



Energy estimate for active systems: application to collective cell movement

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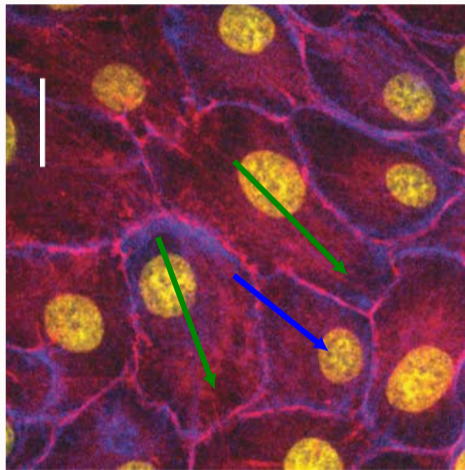
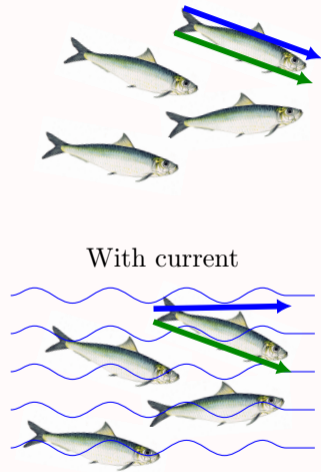
JEARA 2023

Collective cell migration?



[Marchetti et al., Reviews of Modern Physics, 2013]

Polarity p

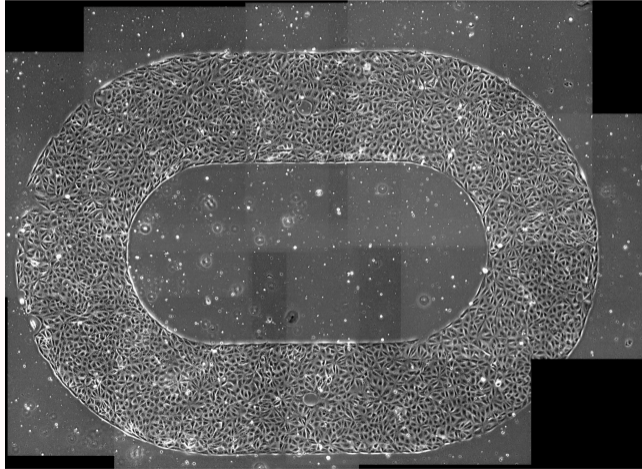


[Durande et al. 2020]



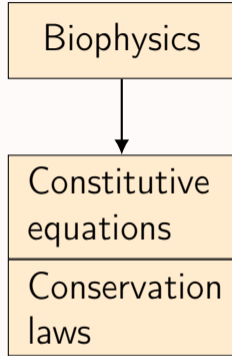
Collective cell movement in a racetrack

Top view of a monolayer of cells

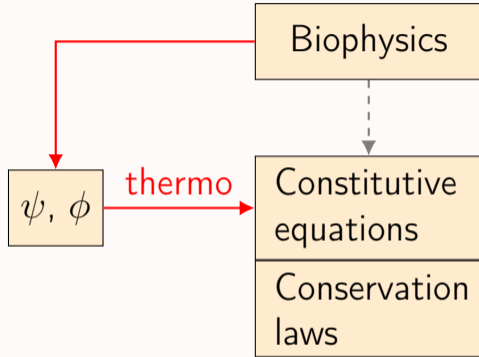


[Durande et al., thesis, 2020]

