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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Contents

Overview - Bachelor's thesis

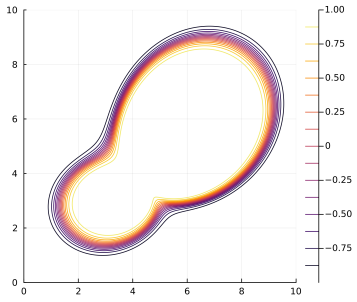
Cell models

Definitions of continuous **Centre Radius Form (CRF)**:

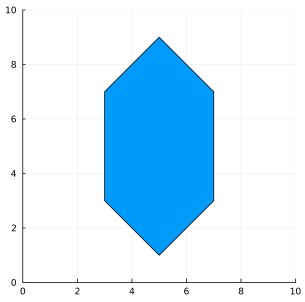
Definition 0.1. Centre radius form (CRF)
For a given point $\vec{c} \in \mathbb{R}^2$ and function $r : [0, 2\pi) \to (0, \infty)$ so that $r \in C^1([0, 2\pi))$, $r(0) = r(2\pi)$ and $r'(0) = r'(2\pi)$, the tuple $(\vec{c}, r)$ describes a cell in its centre radius form (CRF) with centre point $\vec{c}$ and radius $r(\phi)$ at angle $\phi \in [0, 2\pi)$ that is taken with the x axis.

and **Discrete Form (DF)**:

Definition 0.2. Discrete form (DF)
An ordered sequence of points $C = (\vec{x}_1, \ldots, \vec{x}_N)$ 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.



(a) A contour plot of a phase field variable ϕ illustrates how cells can be modeled through phase field models. The cell's inside is the area where $\phi > 0$. The cell wall sits on the red line where $\phi = 0$. The outer lines display the smooth transition to the outside.



(b) Another possibility to model cell forms are Vertex models. An example of this is shown here. This cell has six vertices. In order to model cell deformations, one can define forces that act on each vertex separately and thus cause them to move in an according direction.

Figure 1: To illustrate the models from the introduction, we can see a corresponding plot for each model. The sub figures (a) and (b) are concerned with the representation of cell shapes. In all sub figures, the axes denote the spatial x and y coordinates.

Derivation of forces

First, we derived methods for area computation of both models. I will just focus on DF cells from now on. For DF cells, we can just apply the **shoelace lemma**:

$$A_C = \sum_{i=1}^{N} T_i = \frac{1}{2} \sum_{i=1}^{N} (y_i + y_{i+1})(x_i - x_{i+1}) = \frac{1}{2} \sum_{i=1}^{N} (x_i y_{i+1} - x_{i+1} y_i).$$

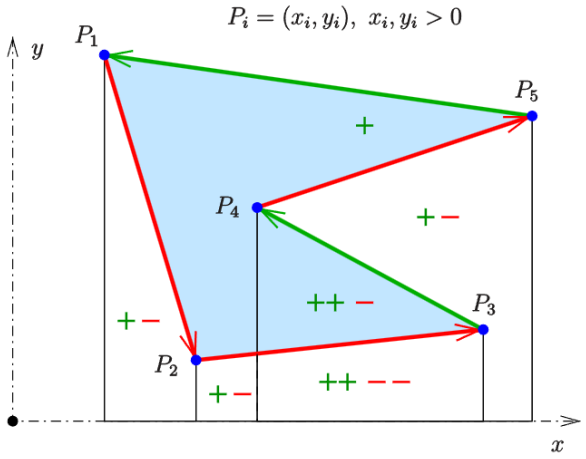


Figure 2: This figure shows a geometrical interpretation of the shoelace formula. In difference to the proposition, here the vertices are called P_i and not $\vec{x}_i$.
Source: [**?**]

Next, we derived a way to compute the **overlap** for DF cells:

Algorithm 0.3. ***Computation of a discrete overlaps***

INPUT:

