Macrophage trajectories smoothing by evolving curves

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Slovak University of Technology

Discrete Duality Finite Volume Method and Applications
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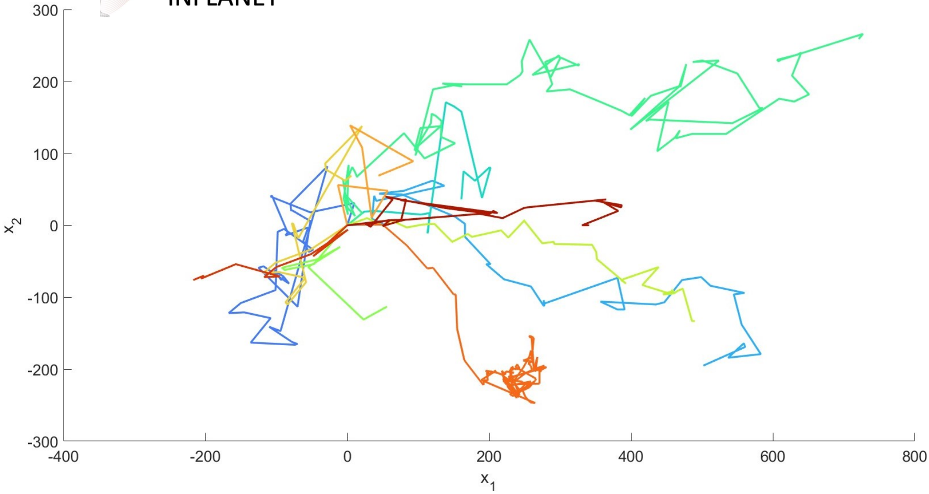
Motivation



Presentation Overview

1. Mathematical Model

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2. Numerical Discretization
   - Space Discretization
   - Inflow-implicit/Outflow-explicit scheme
   - Overall time discretization
   - Attracting term

Presentation Overview

General Equation

$$\Gamma : [0,1] \to \mathbb{R}^2 \\ u \mapsto \mathbf{x}(u) \qquad (1)$$

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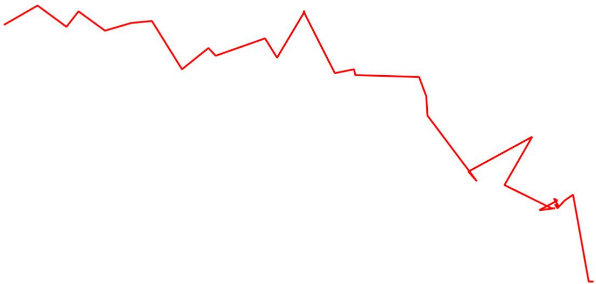
$$\frac{\partial \mathbf{x}}{\partial t} = \underbrace{-\delta k \vec{\mathbf{N}}}_{\textit{diffusion term}} + \lambda[(\mathbf{x}_0 - \mathbf{x}) \cdot \vec{\mathbf{N}}]\vec{\mathbf{N}} + \alpha \vec{\mathbf{T}} \qquad (2)$$

- $\delta > 0$ constant, k curvature, **N** unit normal vector

General Equation



$$\begin{aligned} \Gamma : [0,1] &\to \mathbb{R}^2 \\ u &\mapsto \mathbf{x}(u) \end{aligned} \qquad (1)$$

$$\frac{\partial \mathbf{x}}{\partial t} = -\delta k \vec{\mathbf{N}} + \underbrace{\lambda[(\mathbf{x}_0 - \mathbf{x}) \cdot \vec{\mathbf{N}}]\vec{\mathbf{N}}}_{\text{attracting term}} + \alpha \vec{\mathbf{T}} \qquad (2)$$

- $\delta > 0$ constant, k curvature, $\mathbf{N}$ unit normal vector
- $\lambda > 0$ constant, $\mathbf{x}_0$ initial condition, $(\mathbf{x}_0 - \mathbf{x})$ smooth function, $\cdot$ scalar product

