyses these dynamics on the domain

$$\Omega_{BC} = [-0.5, 0.5]^2,$$

on which $N_{BC} = 400$ particles are located.
The movement of each point particle $\vec{x}_i$ in the simulation is given by the stochastic differential equation (SDE)

$$\mathrm{d}\vec{x}_i(t) = \sqrt{2}\mathrm{d}B_t^{(i)}, \quad 1 \leqslant i \leqslant N_{BC},$$

which describes a Brownian motion in Ω_{BC}. The reflective boundary condition on $\partial\Omega_{BC}$ is imposed. It is known, that the joint probability density of the particle system in this setup evolves according to the diffusion equation, i.e.

$$(1) \qquad \frac{\partial P}{\partial t}(\vec{X}, t) = \Delta_{\vec{X}}P = \nabla_{\vec{X}} \cdot [\nabla_{\vec{X}}P]$$

inside of the domain.
Since all particles are uncorrelated, we can compute

$$(2) \qquad P(\vec{X}) = \prod_{i=1}^{N_{BC}} p(\vec{x}_i, t).$$

The marginal distribution function the of first particle can then be determined via

$$p(\vec{x}_1, t) = \int P(\vec{X}, t)\mathrm{d}\vec{x}_2 \ldots \mathrm{d}\vec{x}_{N_{BC}}.$$

A next step that results in the hard sphere cell model (HSCM) is to give the cell particles a real size.

Let $0 < \epsilon \ll 1$ be the diameter of all cells that are now two dimensional discs with the same size. This changes the dynamics of the cells immense, since they now have chance to collide into each other which is a form of interaction.

The authors of [Bruna and Chapman, 2012] also did a simulation with the HSCM. The setting is as similar as possible to the point particle model, because a main goal of the paper was to compare the diffusion characteristics of both models. There are still $N_{BC} = 400$ cells located on the domain.

The initial condition of both models follows a two dimensional normal distribution with the addition that the distance of each cell centre to all others is at least ϵ. The used distribution $\mathcal{N}_2(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0.09^2 & 0 \\ 0 & 0.09^2 \end{pmatrix})$ has an integral of one over Ω_{BC}.

We can compute this initial condition with Algorithm 2.1.

Algorithm 2.1. *Computation of the initial cell system*

1. *Generate a point $\vec{x} \sim \mathcal{N}_2(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0.09^2 & 0 \\ 0 & 0.09^2 \end{pmatrix})$.*

2. *If for all already generated centres $\vec{x}_j : \|\vec{x} - \vec{x}_j\|_2 > \epsilon$ is true, use $\vec{x}$ as the next cell centre, otherwise discard the point and restart with step 1 until N_{BC} cell centres are found.*

Since we do not want any overlap to occur during the whole simulation with the HSCM, the feasible domain for the whole cell system is not directly $\Omega_{BC}^{N_{BC}}$, but instead

$$\Omega_{BC}^\epsilon = \Omega_1^\epsilon \times \ldots \times \Omega_{N_{BC}}^\epsilon,$$
$$\Omega_i^\epsilon = \Omega_{BC} \backslash (\cup_{j \neq i} \mathrm{B}_\epsilon(\vec{x}_j)), \quad 1 \leqslant i \leqslant N_{BC},$$

where $\mathrm{B}_\epsilon(\vec{x}_j)$ denotes the ball around $\vec{x}_j$ with radius ϵ.

This domain prevents overlaps between the cells by not allowing each cell to drift closer than ϵ to any other cell.

HSCM cells perform the same Brownian motion as the point particles.

The next question is, how cell collisions are modelled. Unlike in our DCF model where cell interactions are modelled as forces acting inside of the domain, the cell collisions from the HSCM arise from the reflective boundary condition.

Let us assume that two cells i and j are given such that $\|\vec{x}_i - \vec{x}_j\|_2 = \epsilon$ is true. Then, both cell centres are located at the boundary $\partial\Omega_{BC}^\epsilon$. Here, the reflective boundary condition is still imposed and it causes both cells to bounce of from each other in the direction of the outward normal vector from the excluded area of the respectively other cell.

In [Bruna and Chapman, 2012] the authors managed to compute the marginal distribution function of the first particle of the HSCM. In two dimensions it is given by:

(3) $$\frac{\partial p}{\partial t}(\vec{x}_1, t) = \nabla_{\vec{x}_1} \cdot \{\nabla_{\vec{x}_1}[p + \frac{\pi}{2}(N_{BC} - 1)\epsilon^2 p^2]\}.$$

We can see a connection to Equation 1. Let us look at the differential equation

$$\frac{\partial P}{\partial t}(\vec{X}, t) = \nabla_{\vec{X}} \cdot [D_\epsilon(p)\nabla_{\vec{X}}P], \ D_\epsilon(p) = 1 + \frac{\pi}{2}(N_{BC} - 1)\epsilon^2 p \ ????.$$

For $\epsilon = 0$ we can then see that $D_\epsilon(p) = 1$ and Equation 1 is given. If $\epsilon > 0$ on the other hand, we have that $D_\epsilon(p) \geqslant 1$ and we get Equation 3.

Thus, we have a higher diffusion rate for $\epsilon > 0$. In that case, we can see that the diffusivity increases with either:

(a) a larger N_{BC} which would mean more interacting cells,

(b) a larger ϵ that leads to a higher interaction radius per cell,

(c) a locally higher cell concentration p.

Overall, we conclude that the bounce effect of the HSCM enhances the diffusion rate of the system's density.