- *Discrete cells C and ζ*
- *List I of unused intersections of C and ζ*

```
function constructOverlap(C, ζ, I)
    usedIntersections = List{Intersection}(I[1])
    newOverlap = List{Vertices}(I[1])
    currentIntersection = I[1]
    for counter = 1 : length(I) do
        if counter is even then
            newPath, newIntersection = findPath(currentIntersection, C, I)
        else
            newPath, newIntersection = findPath(currentIntersection, ζ, I)
        end if
        append!(newOverlap, newPath)
        if newIntersection == I[1] then
            return newOverlap, usedIntersections
        else
            append!(newOverlap, newIntersection)
            append!(usedIntersections, newIntersection)
            currentIntersection = newIntersection
        end if
    end for
end function
```

OUTPUT:

- *A single intersection 'newOverlap' which occurs between C and ζ and which uses vertices from C and ζ as well as only intersections from I*
- *A list 'usedIntersections' of all intersection that are used in 'newOverlap'*

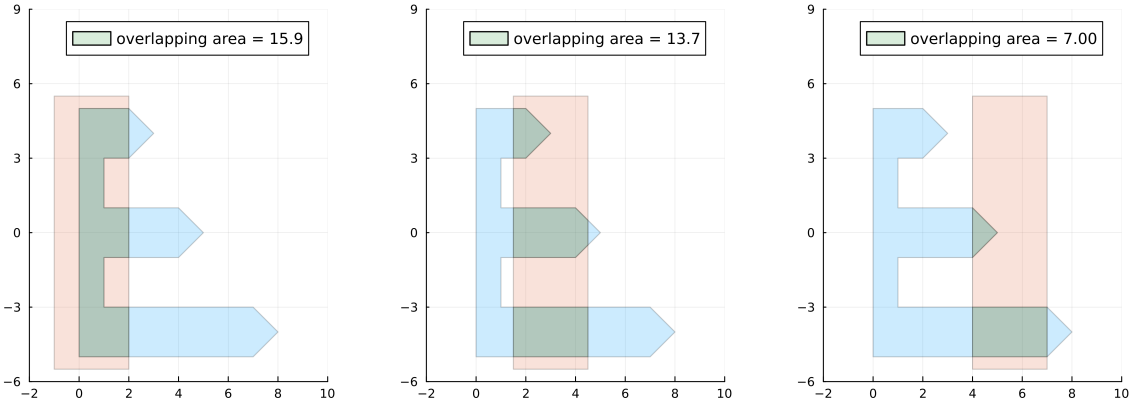


Figure 3: This figure shows 3 plots of 2 DF cells, shown in blue and red, each. One can see the calculated overlap in a green colour and the calculated area of the overlap is shown at the top of the plots. The red cell is shifted to the right in each subsequent plot, resulting in a change of the occurring overlap.

We defined how our **forces** look like using energies:

Definition 0.4. Force function
For a given energy E_i of the ith cell, the force $F_j^{(E_i)}$ that describes the impact of E_i on the jth vertex of the ith cell is given by

$$F_j^{(E_i)}(\vec{C}) := -\alpha_{E_i}(\vec{C})\nabla_{\vec{x}_{ij}} E_i(\vec{C}),$$

where $\alpha_{E_i} > 0$ denotes a positive scaling factor and $\nabla_{\vec{x}_{ij}}$ is the gradient for the jth vertex of cell i.

and introduced the **area force** ...

Proposition 0.5. ***Area force***
The gradient of A_i with respect to the jth vertex of cell i is given by

$$\nabla_{\vec{x}_j} A_i(C_i) = \operatorname{sgn}(a(C_i) - a_i^{(d)})\frac{1}{2}\begin{pmatrix} y_{i,j+1} - y_{i,j-1} \\ x_{i,j-1} - x_{i,j+1} \end{pmatrix}.$$

As a scaling factor, we choose

$$\alpha_{A_i}(C_i) := |a_i^{(d)} - a(C_i)|.$$

Thus, the area force reads

$$F_j^{(A_i)}(C_i) = \frac{1}{2}(a_i^{(d)} - a(C_i))\begin{pmatrix} y_{i,j+1} - y_{i,j-1} \\ x_{i,j-1} - x_{i,j+1} \end{pmatrix}. \tag{1}$$