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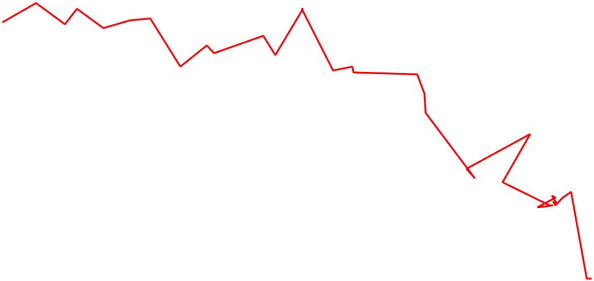

$$\frac{\partial \mathbf{x}}{\partial t} = -\delta k \vec{\mathbf{N}} + \lambda[(\mathbf{x}_0 - \mathbf{x}) \cdot \vec{\mathbf{N}}]\vec{\mathbf{N}} + \underbrace{\alpha \vec{\mathbf{T}}}_{tangential\ velocity} \qquad (2)$$

- $\delta > 0$ constant, k curvature, **N** unit normal vector
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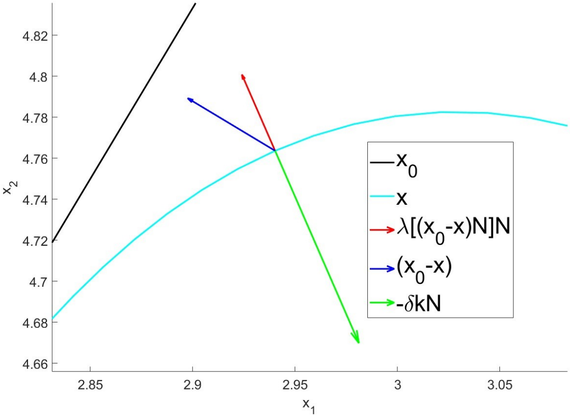
- α tangential velocity, **T** unit tangent vector

Attracting term

Fix a point
$\mathbf{x} = \mathbf{x}(u) \in \Gamma_t$, then

$$(\mathbf{x}_0 - \mathbf{x})(u) = \underset{\mathbf{v} \in \chi_u}{\arg\min} |\mathbf{v}|, \tag{3}$$



where

$$\chi_u = \{\mathbf{x} \in \mathbb{R}^2 : \mathbf{v} = \mathbf{x}_0(q) - \mathbf{x}(u), q \in [0,1]\} \tag{4}$$

Numerical Discretization

Intrinsic form of the PDE

Consider $\mathbf{x}_t = -\delta k\mathbf{N} + \lambda w\mathbf{N} + \alpha\mathbf{T}$, where $w = [(\mathbf{x}_0 - \mathbf{x}) \cdot \vec{\mathbf{N}}]$.

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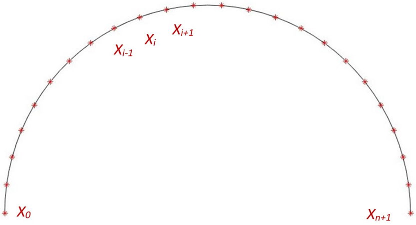

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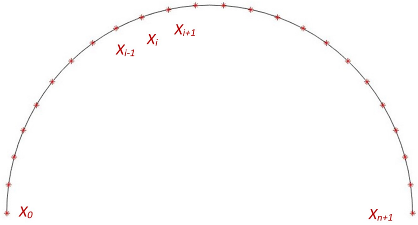

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- Define $\mathbf{T} = \mathbf{x}_s$ and $\mathbf{N} = \mathbf{x}_s^{\perp}$ such that $\mathbf{T} \wedge \mathbf{N} = -1$.

