A new continuum theory for incompressible swelling materials

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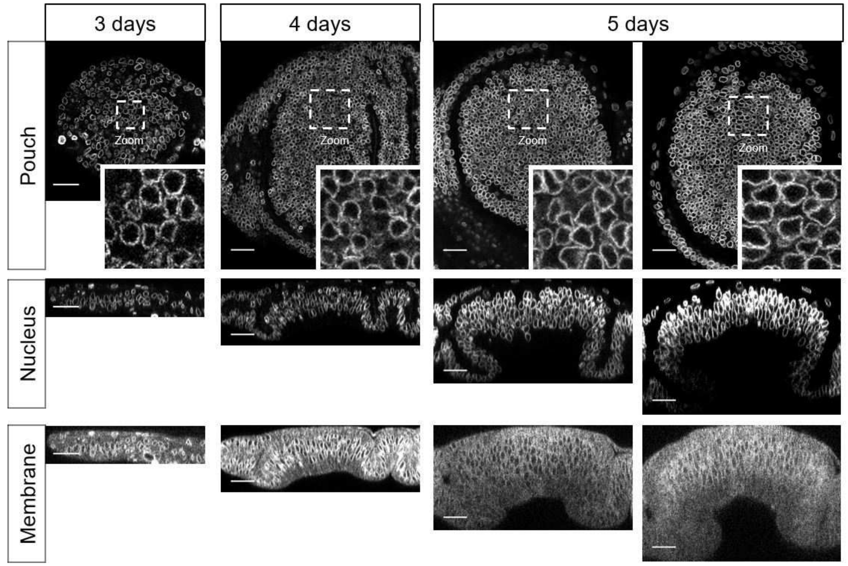
Summary

1. Introduction

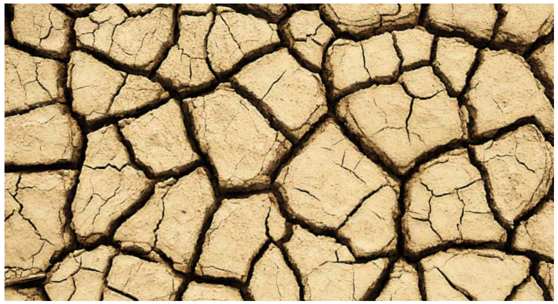
Swelling or drying media



Examples

- Tissues (development)
- Cancer (tumor growth)
- Geosciences (soil)
- Cooking (dough, pasta)

Important applications



Solid mechanics models

- Hyperelasticity + growth tensor
- [Ben Amar, Goriely, Chaplain, . . .]

Fluid mechanics models

- Based on Darcy's law
- [Bertsch, Preziosi, Lowengrub, Oden, Byrne, Spreckels, . . .]

Why Darcy's law ?

General framework

packed medium: uniform density $n = 1$

continuity eq.: $\nabla \cdot v = q =$ growth rate (given)

How to determine the velocity v ? (closure problem)

one scalar equation for a vector

can only determine v in 1-D

Darcy's law: $v = -k \nabla p$ (with $p =$ pressure)

gives the simplest answer

but the simpler needs not be the better

validity discussed in [Ambrosi-Preziosi]

Goal: revisit the closure problem

assuming simple heuristics

assess validity of Darcy's closure

Other modelling features

Packing heuristics: derived from compressible dynamics

incompressible limit [Perthame-Quiros-Vazquez, Hecht-Vauchelet]

Leads to a free boundary problem

for the boundary of the tumor [Friedman]

akin to Hele-Shaw free-boundary problem in fluid mechanics

Cell-based models

off lattice models [Drasdo, . . .],

cellular automata, cellular Potts models [Merks, . . .]

coarse-grained into Hele-Shaw model in [Motsch-Peurichard]

Current work

use packing heuristics

take inspiration from micro model to build continuum one

Modelling assumptions

Rule 1: non-overlapping particles in external potential

minimize mechanical energy under non-overlapping constraints

Potential and particle volume evolve in time

adiabatic particle motion

particles stay at energy minimum under packing constraints

Rule 2: particles cannot swap positions

Rule 3: Displacement between "successive positions" is minimal

Goal: derive particle model (P), then, continuum model (C)

but no formal convergence (P) $\to$ (C)

analogy with crowd models [Maury, Roudneff-Chupin, Santambrogio]