Proof.
To reduce the notation effort, we neglect the subscript i, because we just consider a single cell. In order to compute $\nabla_{\vec{x}_j}|a^{(d)} - a(C)|$, let us first assume that $a^{(d)} \geqslant a(C)$. Then, one can calculate

$$\nabla_{\vec{x}_j}|a^{(d)} - a(C)| = -\nabla_{\vec{x}_j} a(C) = -\tfrac{1}{2}\sum_{j=1}^{N} \nabla_{\vec{x}_j}(x_j y_{j+1} - x_{j+1}y_j)$$
$$= -\tfrac{1}{2}\sum_{j=1}^{N} \begin{pmatrix} \partial_{x_j}(x_j y_{j+1} - x_{j+1}y_j) \\ \partial_{y_j}(x_j y_{j+1} - x_{j+1}y_j) \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} y_{j+1} - y_{j-1} \\ x_{j-1} - x_{j+1} \end{pmatrix}$$

Remember that $a^{(d)}$ is just an independent constant. In the other case, where $a^{(d)} < a(C(t))$, there is just a change in the sign. The combination of both cases yields the expression above.
Since $-|a^{(d)} - a(C)|\,\mathrm{sgn}(a(C) - a^{(d)}) = a^{(d)} - a(C)$, we can conclude the area force. □

... the **edge force** ...

Proposition 0.6. ***Edge force***
The edge force is given by the formula

$$F_j^{(E_{ij})}(C_i) = \frac{e_{j-1} - e_{i,j-1}^{(d)}}{e_{j-1}(C_i)}\begin{pmatrix} x_{j-1} - x_j \\ y_{j-1} - y_j \end{pmatrix} + \frac{e_j - e_{i,j}^{(d)}}{e_j(C_i)}\begin{pmatrix} x_{j+1} - x_j \\ y_{j+1} - y_j \end{pmatrix}. \tag{2}$$

We choose $\alpha_{E_{ij}} := |e_{ij}^{(d)} - e_j(C_i)|$.
Proof.
Since this force acts on each cell individually, we can neglect the subscript i. The searched term has the following structure

$$F_j^{(E_j)}(C) = -\alpha_{E_{j-1}} \nabla_{\vec{x}_j} E_{j-1}(C) - \alpha_{E_j} \nabla_{\vec{x}_j} E_j(C),$$

with the scaling factors α_{E_j} already defined in the proposition.
The partial derivatives of the edge length e_j are

$$\partial_{x_j} e_j(C) = \partial_{x_j}((x_{j+1} - x_j)^2 + (y_{j+1} - y_j)^2)^{\frac{1}{2}} = \frac{x_j - x_{j+1}}{e_j(C)},$$
$$\partial_{y_j} e_j(C) = \frac{y_j - y_{j+1}}{e_j(C)}.$$

This yields

$$\nabla_{\vec{x}_j} E_j = sgn(e_j^{(d)} - e_j(C))\nabla_{\vec{x}_j} - e_j(C) = sgn(e_j^{(d)} - e_j(C))\frac{1}{e_j(C)}\begin{pmatrix} x_{j+1} - x_j \\ y_{j+1} - y_j \end{pmatrix},$$

and analogously

$$\nabla_{\vec{x}_j} E_{j-1} = sgn(e_{j-1}^{(d)} - e_{j-1}(C_i))\frac{1}{e_{j-1}(C)}\begin{pmatrix} x_{j-1} - x_j \\ y_{j-1} - y_j \end{pmatrix}.$$

This yields the edge force

$$F_j^{(E_j)}(C) = \frac{e_{j-1}(C) - e_{j-1}^{(d)}}{e_{j-1}(C)}\begin{pmatrix} x_{j-1} - x_j \\ y_{j-1} - y_j \end{pmatrix} + \frac{e_j(C) - e_j^{(d)}}{e_j(C)}\begin{pmatrix} x_{j+1} - x_j \\ y_{j+1} - y_j \end{pmatrix}.$$

□

... the (interior angle force) ...