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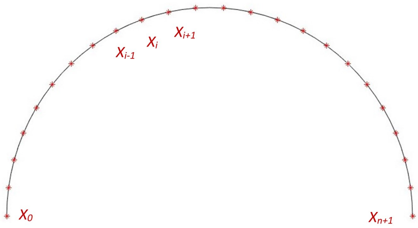

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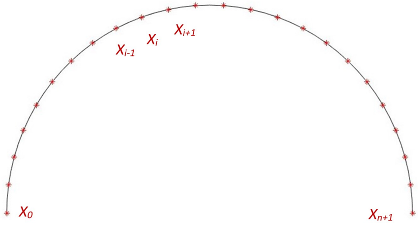

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We obtain the form of the so-called intrinsic partial differential equation: $\mathbf{x}_t = \delta \mathbf{x}_{ss} + \alpha \mathbf{x}_s + \lambda w \mathbf{x}_s^{\perp}$.

Consider the local and the global length of the evolving curve

$$g = |\mathbf{x}_u|, \quad L = \int_0^1 g du, \qquad \frac{g}{L} \approx \frac{\frac{|\mathbf{x}_i - \mathbf{x}_{i-1}|}{h}}{L} = \frac{|\mathbf{x}_i - \mathbf{x}_{i-1}|}{Lh} = \frac{|\mathbf{x}_i - \mathbf{x}_{i-1}|}{\frac{L}{n+1}}$$

where $h = \frac{1}{n+1}$ and $n+1$ is the number of segments.

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Using the Frenet-Serret formulas we obtain

$$(\frac{g}{L})_t = \frac{g}{L}(k\beta + \alpha_s - \langle k\beta \rangle_\Gamma)$$

where $\langle k\beta \rangle_\Gamma = \frac{1}{L}\int_\Gamma k\beta$.

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Define

$$(\frac{g}{L})_t = \omega(1 - \frac{g}{L}) \qquad \omega > 0$$

Numerical Discretization

Choice of the tangential velocity

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Define

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We obtain

$$\alpha_s = \langle k\beta\rangle_\Gamma - k\beta + \omega\left(\frac{L}{g} - 1\right)$$

Space Discretization

Flowing finite volume method

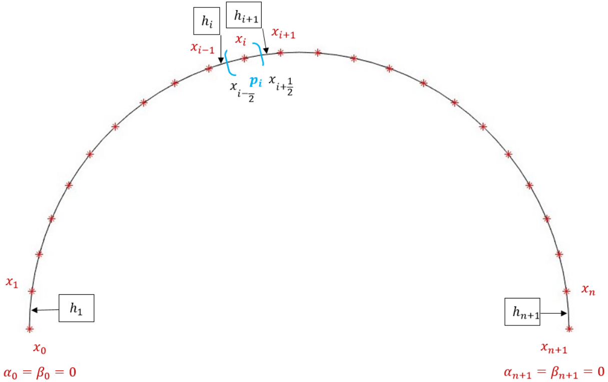
Let us consider the intrinsic form of the PDE

$$\mathbf{x}_t - \alpha \mathbf{x}_s = \delta \mathbf{x}_{ss} + \lambda w \mathbf{x}_s^{\perp}$$

$$h_i = |\mathbf{x}_i - \mathbf{x}_{i-1}|$$

$$\mathbf{p}_i = [\mathbf{x}_{i-\frac{1}{2}}, \mathbf{x}_{i+\frac{1}{2}}]$$

$$\mathbf{x}_{i+\frac{1}{2}} = \frac{\mathbf{x}_i + \mathbf{x}_{i+1}}{2}$$



Space Discretization

Flowing finite volume method

Integrating over the finite volume $\mathbf{p}_i$ we obtain

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{x}_t ds - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \alpha \mathbf{x}_s ds = \delta \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{x}_{ss} ds + \lambda \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} w \mathbf{x}_s^{\perp} ds \quad (5)$$

The values α, w are considered to be constant over the finite volume and will be indicated as α_i, w_i.