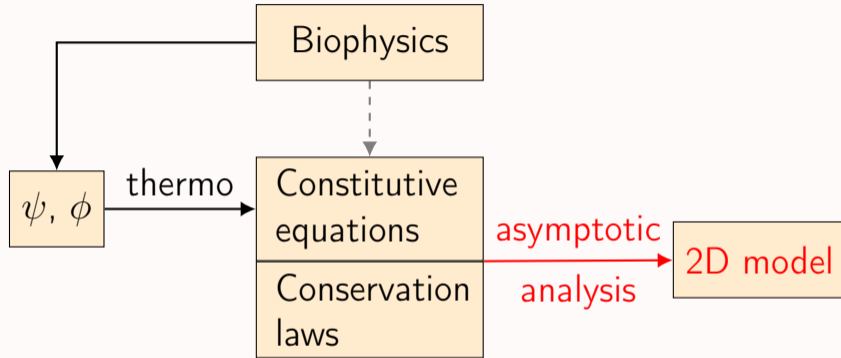
Framework



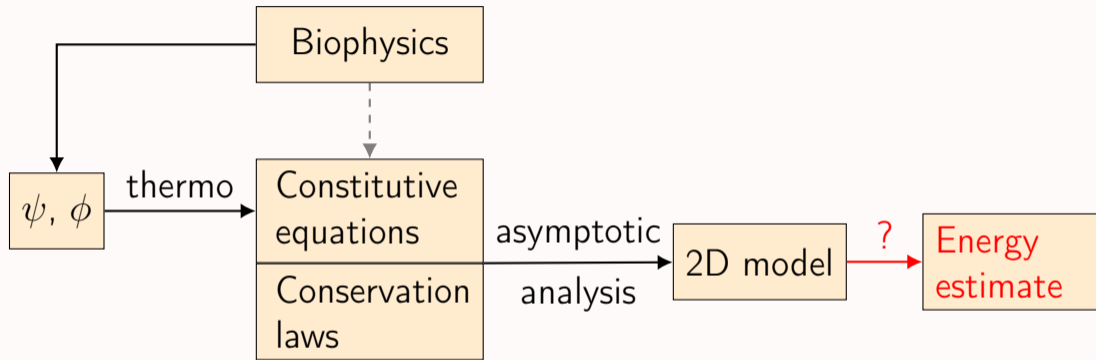
Framework



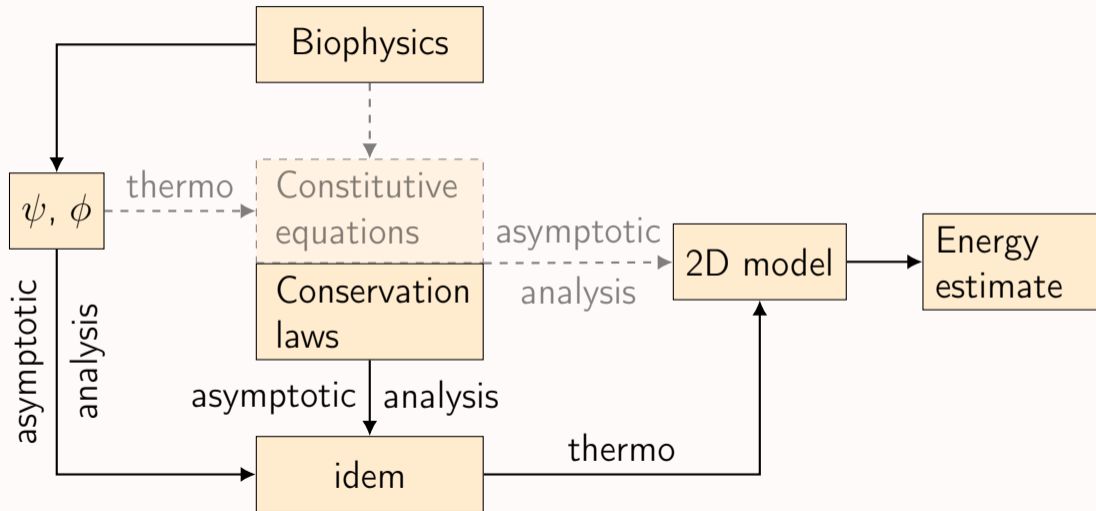
Framework



Framework



Framework



Contents

1. 2D thermodynamic framework
2. Energy estimate
3. Numerical illustrations

1. 2D thermodynamic framework

Free energy

$$\mathcal{F}(\rho, \mathbf{p}) = \int_{\Omega} \rho \psi(\rho, \mathbf{p}, \nabla \mathbf{p})$$

$$\psi(\rho, \mathbf{p}, \nabla \mathbf{p}) = \frac{c_0}{\gamma} \rho^\gamma$$

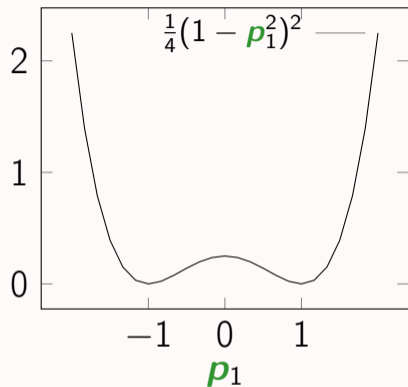
$$+ B \left(\frac{1}{4} \left(|\mathbf{p}|^2 - 1 \right)^2 + \frac{\kappa^2}{2} |\nabla \mathbf{p}|^2 \right)$$

where

Ω : migration domain ρ : density

c_0 & γ : density penalization coefficients

B : resistance of \mathbf{p} to viscous forces κ : correlation length



Free energy

$$\mathcal{F}(\rho, \mathbf{p}) = \int_{\Omega} \rho \psi(\rho, \mathbf{p}, \nabla \mathbf{p})$$

$$\psi(\rho, \mathbf{p}, \nabla \mathbf{p}) = \frac{c_0}{\gamma} \rho^\gamma$$

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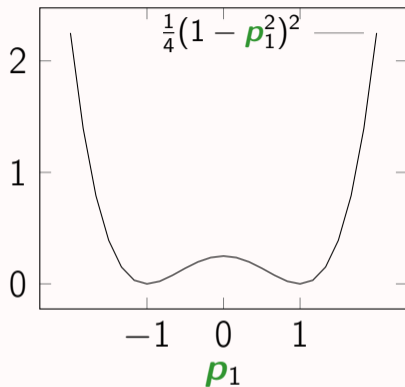
double-well

where

Ω : migration domain ρ : density

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B : resistance of \mathbf{p} to viscous forces κ : correlation length