2. Microscopic background

N spheres, positions $x_i \in \mathbb{R}^d$; radii $R_i > 0$, $i = 1, \ldots, N$

Denote $\mathcal{X} = (x_i)_{i=1,\ldots,N}$, $\mathcal{R} = (R_i)_{i=1,\ldots,N}$

External potential $V(x, R)$

Energy $E_{\mathcal{R}}(\mathcal{X}) = \sum_{i=1}^{N} V(x_i, R_i)$

Admissible (non-overlapping) configurations:

$$\mathcal{A}_{\mathcal{R}} = \{\mathcal{X} \mid |x_i - x_j| \geq R_i + R_j, \forall i \neq j\}$$

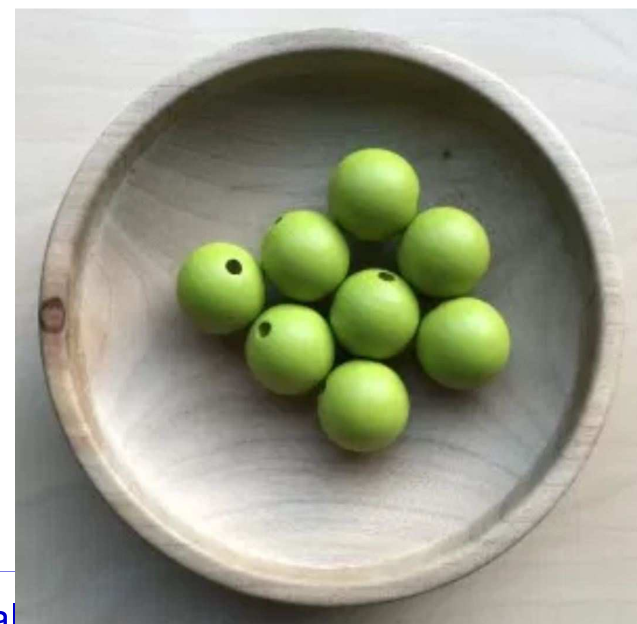
Seek $\mathcal{X}$ a solution of the problem $\min_{\mathcal{X} \in \mathcal{A}_{\mathcal{R}}} E_{\mathcal{R}}(\mathcal{X})$

Non-convex problem

multiple solutions

for numerical resolution:

[Maury, D-Ferreira-Motsch, ...]



Adiabatic evolution problem

Time-varying potential $V = V(x, R, t)$ and radii $\mathcal{R} = \mathcal{R}(t)$

Energy $E_{\mathcal{R},t}(\mathcal{X}) = \sum_{i=1}^N V(x_i, R_i, t)$

$\mathcal{X}(t)$ a solution of $\min_{\mathcal{X} \in \mathcal{A}_{\mathcal{R}(t)}} E_{\mathcal{R}(t),t}(\mathcal{X})$

Problem: find a smooth trajectory $\mathcal{X}(t)$ and define $\mathcal{V}(t) = \frac{d}{dt}\mathcal{X}(t)$

Time-discretization Δt; define $t^k = k\Delta t$, $\mathcal{X}^k = \mathcal{X}(t^k)$, ...

$\mathcal{X}^k$ solves $\min_{\mathcal{X} \in \mathcal{A}_{\mathcal{R}^k}} E_{\mathcal{R}^k,t^k}(\mathcal{X})$

increment $k \to k+1$

$\mathcal{X}^k$ not a solution of $\min_{\mathcal{X} \in \mathcal{A}_{\mathcal{R}^{k+1}}} E_{\mathcal{R}^{k+1},t^{k+1}}(\mathcal{X})$

Find a solution $\mathcal{X}^{k+1}$ as close as possible to $\mathcal{X}^k$

i.e. $\mathcal{V}^{k+1/2} = \frac{1}{\Delta t}(\mathcal{X}^{k+1} - \mathcal{X}^k)$ as small as possible

stated as "minimal displacement rule"

$\Rightarrow$ "non-swapping rule" (otherwise large displacements)

Comments on microscopic description

Strategy proposed for crowd motion

[Maury, Venel, Roudneff-Chupin, Santambrogio, Al Reda . . .]

Strategy applied for tumor growth modelling

[Leroy-Leretre, . . .]