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The values α, w are considered to be constant over the finite volume and will be indicated as α_i, w_i.
Using the Newton-Leibniz formula and approximating $\mathbf{x}_s$ by a finite difference we obtain

$$\begin{aligned} &\frac{h_i + h_{i+1}}{2}(\mathbf{x}_i)_t + \frac{\alpha_i}{2}(\mathbf{x}_i - \mathbf{x}_{i+1}) - \frac{\alpha_i}{2}(\mathbf{x}_i - \mathbf{x}_{i-1}) = \\ &= \delta\left(\frac{\mathbf{x}_{i+1} - \mathbf{x}_i}{h_{i+1}} - \frac{\mathbf{x}_i - \mathbf{x}_{i-1}}{h_i}\right) + \lambda w_i \left(\frac{\mathbf{x}_{i+1} - \mathbf{x}_{i-1}}{2}\right)^{\perp} \end{aligned} \tag{6}$$

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Space Discretization
Inflow-implicit/Outflow-explicit scheme

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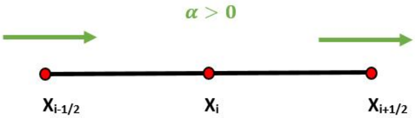

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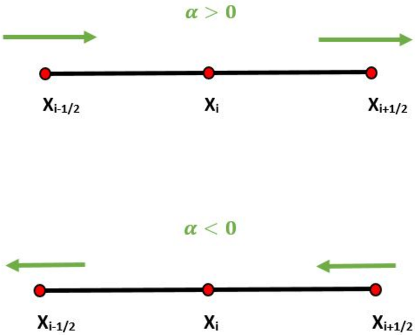

Space Discretization

Inflow-implicit/Outflow-explicit scheme

$$\frac{h_i + h_{i+1}}{2}(\mathbf{x}_i)_t + \frac{\alpha_i}{2}(\mathbf{x}_i - \mathbf{x}_{i+1}) - \frac{\alpha_i}{2}(\mathbf{x}_i - \mathbf{x}_{i-1}) = \\ = \delta_i\left(\frac{\mathbf{x}_{i+1} - \mathbf{x}_i}{h_{i+1}} - \frac{\mathbf{x}_i - \mathbf{x}_{i-1}}{h_i}\right) + \lambda w_i\left(\frac{\mathbf{x}_{i+1} - \mathbf{x}_{i-1}}{2}\right)^{\perp} \tag{7}$$

Space Discretization

Inflow-implicit/Outflow-explicit scheme

$$
\begin{aligned}
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\end{aligned} \tag{7}
$$

$$
\mathbf{x}_t - \alpha \mathbf{x}_s = \delta \mathbf{x}_{ss} + \lambda w \mathbf{x}_s^{\perp}
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Space Discretization

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Space Discretization
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$$\frac{h_i + h_{i+1}}{2}(\mathbf{x}_i)_t + \frac{1}{2}(b^{in}_{i+\frac{1}{2}} + b^{out}_{i+\frac{1}{2}})(\mathbf{x}_i - \mathbf{x}_{i+1}) + \frac{1}{2}(b^{in}_{i-\frac{1}{2}} + b^{out}_{i-\frac{1}{2}})(\mathbf{x}_i - \mathbf{x}_{i-1}) \\ = \delta\left(\frac{\mathbf{x}_{i+1} - \mathbf{x}_i}{h_{i+1}} - \frac{\mathbf{x}_i - \mathbf{x}_{i-1}}{h_i}\right) + \lambda w_i\left(\frac{\mathbf{x}_{i+1} - \mathbf{x}_{i-1}}{2}\right)^{\perp} \tag{9}$$

Overall time discretization

Let m be the time step index and τ the length of the discrete time step.