Free energy

$$\mathcal{F}(\rho, \mathbf{p}) = \int_{\Omega} \rho \psi(\rho, \mathbf{p}, \nabla \mathbf{p})$$

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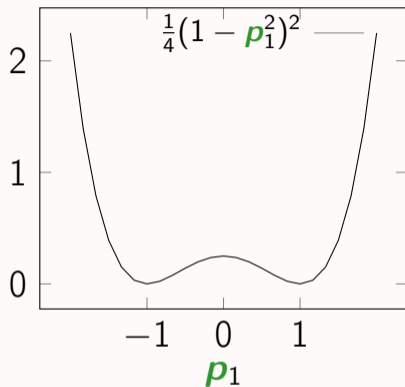
$$+ B \left(\frac{1}{4} (|\mathbf{p}|^2 - 1)^2 + \frac{\kappa^2}{2} |\nabla \mathbf{p}|^2 \right)$$

where

Ω : migration domain ρ : density

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Dissipation potential

$$\phi(\mathbf{D}(\mathbf{v}), \overset{\nabla}{\mathbf{p}}) = \rho \left(|\mathbf{D}(\mathbf{v})|^2 + |\operatorname{div} \mathbf{v}|^2 + \frac{Pe}{2} |\overset{\nabla}{\mathbf{p}}|^2 \right)$$

where

$\mathbf{D}(\mathbf{v}) = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$: deformation rate tensor

$\overset{\nabla}{\mathbf{p}} = \frac{\partial \mathbf{p}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{p} - \nabla \mathbf{v} \cdot \mathbf{p}$: upper convective derivative

Pe : relaxation time

Constitutive equations: abstract case

$$\rho\boldsymbol{\sigma} = -\rho^2 \frac{\partial\psi}{\partial\rho} \mathbf{I} + \frac{\partial\phi}{\partial\mathbf{D}(\mathbf{v})} - \rho \nabla \mathbf{p}^\top \cdot \frac{\partial\psi}{\partial\nabla\mathbf{p}} + \mathbf{p} \otimes \frac{\partial\mathcal{F}}{\partial\mathbf{p}} \quad (1a)$$

$$0 = \frac{\partial\mathcal{F}}{\partial\mathbf{p}} + \frac{\partial\phi}{\partial\nabla\mathbf{p}} \quad (1b)$$

where

$$\boldsymbol{\sigma}: \text{stress tensor} \quad \frac{\partial\mathcal{F}}{\partial\mathbf{p}} = \rho \frac{\partial\psi}{\partial\mathbf{p}} - \text{div} \left(\rho \frac{\partial\psi}{\partial\nabla\mathbf{p}} \right)$$

[Stokes, Springer, 1984] [Saramito, book to appear, 2023]

Constitutive equations: concrete case

$$\rho \boldsymbol{\sigma} = -c_0 \rho^{\gamma+1} \mathbf{I} + 2\rho (\mathbf{D}(\mathbf{v}) + \text{div}(\mathbf{v})\mathbf{I}) - \kappa^2 B \rho \nabla \mathbf{p}^\top \cdot \nabla \mathbf{p} \quad (1a)$$
$$+ B \mathbf{p} \otimes \left[\rho (|\mathbf{p}|^2 - 1) \mathbf{p} - \kappa^2 \text{div}(\rho \nabla \mathbf{p}) \right]$$

$$0 = \rho (|\mathbf{p}|^2 - 1) \mathbf{p} - \kappa^2 \text{div}(\rho \nabla \mathbf{p}) + Pe \rho \overset{\nabla}{\mathbf{p}} \quad (1b)$$

Non-symmetric stress tensor

Microrotation [Cosserat and Cosserat, A. Hermann et Fils, 1909]

Couple stress theory [Stokes, Springer, 1984]

Liquid crystals [de Gennes and Prost, Clarendon Press Publication, 1993]

Microcontinuum field theory [Eringen, Springer-Verlag New York, 1999]

Conservation laws

mass

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0$$

linear momentum

$$\operatorname{div}(\rho \boldsymbol{\sigma}^T) + \mathbf{f}_{\text{ext}} = 0$$

Definitions:

ρ : density

\mathbf{v} : velocity

$\boldsymbol{\sigma}$: stress tensor

\mathbf{f}_{ext} : external forces

Resulting equations

Find \mathbf{v} (velocity), ρ (density) and \mathbf{p} (polarity) s.t.

$$\left\{ \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0 \right.$$

mass

Resulting equations

Find \mathbf{v} (velocity), ρ (density) and \mathbf{p} (polarity) s.t.

$$\begin{cases} \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0 & \text{mass} \\ \operatorname{div}(\rho \boldsymbol{\sigma}^\top) + \mathbf{f}_{\text{ext}} = 0 & \text{momentum} \end{cases}$$

where the total stress is given by

$$\begin{aligned} \rho \boldsymbol{\sigma} = & 2\rho(\mathbf{D}(\mathbf{v}) + \operatorname{div}(\mathbf{v})\mathbf{I}) - c_0\rho^{\gamma+1}\mathbf{I} - \kappa^2 B\rho \nabla \mathbf{p}^\top \cdot \nabla \mathbf{p} \\ & + B\mathbf{p} \otimes \left[\rho(|\mathbf{p}|^2 - 1)\mathbf{p} - \kappa^2 \operatorname{div}(\rho \nabla \mathbf{p}) \right] \end{aligned}$$