Proposition 0.7. ***Interior angle force***
The interior angle force is given by

$$F_j^{(I_{ij})}(C_i) = (\iota_{ij}^{(d)} - \iota_j(C_i)) \left(\frac{1}{\|\vec{v}_1\|_2^2} \begin{pmatrix} v_{1,y} \\ -v_{1,x} \end{pmatrix} + \frac{1}{\|\vec{v}_2\|_2^2} \begin{pmatrix} -v_{2,y} \\ v_{2,x} \end{pmatrix} \right),$$

where $\vec{v}_1 = (v_{1,x}, v_{1,y})^T := \vec{x}_{j-1} - \vec{x}_j$ *and* $\vec{v}_2 = (v_{2,x}, v_{2,y})^T := \vec{x}_{j+1} - \vec{x}_j$.
The scaling factor is defined as $\alpha_{I_{ij}} := |\iota_{ij}^{(d)} - \iota_j(C)|$.
Proof.
Again, we neglect the i, because we just consider one cell. The goal is to determine the interior angle force

$$F_j^{(I_j)}(C) = -|\iota_j^{(d)} - \iota_j(C)| \nabla_{\vec{x}_j} I_j(C)$$

Just like in the last forces, we use the sgn *function to get rid of the absolute value, yielding*

$$\nabla_{\vec{x}_j} I(C) = \operatorname{sgn}(\iota_j^{(d)} - \iota_j(C)) \nabla_{\vec{x}_j}(-\iota_j(C)),$$

since the desired state is just a constant number. Since we have a minus in front of the gradient at the end of the equation, the searched force can be written as

$$F_j^{(I_j)}(C) = (\iota_j^{(d)} - \iota_j(C)) \nabla_{\vec{x}_j} \iota_j(C).$$

The gradient of $\iota_j(C)$ *is still missing. We will neglect the not differentiable modulo operator and must then compute*

$$\nabla_{\vec{x}_j}(\operatorname{arctan2}(\vec{v}_1(C)) - \operatorname{arctan2}(\vec{v}_2(C))),$$

where $\vec{v}_1(C) = (x_{j-1} - x_j, y_{j-1} - y_j)^T$ *and* $\vec{v}_2(C) = (x_{j+1} - x_j, y_{j+1} - y_j)^T$.
The function arctan2 *is partly defined and not truly differentiable. We still want to compute a gradient to use it for our interior angle force. Since* $\operatorname{arctan2}(x, y) = \arctan(\frac{y}{x}) +$ *constant almost everywhere, we will use the function* $g(x, y) = \arctan(\frac{y}{x})$ *for the derivation, because the different constants do not matter in the derivation. With g, we can rewrite* $\iota_j(C) = g(x, y) \circ \vec{v}_1(C) - g(x, y) \circ \vec{v}_2(C)$.
Thus, we need to determine

$$\nabla_{\vec{x}_j}(g(x, y) \circ \vec{v}_1(C) - g(x, y) \circ \vec{v}_2(C)).$$

The partial derivatives of g are

$$\partial_x \arctan(\tfrac{y}{x}) = -\frac{y}{x^2} \frac{1}{1 + (\frac{y}{x})^2} = -\frac{y}{x^2 + y^2},$$
$$\partial_y \arctan(\tfrac{y}{x}) = \frac{1}{x} \frac{1}{1 + (\frac{y}{x})^2} = \frac{x}{x^2 + y^2}.$$

It is easy to see that

$$\partial_{x_j} \vec{v}_1(C) = \partial_{x_j} \vec{v}_2(C) = (-1, 0)^T, \partial_{y_j} \vec{v}_1(C) = \partial_{y_j} \vec{v}_2(C) = (0, -1)^T.$$

This implies

$$\begin{aligned}\partial_{x_j}\iota_j(C) &\triangleq \partial_{x_j}(g\circ\vec{v}_1(C) - g\circ\vec{v}_2(C))\\ &= (g'(\vec{v}_1(C))\partial_{x_j}\vec{v}_1(C) - g'(\vec{v}_2(C))\partial_{x_j}\vec{v}_2(C)\\ &= -(\partial_x g)(\vec{v}_1(C)) + (\partial_x g)(\vec{v}_2(C))\\ &= \frac{v_{1,y}}{v_{1,x}^2+v_{1,y}^2} - \frac{v_{2,y}}{v_{2,x}^2+v_{2,y}^2},\end{aligned}$$

using the multidimensional chain rule. In a similar fashion, we obtain

$$\partial_{y_j}\iota_j(C) = -\frac{v_{1,x}}{v_{1,x}^2+v_{1,y}^2} + \frac{v_{2,x}}{v_{2,x}^2+v_{2,y}^2}.$$