- time derivative: finite difference $\mathbf{x}_t = \frac{\mathbf{x}_i^{m+1} - \mathbf{x}_i^m}{\tau}$

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- attracting term explicitly

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- unknowns in the outflow part of the advection term explicitly
- diffusion term implicitly
- attracting term explicitly

We obtain

$$\mathbf{x}_{i-1}^{m+1}\left(-\frac{\delta}{h_i^m} - \frac{b_{i-\frac{1}{2}}^{in^m}}{2}\right) + \mathbf{x}_{i+1}^{m+1}\left(-\frac{\delta}{h_{i+1}^m} - \frac{b_{i+\frac{1}{2}}^{in^m}}{2}\right) +$$

$$+ \mathbf{x}_i^{m+1}\left(\frac{h_{i+1}^m + h_i^m}{2\tau} + \frac{\delta}{h_i^m} + \frac{\delta}{h_{i+1}^m} + \frac{b_{i-\frac{1}{2}}^{in^m}}{2} + \frac{b_{i+\frac{1}{2}}^{in^m}}{2}\right) = \mathbf{x}_i^m \frac{h_{i+1}^m + h_i^m}{2\tau} +$$

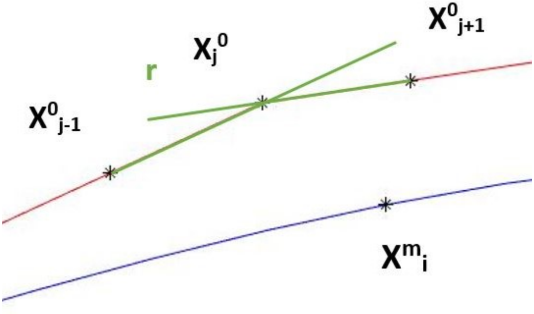
$$- \frac{b_{i+\frac{1}{2}}^{out^m}}{2}(\mathbf{x}_i^m - \mathbf{x}_{i+1}^m) - \frac{b_{i-\frac{1}{2}}^{out^m}}{2}(\mathbf{x}_i^m - \mathbf{x}_{i-1}^m) + \lambda w_i^m \left(\frac{\mathbf{x}_{i+1}^m - \mathbf{x}_{i-1}^m}{2}\right)^{\perp} \quad (10)$$

Overall time discretization

Attracting term

Fix $\mathbf{x}_i^m$ and for $j = 1, .., n+1$

- Consider the line r passing through the points $\mathbf{x}_{j-1}^0, \mathbf{x}_j^0$,



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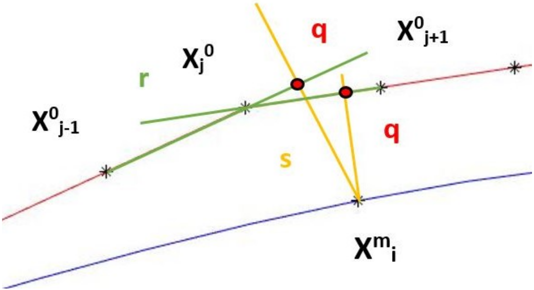

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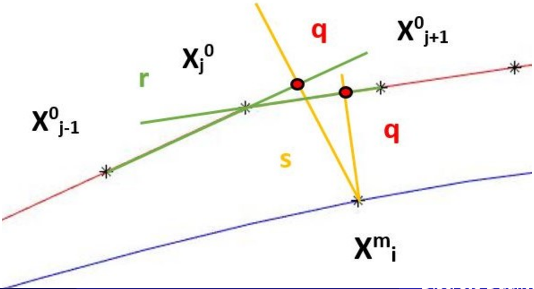
- Find the line s such that:$s \perp r$ and $\mathbf{x}_i^m \in s$. Find $\mathbf{q} \in r \cap s$.
- Consider $d = d(\mathbf{q}, \mathbf{x}_i^m)$. If $\mathbf{q} \in [\mathbf{x}_{j-1}^0, \mathbf{x}_j^0]$ and $d < minD$ then: $\mathbf{x}^0 - \mathbf{x}_i^m = \mathbf{q} - \mathbf{x}_i^m$