Finding a theoretical solution is difficult

minimization problem non-convex

solution not unique

many closeby local minima

Problem is simpler in a continuum description

goal of this work

3. Continuum model: equilibrium

Continuum equilibrium problem

Given: particle average volume $\tau(x)$; external potential $V(x,\tau)$

unknown is particle density $n(x)$

Total number of particles $\int n(x)\,dx = N$ is fixed

energy $F_\tau[n] = \int V(x,\tau(x))\,n(x)\,dx$

non-overlapping condition $n\,\tau \leq 1$

admissible config: $\mathcal{A}_{\tau,N} = \{n \mid n \geq 0,\ n\tau \leq 1,\ \int n(x)\,dx = N\}$

seek a solution n to $\quad \min_{n \in \mathcal{A}_{\tau,N}} F_\tau[n]$

Assumptions

define $W(x) = V(x,\tau(x))$ (effective potential). Assume:

$W \to \infty$ as $|x| \to \infty$

$W(0) = 0$, $W(x) \geq 0$ and 0 is the only critical point of W

level sets $\{W(x) = u\}$ compact, connected, > 0 measure

$\int \tau^{-1}(x)dx \geq N$

Equilibrium problem: solution

Under the previous assumptions

and other technical assumptions (skipped)

problem $\min_{n\in\mathcal{A}_{\tau,N}} F_\tau[n]$ has a unique solution

Given by

$$n(x) = \begin{cases} \tau^{-1}(x) & \text{if } x \in \Omega_N \\ 0 & \text{otherwise} \end{cases}$$

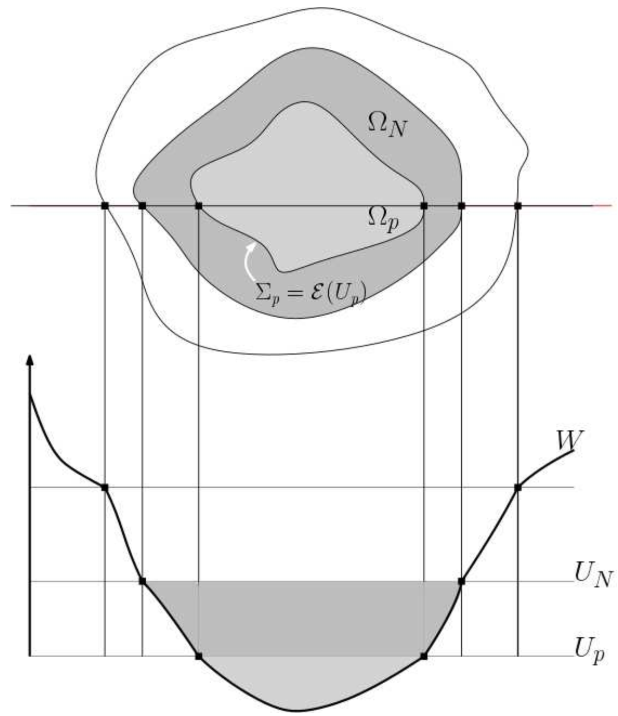
$\Omega_N = \{x \in \mathbb{R}^d \mid 0 \le W(x) \le U_N\}$

U_n s.t. $P(U_n) = N$

$P(u) = \int_{0\le W(x)\le U} \tau^{-1}(x)\, dx$

$P(u) =$ number of particles enclosed

by level set $\{W(x) = u\}$



4. Movement: non-swapping condition

Suppose $V = V(x,t,\tau)$, $\tau = \tau(x,t)$

at each t, gives solution $n(t) = n(\cdot,t)$ of previous min problem

with frozen t, i.e. with $V(t) = V(\cdot,t,\cdot)$, $\tau(t) = \tau(\cdot,t)$

and $\int n(x,t)\,dx = N =$ constant (no source/sink of particles)