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Pe :
relaxation
time

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Pe :
relaxation
time

κ :
correlation
length

where the total stress is given by

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Pe :
relaxation
time

κ : correlation
length

\mathbf{B} : resistance
of \mathbf{p} to
viscous forces

Activity

$$\mathbf{f}_{\text{ext}} = \mathbf{f}_a - C_F \mathbf{v} + \text{div}(\rho \boldsymbol{\sigma}_a)$$

$$\mathbf{f}_a = T_a \mathbf{p}$$

$$\boldsymbol{\sigma}_a = -\sigma_a \left(\mathbf{p} \otimes \mathbf{p} + |\mathbf{p}|^2 \mathbf{I} \right)$$

external forces

active force

active stress

where

C_F : friction

T_a : active force coefficient

σ_a : active stress coefficient

Complete system

Find \mathbf{v} (velocity), ρ (density) and \mathbf{p} (polarity) s.t.

$$\left\{ \begin{array}{ll} \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0 & \text{mass} \\ -\operatorname{div}(\rho \boldsymbol{\sigma}^\top) + C_F \mathbf{v} = T_a \mathbf{p} + \operatorname{div}(\rho \boldsymbol{\sigma}_a) & \text{momentum} \\ Pe \rho \nabla \cdot \mathbf{p} + \rho (|\mathbf{p}|^2 - 1) \mathbf{p} - \kappa^2 \operatorname{div}(\rho \nabla \mathbf{p}) = 0 & \text{polarity} \end{array} \right.$$

where the stresses are given by

$$\begin{aligned} \rho \boldsymbol{\sigma} &= 2\rho (\mathbf{D}(\mathbf{v}) + \operatorname{div}(\mathbf{v}) \mathbf{I}) - c_0 \rho^{\gamma+1} \mathbf{I} - \kappa^2 B \rho \nabla \mathbf{p}^\top \cdot \nabla \mathbf{p} \\ &\quad + B \mathbf{p} \otimes \left[\rho (|\mathbf{p}|^2 - 1) \mathbf{p} - \kappa^2 \operatorname{div}(\rho \nabla \mathbf{p}) \right] \\ \boldsymbol{\sigma}_a &= -\sigma_a (\mathbf{p} \otimes \mathbf{p} + |\mathbf{p}|^2 \mathbf{I}) \end{aligned}$$

2. Energy estimate

Energy estimate

(linear momentum) $\cdot \mathbf{v}$ + (polarity equation) $\cdot \frac{1}{\rho Pe} \frac{\partial \mathcal{F}}{\partial \mathbf{p}}$ gives

$$\frac{d\mathcal{F}}{dt} + \int_{\Omega} \left(2\rho |\mathbf{D}(\mathbf{v})|^2 + 2\rho |\operatorname{div} \mathbf{v}|^2 + \frac{1}{Pe\rho} \left| \frac{\partial \mathcal{F}}{\partial \mathbf{p}} \right|^2 + C_F |\mathbf{v}|^2 \right) = \int_{\Omega} \left(T_a \mathbf{p} \cdot \mathbf{v} + \sigma_a \rho \mathbf{p} \otimes \mathbf{p} : \mathbf{D}(\mathbf{v}) + \sigma_a \rho |\mathbf{p}|^2 \operatorname{div} \mathbf{v} \right) \quad (7)$$

dissipation

activity

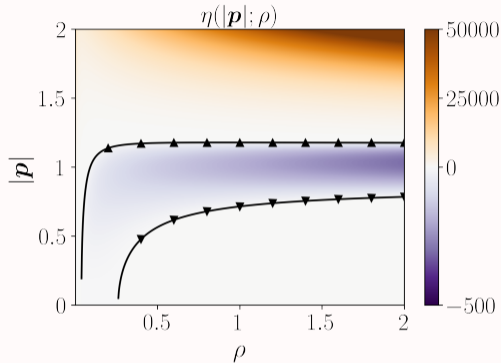
where $\frac{\partial \mathcal{F}}{\partial \mathbf{p}} = \rho B (|\mathbf{p}|^2 - 1) \mathbf{p} - \kappa^2 B \operatorname{div}(\rho \nabla \mathbf{p})$

Balance between dissipation & activity (1)