Together this yields

$$\nabla_{\vec{x}_j}\iota_j(C) = \frac{1}{\|\vec{v}_1\|_2^2}\begin{pmatrix} v_{1,y}\\ -v_{1,x}\end{pmatrix} + \frac{1}{\|\vec{v}_2\|_2^2}\begin{pmatrix} -v_{2,y}\\ v_{2,x}\end{pmatrix},$$

which corresponds to the term from the proposition.

□

. . . and last but not least the **overlap force**

Proposition 0.8. ***Overlap force***
The overlap force $F_j^{(O_i)}$ that acts on $\vec{x}_{ij}$ is given by

$$F_j^{(O_i)}(\vec{C}) = \sum_{m=1,m\neq i}^{M}\Big(\sum_{D_k\in\Omega_{im}} -\mathbb{1}_{\omega_{ik}}(\vec{x}_{ij})a(D_k)\nabla_{\vec{d}_l}a(D_k)\Big), \tag{3}$$

with $\nabla_{\vec{d}_l}a(D_k)$ given as

$$\nabla_{\vec{d}_l}a(D_k) = \frac{1}{2}\begin{pmatrix} d_{l+1}^y - d_{l-1}^y\\ d_{l-1}^x - d_{l+1}^x\end{pmatrix},$$

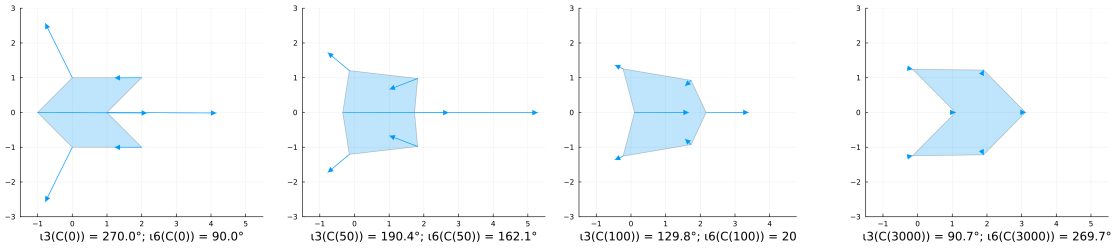


Figure 4: This figure shows how the interior angle force acts on the vertices of a DF cell. The initial state can be seen in the first diagram. The desired state is the horizontally mirrored version of the initial state. Below each chart, we can see the current interior angles at $t \in \{0, 50, 100, 3000\}$ of the two vertices that have the y value zero. The desired states are 90° for the right and 270° for the left considered vertex. The interior angle force ensures that each interior angle transitions to the desired state over time, as we can see in this figure.

with $\vec{d_l}$ being the corresponding vertex to $\vec{x}_{ij}$ in the according overlap and $\vec{d}_{l-1}$ and $\vec{d}_{l+1}$ being the vertices before and after $\vec{d_l}$.
Proof.
Instead of just using one scaling factor for each vertex, we will use a scaling factor $\alpha_{O_i,D_k} = a(D_k)$ for each individual overlap D_k.
For all vertices $\vec{x}_{ij} \notin \omega_{ik}$, that are not included in the overlap D_k, the force is zero, because a change of position would not impact the area of the overlap in this case. This produces the indicator function $\mathbb{1}_{\omega_{ik}}(\vec{x}_{ij})$ in the formula, that makes the force vanish for $\vec{x}_{ij} \notin \omega_{ik}$.
Per definition of ω_{ik}, we can always find an overlap vertex $\vec{d_l}$ that corresponds to $\vec{x}_{ij}$ if $\vec{x}_{ij} \in \omega_{ik}$. In this case, we can apply the gradient with respect to $\vec{d_l}$ on the area functional of D_k, to compute the direction of the fastest descent.
Thus, we must solve

$$F_j^{(O_i)}(\vec{C}) = \sum_{l=1, l\neq i}^{M} \Big(\sum_{D_k \in \Omega_{il}} -\mathbb{1}_{\omega_{ik}}(\vec{x}_{ij}) a(D_k) \nabla_{\vec{d_l}} a(D_k) \Big).$$