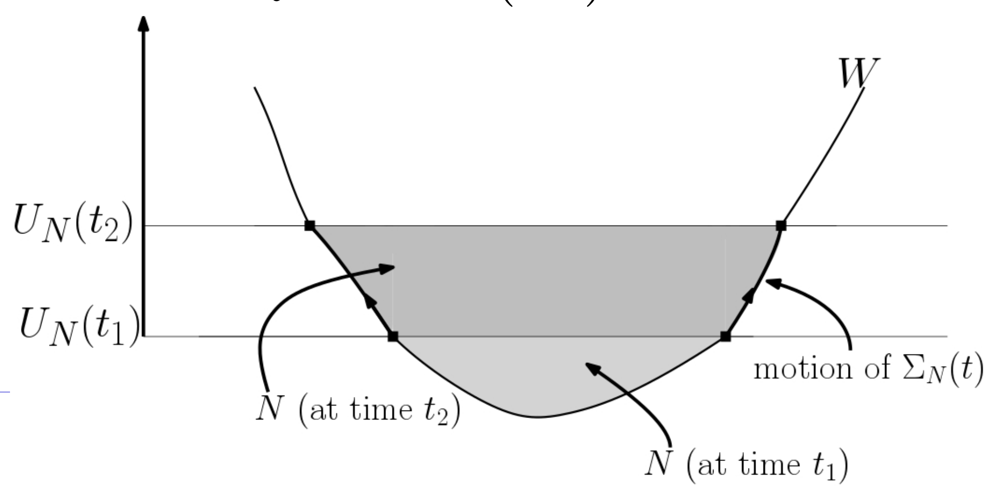
energy $F_{\tau(t),t}[n] = \int V(x,\tau(x,t),t)\,n(x)\,dx$

admissible configuration: $\mathcal{A}_{\tau(t),N} =$

$\{n \mid n \geq 0,\, n\tau(t) \leq 1,\, \int n(x)\,dx = N\}$

$n(t) =$ the solution to $\min_{n \in \mathcal{A}_{\tau(t),N}} F_{\tau(t),t}[n]$

Goal: define v s.t. $\partial_t n + \nabla \cdot (nv) = 0$



Continuity eq. is an eq. for v since n is known

But scalar eq. for a vector quantity v: requires more conditions

Note $\Pi(x,t) = P(W(x,t),t) = \#$ of particles in domain limited

by level set $\Sigma_p(t) = \{y \,|\, W(y,t) = W(x,t)\}$ with $p = \Pi(x,t)$

$\Sigma_p(t) = \{y \,|\, \Pi(y,t) = p\} = \partial\Omega_(t)$, $\quad \Omega_p(t) = \{y \,|\, \Pi(y,t) \leq p\}$

Non-swapping condition:

Two close particles are on the same level set $\Sigma_{p_0}(t_0)$ at time t_0 iff

they are on the same level set $\Sigma_{p(t)}(t)$ for all t close to t_0

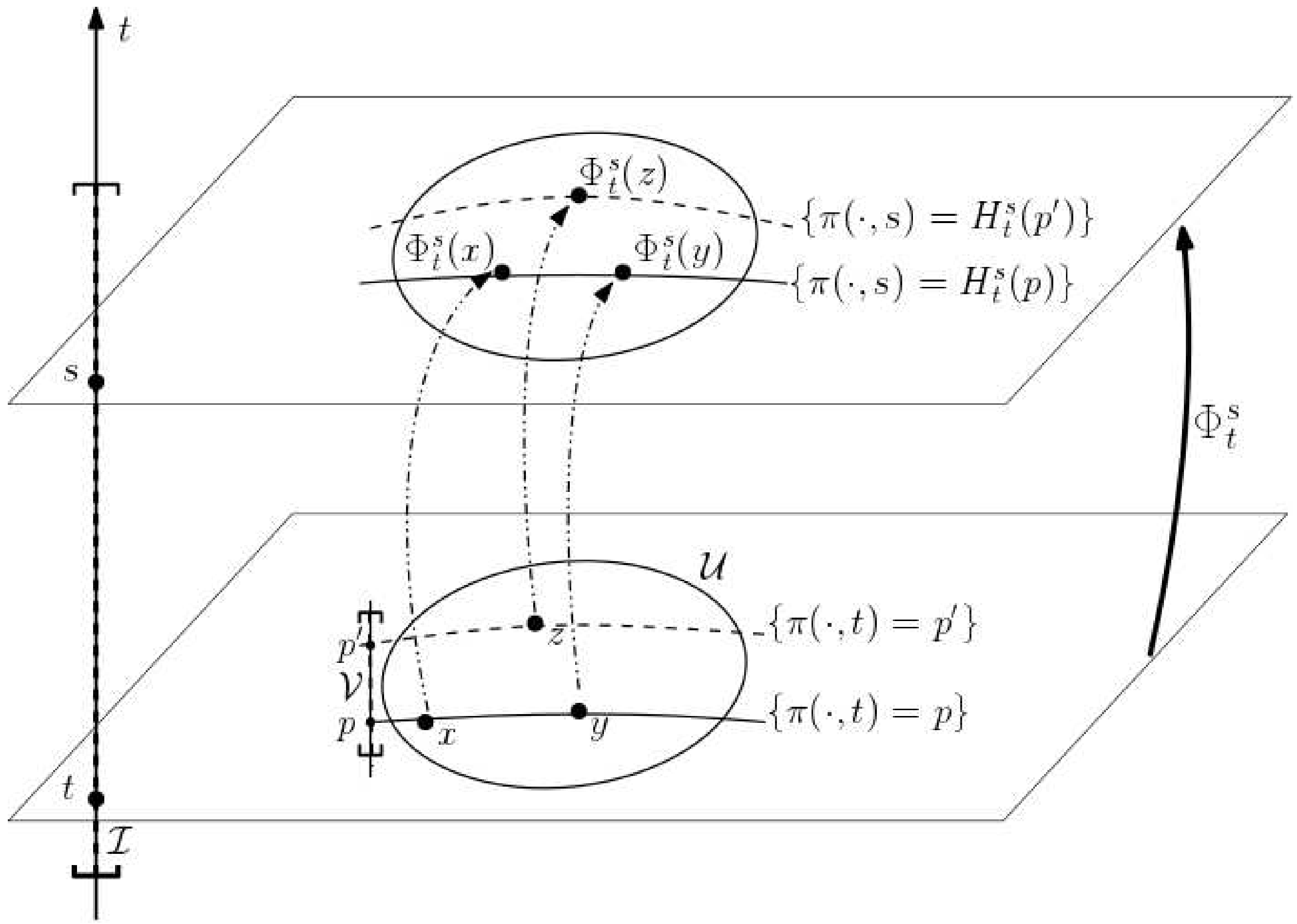
In dimension $d = 1$: non-swapping condition trivially satisfied