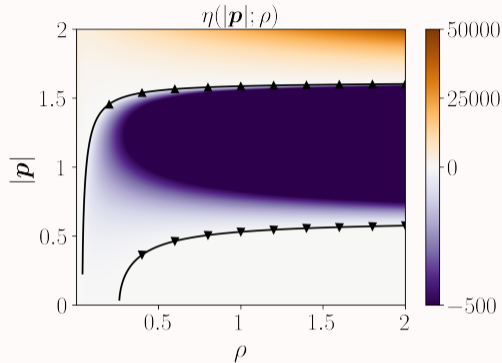
$$\frac{d\mathcal{F}}{dt} + \int_{\Omega} \underbrace{\left[\frac{1}{Pe\rho} \left| \frac{\partial \mathcal{F}}{\partial \mathbf{p}} \right|^2 - \left(\frac{T_a^2}{4C_F} |\mathbf{p}|^2 + \frac{\sigma_a^2}{4} \rho |\mathbf{p}|^4 \right) \right]}_{=\eta(|\mathbf{p}|; \rho)} \leq 0 \quad (8)$$

When $\kappa = 0$, $\eta(|\mathbf{p}|; \rho)$ is a polynomial in $|\mathbf{p}|$ and in ρ

Balance between dissipation & activity (2)



(a) $\sigma_a = 20$



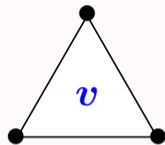
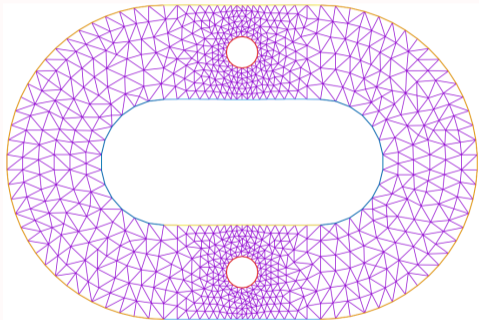
(b) $\sigma_a = 20\sqrt{10} \approx 63.25$

$\eta(|\mathbf{p}|; \rho)$ for $T_a^2/C_F = 400$, $Pe = 1/10$ and $B = 10$

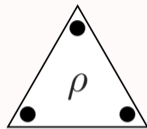
$\eta < 0$ is a necessary but not sufficient condition to have $d\mathcal{F}/dt > 0$

3. Numerical illustrations

Spatial discretization



\mathcal{P}^1 cont.



\mathcal{P}^1 discont.



\mathcal{P}^2 discont.

Time discretization

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0 \\ -\operatorname{div}(\rho \boldsymbol{\sigma}(\rho, \mathbf{v}, \mathbf{p})^\top) + C_F \mathbf{v} &= T_a \mathbf{p} + \operatorname{div}(\rho \boldsymbol{\sigma}_a(\mathbf{p})) \\ Pe_\rho \left(\frac{\partial \mathbf{p}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{p} - \nabla \mathbf{v} \cdot \mathbf{p} \right) + \frac{\partial \mathcal{F}}{\partial \mathbf{p}}(\rho, \mathbf{p}) &= 0\end{aligned}$$

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→ nonlinear problem in $X_h^n = (\mathbf{v}_h^n, \rho_h^n, \mathbf{p}_h^n)$: $X_h^n = G(X_h^n)$

Time discretization

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0 \\ -\operatorname{div}(\rho \boldsymbol{\sigma}(\rho, \mathbf{v}, \mathbf{p})^\top) + C_F \mathbf{v} &= T_a \mathbf{p} + \operatorname{div}(\rho \boldsymbol{\sigma}_a(\mathbf{p})) \\ Pe_\rho \left(\frac{\partial \mathbf{p}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{p} - \nabla \mathbf{v} \cdot \mathbf{p} \right) + \frac{\partial \mathcal{F}}{\partial \mathbf{p}}(\rho, \mathbf{p}) &= 0 \end{aligned}$$

→ nonlinear problem in $X_h^n = (\mathbf{v}_h^n, \rho_h^n, \mathbf{p}_h^n)$: $X_h^n = G(X_h^n)$

→ fixed-point loop: $X_h^{n,k} = G(X_h^{n,k-1})$

Positivity preserving time scheme for ρ

A-BDF of order 2:

$$\left(\text{Id} - \frac{2\Delta t}{3(1-\theta)} A_h^{\text{upw},n} \right) \rho_h^n = \frac{4}{3(1-\theta)} \rho_h^{n-1} - \frac{1+3\theta}{3(1-\theta)} \rho_h^{n-2} - \frac{2\theta\Delta t}{1-\theta} A_h^{\text{upw},n-1} \rho_h^{n-1}$$

where $A_h^{\text{upw},n}$ is a positivity-preserving operator discretising transport terms using the dG upwind method at time n

Positivity preserving time scheme for ρ

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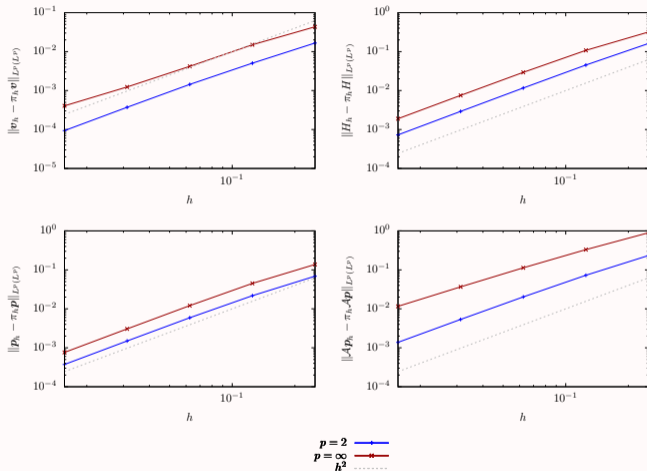
where $\mathbf{A}_h^{\text{upw},n}$ is a positivity-preserving operator discretising transport terms using the dG upwind method at time n