We can use the gradient computation shown in the area force, to determine

$$\nabla_{\vec{d_l}} a(D_k) = \tfrac{1}{2} \begin{pmatrix} d_{l+1}^y - d_{l-1}^y \\ d_{l-1}^x - d_{l+1}^x \end{pmatrix}.$$

□

The interactive system

Model 0.9. ***First interacting system***
The sum of all derived forces yields the first interacting system

$$d\vec{x}_{ij}(t) = F_j^{(A_i)}(C_i) + F_j^{(E_{ij})}(C_i) + F_j^{(I_{ij})}(C_i) + 10F_j^{(O_i)}(C_i) + \sqrt{2D}dB_t^{(i)}, \tag{4}$$

where $\vec{x}_{ij}$ *again stands for the vertex* j *of the* i*th cell,* $(1 \leqslant i \leqslant 9,\ 1 \leqslant j \leqslant 20)$.

and then made a rescaling which balanced all forces

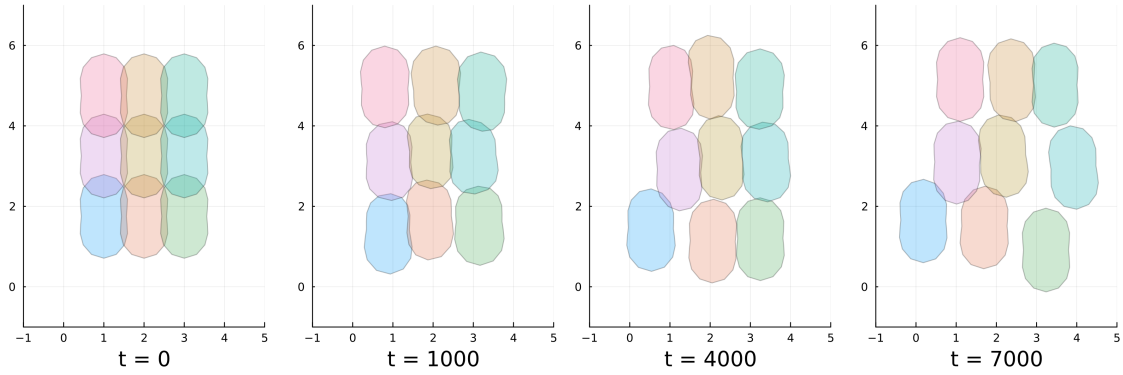


Figure 5: This figure shows different plots of a solution to the explained SDE (**??**) with the rescaled force configuration. We can see the cells at the times $t \in \{0, 1000, 4000, 7000\}$.