Influence of the attracting term

Comparison

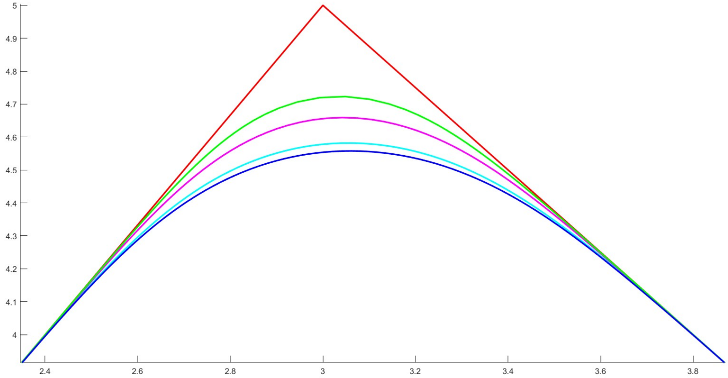
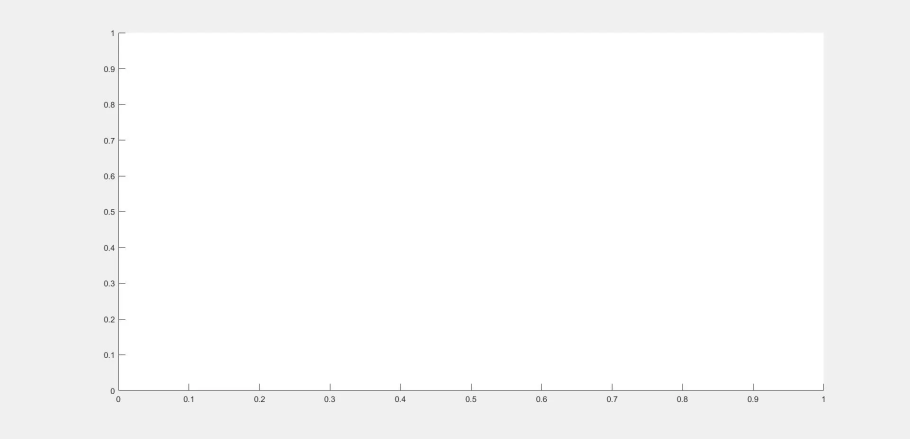
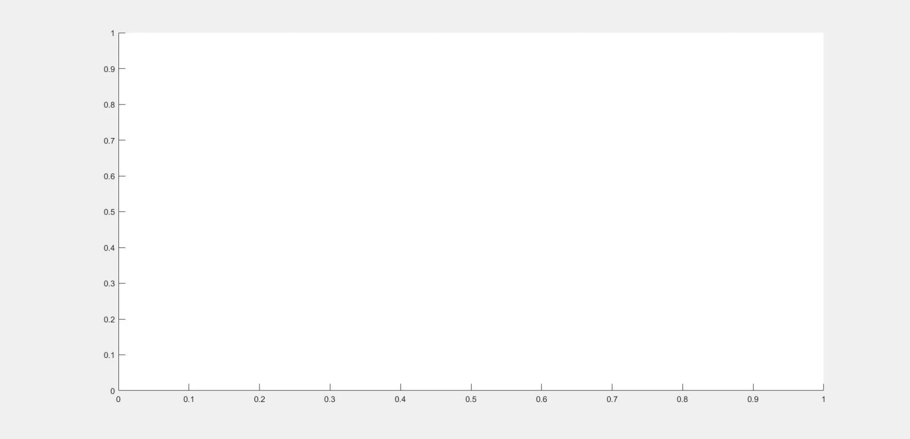


Figure: Comparison of the evolution of the initial curve (red) for δ fixed and different values of λ after 400 time steps.Results are shown for $\lambda = 0$ (blue),$\lambda = 1$(light blue),$\lambda = 5$(pink) and $\lambda = 10$(green)