Positivity limiter (mean conservative):

$$\tilde{\rho}_{h|K}(\mathbf{x}) = \nu_K (\rho_{h|K}(\mathbf{x}) - \langle \rho_h \rangle_K) + \langle \rho_h \rangle_K$$

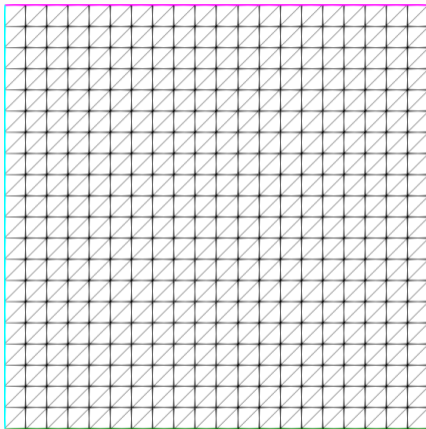
where $\nu_K = \min_{\text{nodes } \mathbf{v}_K \text{ of } K} \min \left(1, \frac{\langle \rho_h \rangle_K}{\langle \rho_h \rangle_K - \rho_{h|K}(\mathbf{v}_K)} \right)$

Numerical convergence



$L^2(L^2)$ and $L^\infty(L^\infty)$ errors in 2D, with respect to h . $A p$ denotes $\kappa^2 \operatorname{div}(\rho \nabla p)$.

Boundary conditions



800 triangles, $h_{\min} = 0.1$, $h_{\max} = \sqrt{2}/10$

No-penetration condition:

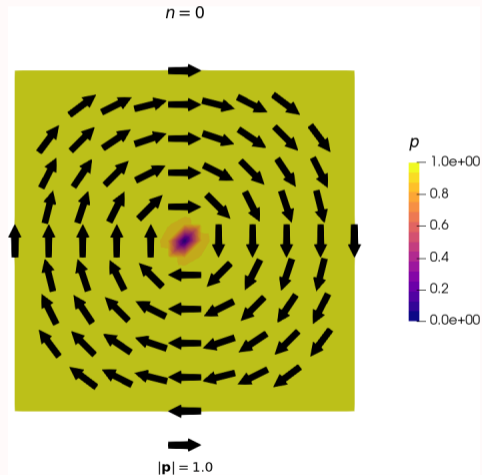
$$\mathbf{v} \cdot \mathbf{n} = 0$$

$$\mathbf{n} \cdot \boldsymbol{\sigma} = (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n}$$

Neumann condition for the polarity:

$$\kappa^2 \rho \frac{\partial \mathbf{p}}{\partial \mathbf{n}} = 0$$

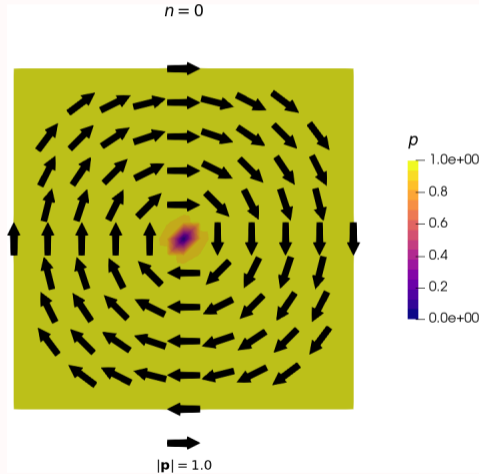
Numerical experiment (1)



Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
0.4	0.4	0.89	0.1	0.316	0	2	100

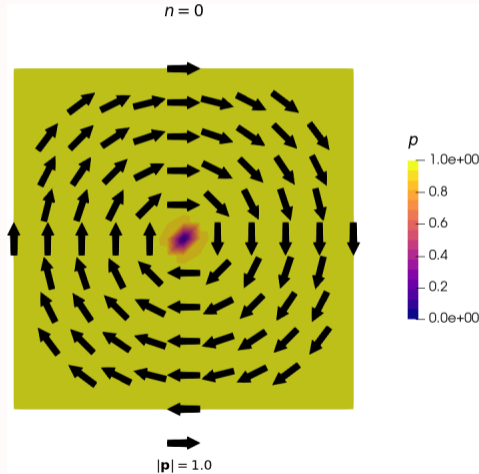
Numerical experiment (2)



Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
0.4	0.4	2.83	0.1	0.316	0	2	100