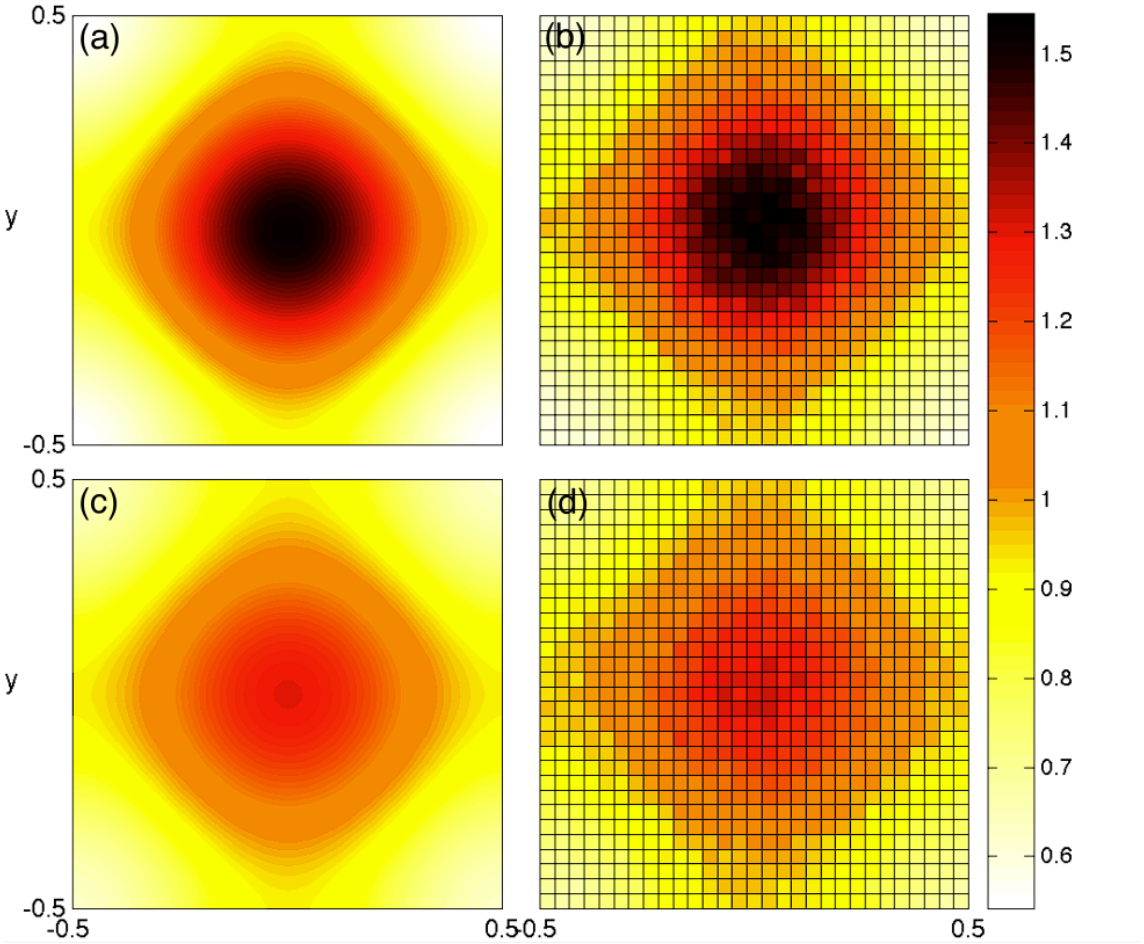
The **result of the bachelor's thesis** is a serviceable dynamic with interactions of an entire cellular system.

Outlook of bachelor's thesis

In [**?**] Bruna, Chapman and Schmidtchen studied a macroscopic model for Brownian hard needles. Similar to the hard sphere model in the paper [**?**] from the introduction, there are exclusion effects for the different needle particles. The authors managed to derive an effective PDE that describes the probability density $\rho(t, \vec{x}, \theta)$ of finding a needle with rotation θ at position $\vec{x}$ and time t. An interesting next step for the development of the theory in this thesis would be to derive an effective PDE for our energy dynamic model of the DF cells.

Overview - Master's thesis

The first task of the Master's thesis is to do a sanity check with the paper [**?**]. Until

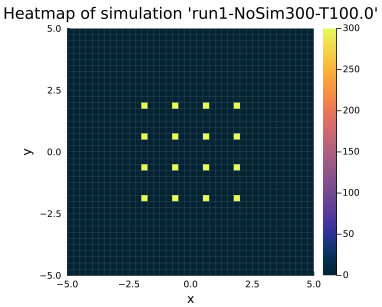


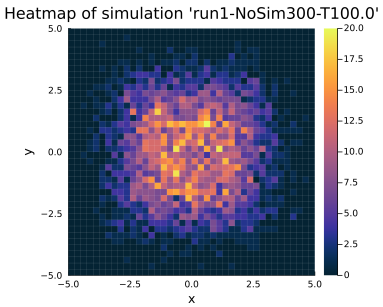
now, we made 2 bigger simulations. We neglected the interior angle force, because it caused stability problems.