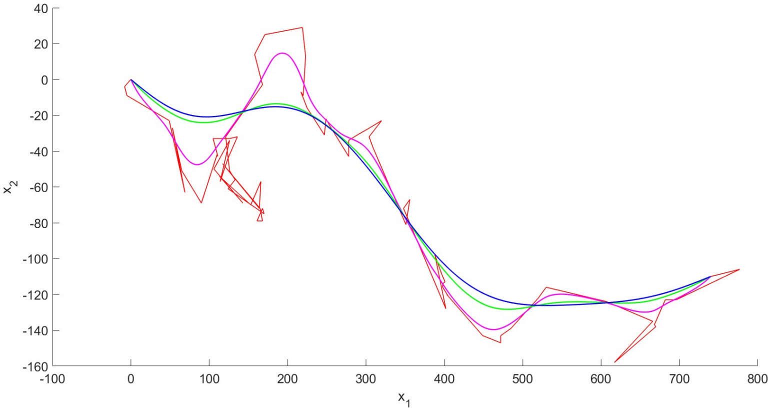
Macrophages trajectories



Macrophages trajectories



Macrophages trajectories

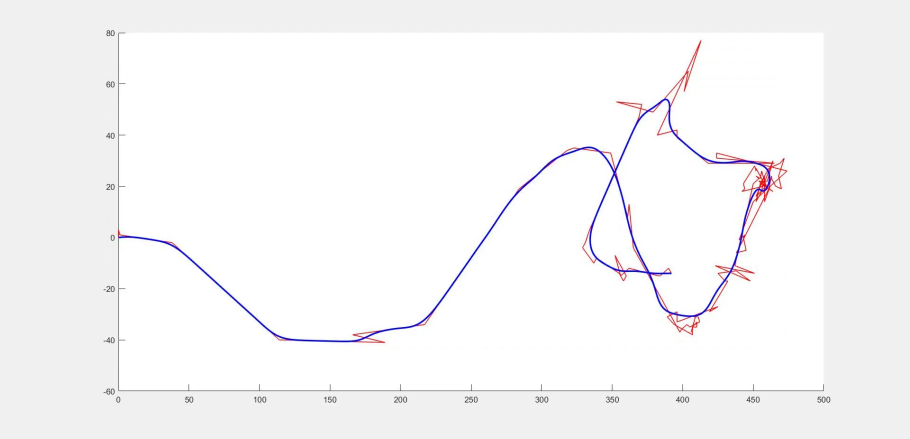


We considered the mean Hausdorff distance between two discrete curves $\mathcal{A}, \mathcal{B}$ defined as

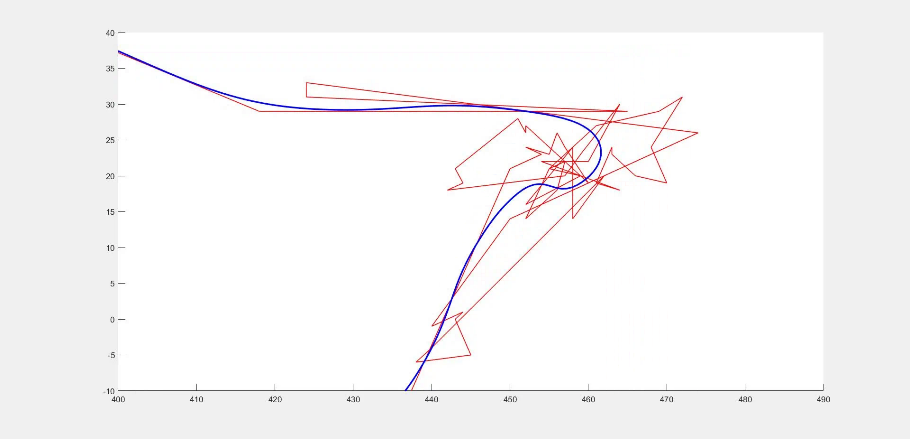
$$
\begin{aligned}
\bar{\delta}_H(\mathcal{A}, \mathcal{B}) &= \frac{1}{n} \sum_{i=1}^{n} \min_{\mathbf{b} \in B} d(a_i, \mathbf{b}), \\
\bar{\delta}_H(\mathcal{B}, \mathcal{A}) &= \frac{1}{n} \sum_{i=1}^{n} \min_{\mathbf{a} \in A} d(b_i, \mathbf{a}), \\
\bar{d}_H(\mathcal{A}, \mathcal{B}) &= \frac{\bar{\delta}_H(\mathcal{A}, \mathcal{B}) + \bar{\delta}_H(\mathcal{B}, \mathcal{A})}{2},
\end{aligned}
\tag{11}
$$