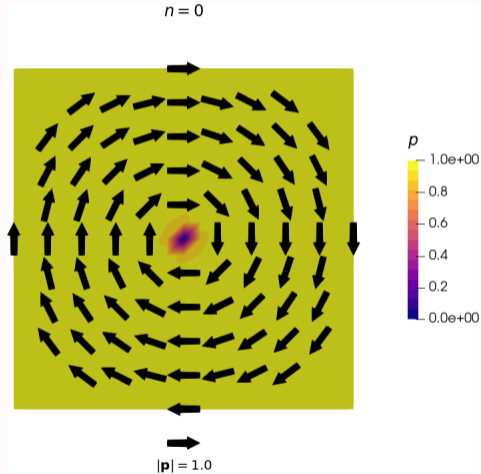
Numerical experiment (3)



Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
0.4	0.4	8.94	0.1	0.316	0	2	100

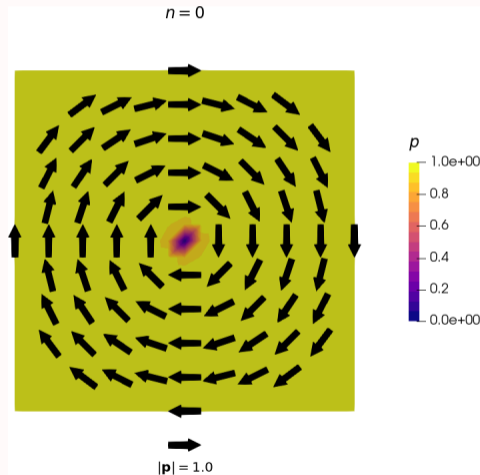
Numerical experiment (4)



Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
0.4	0.4	0.89	10	0.316	0	2	100

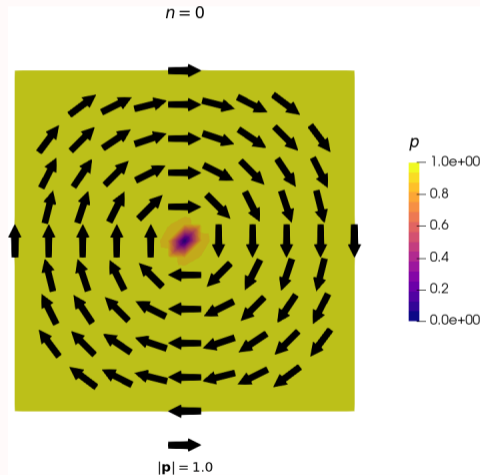
Numerical experiment (5)



Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
0.4	0.4	2.83	10	0.316	0	2	100

Numerical experiment (6)

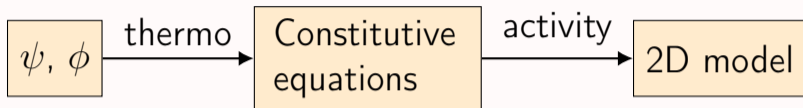


Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
0.4	0.4	2.83	10	0.316	0.01	2	100

To sum up

1. 2D thermodynamic framework:



2. Energy estimate:

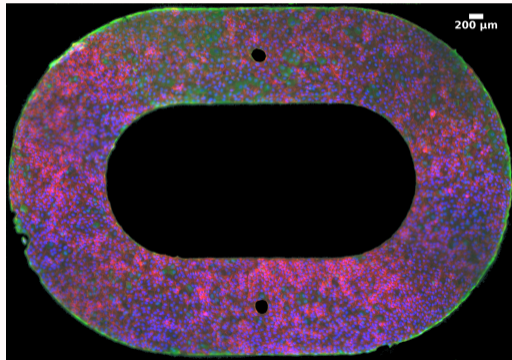
$$\frac{d\mathcal{F}}{dt} + \int_{\Omega} \left(2\rho |\mathbf{D}(\mathbf{v})|^2 + 2\rho |\operatorname{div} \mathbf{v}|^2 + \frac{1}{Pe\rho} \left| \frac{\partial \mathcal{F}}{\partial \mathbf{p}} \right|^2 + C_F |\mathbf{v}|^2 \right) \quad \text{dissipation}$$
$$= \int_{\Omega} \left(T_a \mathbf{p} \cdot \mathbf{v} + \sigma_a \rho \mathbf{p} \otimes \mathbf{p} : \mathbf{D}(\mathbf{v}) + \sigma_a \rho |\mathbf{p}|^2 \operatorname{div} \mathbf{v} \right) \quad \text{activity} \quad (7)$$

Future work: model exploration and comparisons with experiments

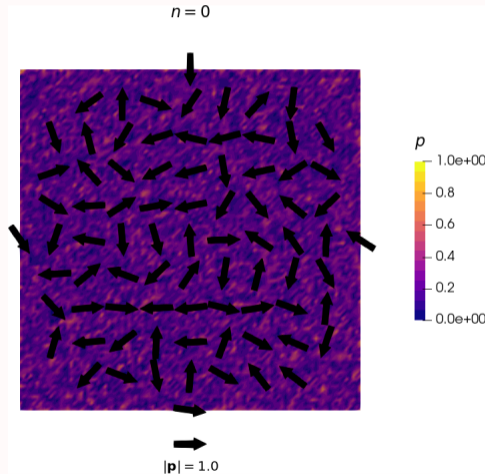
Role of domain size and correlation length κ