Another evidence of this behavior is shown in Figure 2 in [Bruna and Chapman, 2012]. This figure contains the following four plots:

(a) shows the solution of the linear diffusion equation 1 for point particles.

(b) shows the histogram of a Monte Carlo simulation of the point particle model.

(c) shows the solution of the nonlinear diffusion equation 3 for finite-sized particles.

(d) shows the histogram of a Monte Carlo simulation of the HSCM.

In a Monte Carlo simulation, a stochastic process is simulated many times in order to analyse whether the results follow a specific stochastic distribution. In our case that specific stochastic distribution is the density

* 400 particles/cells * initial distribution ~ N(0,0.09) + no overlaps for hard discs

The domain of the system is

a square with side length 1 around the origin and the time step size is 10^-5.

Figure 2 in [Bruna and Chapman, 2012] shows the marginal distribution function $p(x_1, t)$ at time $t = 0.05$. The figure compares the solution of the nonlinear diffusion equation (11) for finite-sized particles with the solution of the linear diffusion equation (4) for point particles.

The figure consists of four plots:

The figure is a useful tool for understanding the behavior of the system and the effects of excluded-volume interactions on the collective diffusion rate. The the heat equation and Equation (4) and in Figure $2a$ and $2c$ show similar characteristics as the stochastic simulations in $2b$ and $2d$. We can observe that the excluded-volume effects enhance the overall collective diffusion rate.
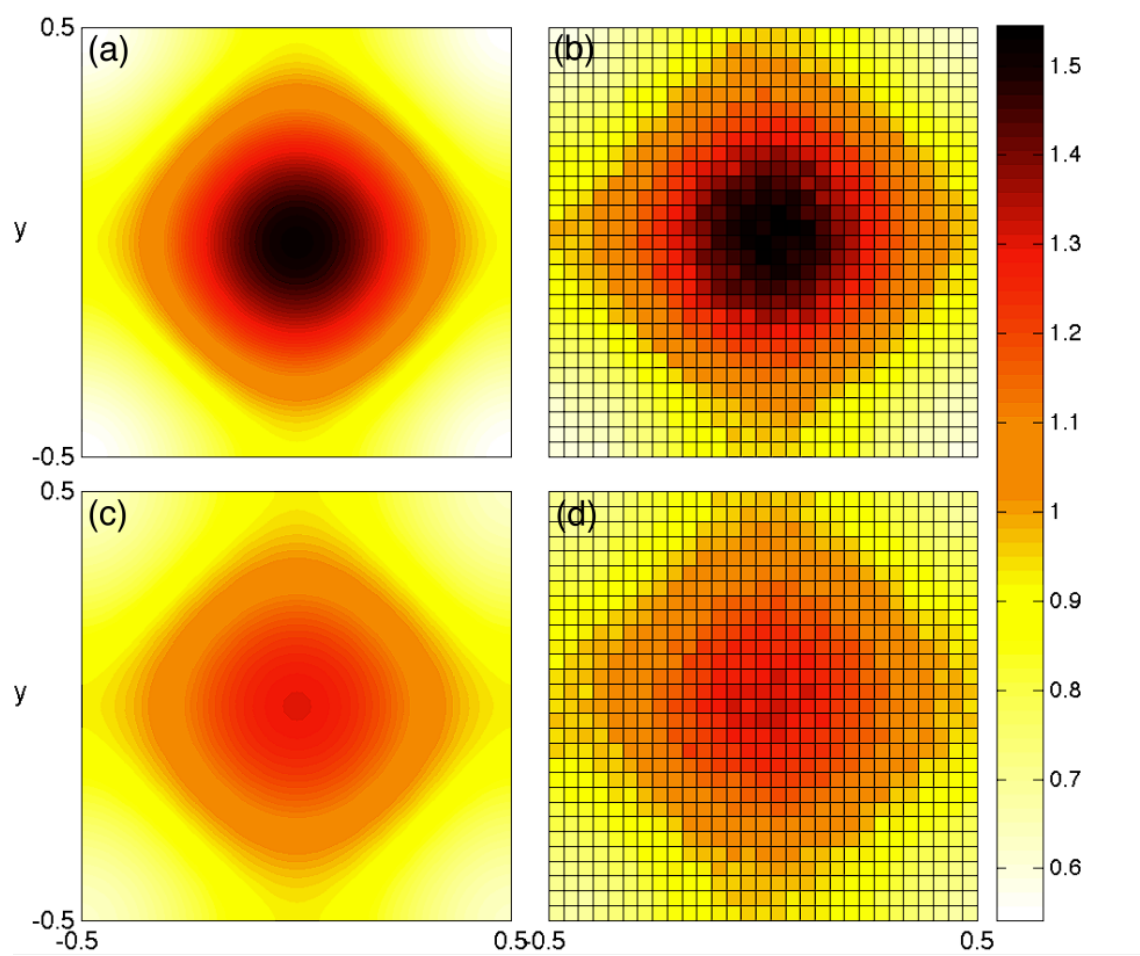
References

[Bruna and Chapman, 2012] Bruna, M. and Chapman, S. J. (2012). Excluded-volume effects in the diffusion of hard spheres. *Phys. Rev. E*, 85:011103.

Statement of authorship

I hereby declare that I have written this thesis (*Diffusitivity of deformable cells*) under the supervision of Jun.-Prof. Dr. Markus Schmidtchen independently and have listed all used sources and aids. I am submitting this thesis for the first time as part of an examination. I understand that attempted deceit will result in the failing grade „not sufficient" (5.0).

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Dresden, April 18, 2025
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