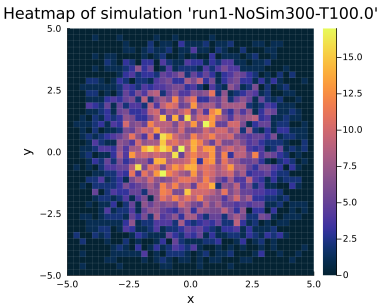
First big simulation

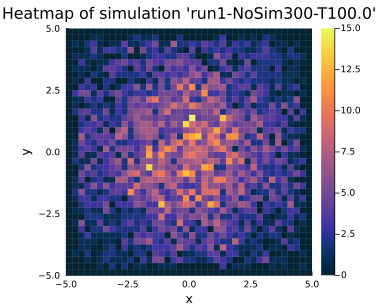
Here is our most recent simulation parameters:

- 16 cells are spawned at a fixes 4x4 initial state
- 40 wall points per cell
- Diffusitivity constant $D = 5.0$
- bachelor scalings, but wihtout interior angle force for better stability
- $timeinterval = [0, 100]$
- $timestepsize = 2^{-8}$
- used bachelor overlap
- 300 simulations ran
- $grid = [-5, 5]^2$ with discretisation step size $\delta x = 0.25$





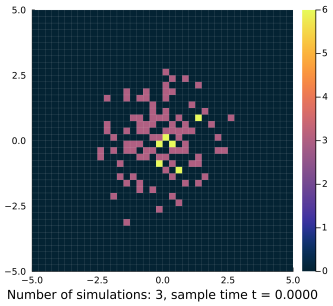


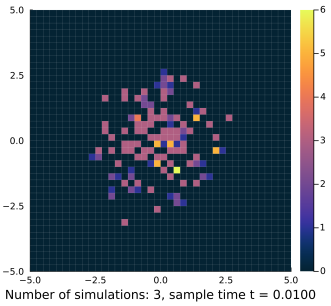


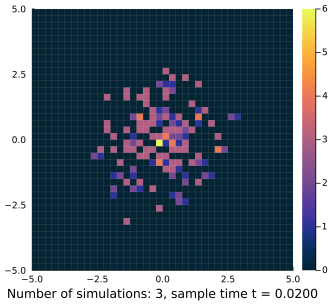
Second big simulation

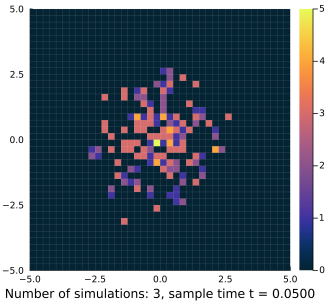
Here is our most recent simulation parameters:

- 100 cells are spawned normally distributed at the domain but without overlaps
- 20 wall points per cell
- Diffusitivity constant $D = 100.0$
- bachelor scalings, but wihtout interior angle force for better stability
- $timeinterval = (0.0, 0.05)$
- $timestepsize = 10^{-4} = 0.0001$
- used radius billiard overlap
- 3 simulations ran
- $grid = [-5, 5]^2$ with discretisation step size $\delta x = 0.25$









Overlaps

bachelor overlap (l 441 in energies.jl) billiard overlap (l 474 in energies.jl) combination of first 2 overlap (l 539 in energies.jl) radiusOverlapForceCells overlap (l 506 in energies.jl)

Next Steps

- Recreate chapman12 heatmap
-

initial condition: X' = $\sqrt{10}X$, where $X \sim N(0, 0.09^2)$

NoCells' = x (NoCells = 400)
radius' = y (radius = 0.005)
(N-1) $\epsilon^2 must be constant$AND ALSO$radius' = 0$ and without interaction [other parameters the same?]

time = [0.00,0.05], $\delta t = 10^{-5}, we could choose \delta t' = 10^{-4}$
$NoSimulations = 10^4$
$NoSimulations' = 10^3 (TODO check)$

$DOIT FOR THE DIFFERENT OVERLAPS Radius Overlap for paper like Look at bachelor overlap$
$ALSO do the smooth plots from left side \ May be run on linux workstation in Z21$

- parallelize code
- use same color grading as in chapman12 (name?)

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, January 30, 2025
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