Influence of density ρ on the dynamics (for smaller c_0)

Does the polarity p remain bounded? Role of B



Topological defects



Parameters:

C_F	T_a	σ_a	Pe	κ	B	γ	c_0
40	40	2.83	0.1	0.01	0	2	100

Asymptotic: example

$$-\operatorname{div} \boldsymbol{\sigma}^\top = 0$$

$$x_3 = x_3^{(1)} \epsilon$$

$$\boldsymbol{\sigma}_{ss} = \boldsymbol{\sigma}_{ss}^{(0)} + \boldsymbol{\sigma}_{ss}^{(1)} \epsilon + \mathcal{O}(\epsilon^2)$$

$$\boldsymbol{\sigma}_{3s} = \boldsymbol{\sigma}_{3s}^{(0)} + \boldsymbol{\sigma}_{3s}^{(1)} \epsilon + \mathcal{O}(\epsilon^2)$$

$$\Rightarrow -\operatorname{div}_s(\boldsymbol{\sigma}_{ss}^{(0)}) = \partial \boldsymbol{\sigma}_{3s}^{(1)} / \partial x_3^{(1)}$$

$$\Rightarrow -\operatorname{div}_s(h \langle \boldsymbol{\sigma}_{ss}^{(0)} \rangle_h) = \boldsymbol{\sigma}_{3s}^{(1)}(x_3 = h) - \boldsymbol{\sigma}_{3s}^{(1)}(x_3 = 0)$$

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$$\Rightarrow -\operatorname{div}_s(h \langle \boldsymbol{\sigma}_{ss}^{(0)} \rangle_h) = \cancel{\boldsymbol{\sigma}_{3s}^{(1)}(x_3 = h)} - \boldsymbol{\sigma}_{3s}^{(1)}(x_3 = 0)$$

Edelen's decomposition

Let $(E, (\cdot | \cdot))$ be a Euclidean vector space and $\mathcal{J} \in \mathcal{C}^1(E)$.

$$(\mathcal{X} | \mathcal{J}(\mathcal{X})) \geq 0 \iff \begin{cases} \exists! \phi: E \rightarrow \mathbb{R}^+ \text{ and } \mathcal{U}: E \rightarrow E \text{ s.t.} \\ \phi(0_E) = 0 \text{ and } \mathcal{U}(0_E) = 0_E \\ (\mathcal{X} | \mathcal{U}(\mathcal{X})) = 0 \\ \mathcal{J}(\mathcal{X}) = \frac{\partial \phi}{\partial \mathcal{X}}(\mathcal{X}) + \mathcal{U}(\mathcal{X}) \end{cases}$$

Conservation laws

linear momentum

$$\operatorname{div}(\rho \boldsymbol{\sigma}) + \mathbf{f}_{\text{ext}} = 0$$

angular momentum

$$\sigma_{12} - \sigma_{21} = 0$$

Conservation laws

linear momentum

$$\operatorname{div}(\rho \boldsymbol{\sigma}^{\top}) + \mathbf{f}_{\text{ext}} = 0$$

angular momentum

$$\operatorname{div}(\rho \mathbf{c}) + \rho(\sigma_{12} - \sigma_{21}) = 0$$

where

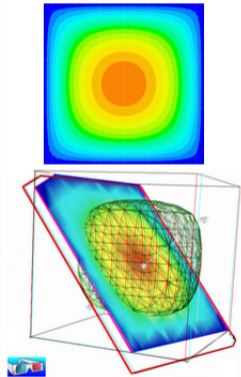
\mathbf{c} : couple stress

$\mathbf{k} = \nabla \omega$: curvature-twist rate

$\omega = \frac{1}{2} \operatorname{curl} \mathbf{v} = \frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2}$: vorticity

Rheolef (C++)

<http://www-ljk.imag.fr/membres/Pierre.Saramito/rheolef>



Example: find u such that $-\Delta u = 1$ in Ω and $u = 0$ on $\partial\Omega$

```
int main (int argc, char** argv) {  
  environment rheolef (argc, argv);  
  geo omega (argv[1]);  
  space Xh (omega, argv[2]);  
  Xh.block ("boundary");  
  trial u (Xh); test v (Xh);  
  form a = integrate (dot(grad(u), grad(v)));  
  field lh = integrate (v);  
  field uh (Xh);  
  uh ["boundary"] = 0;  
  problem p (a);  
  p.solve (lh, uh);  
  dout << uh;  
}
```

Let $\Omega \subset \mathbb{R}^N$, $N = 1, 2, 3$

$X_h = \{v \in H^1(\Omega); v|_K \in P_k, \forall K \in \mathcal{T}_h\}$

$V_h = X_h \cap H_0^1(\Omega)$

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx$$

$$l(v) = \int_{\Omega} v \, dx$$

(P) : find $u_h \in V_h$ such that

$$a(u_h, v_h) = l(v_h), \quad \forall v_h \in V_h$$