where $\mathcal{A} = \{a_0, ..., a_{n+1}\}$, $\mathcal{B} = \{b_0, ..., b_{n+1}\}$ are discrete sets and $A = \{\mathbf{a}_1, ..., \mathbf{a}_{n+1}\}$, $B = \{\mathbf{b}_1, ..., \mathbf{b}_{n+1}\}$ are sets of segments

Macrophage trajectories



Macrophage trajectories



Smoothed Velocity Estimation

Time Estimation

The formula for the new real-time is given by

$$T_i^{n+1} = T_i^n + \frac{\alpha_i^n \tau}{L^{n+1}} \tag{12}$$

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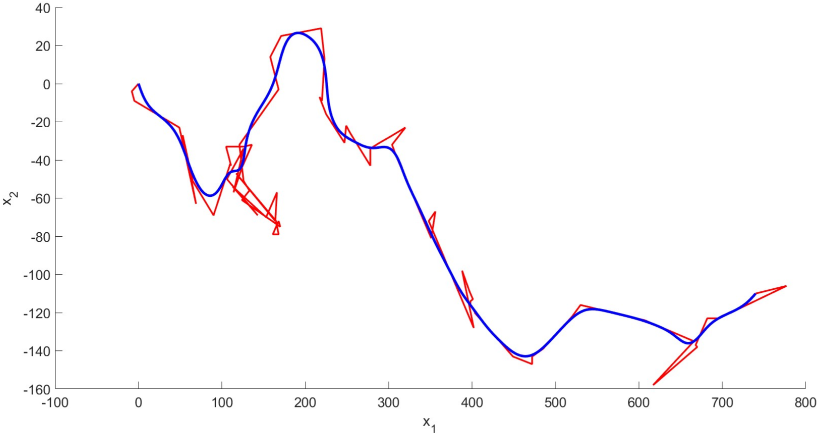
- α_i^n is the tangential velocity
- τ the time step
- L^{n+1} is the total length of the curve in the current time step

Finally, we calculated the velocity using the central difference scheme

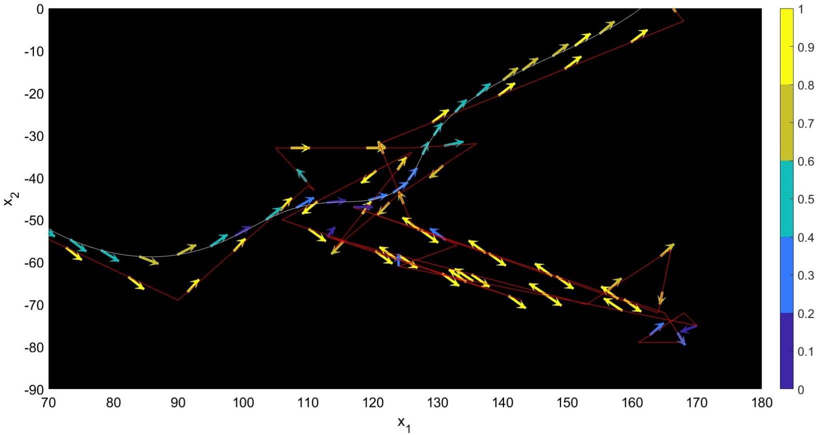
$$V(x,y) = \left(\frac{\mathbf{x}_1^{i+1} - \mathbf{x}_1^{i-1}}{T_{i+1} - T_{i-1}}, \frac{\mathbf{x}_2^{i+1} - \mathbf{x}_2^{i-1}}{T_{i+1} - T_{i-1}}\right) \tag{13}$$



40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
x2
-100
0
100
200
300
400
500
600
700
800
x1

Time and Velocity Estimation

Velocity Estimation



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