v uniquely determined by continuity condition

In dimension $d \geq 2$: non-swapping condition non-trivial

determines the component of v normal to $\Sigma_p(t)$

Graphical view of non-swapping condition



Thm ($d \geq 2$): Non-swapping condition $\Leftrightarrow$

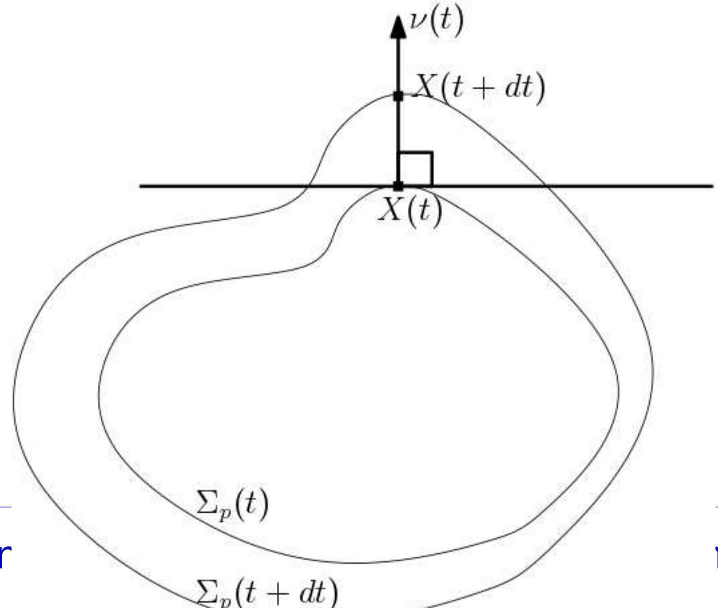
For each particle, $\exists$ unique p s.t. particle $\in \Sigma_p(t)$, $\forall t$

$\Leftrightarrow$ let $X(t)$ satisfy $\dot{X}(t) = v(X(t), t)$ with v satisfying continuity eq. Then $\exists p \geq 0$ such that $\Pi(X(t), t) = p$, $\forall t$

$\Rightarrow$ Normal velocity to $\Sigma_p(t)$ uniquely determined

$$v \cdot \nu = -\frac{\partial_t \Pi}{|\nabla \Pi|}$$

where $\nu = \frac{\nabla \Pi}{|\nabla \Pi|}$ = normal to $\Sigma_p(t)$ with $p = \Pi(x,t)$



5. Movement: minimal displacement condition

$$v = v_\perp + v_\parallel, \quad v_\perp = (v \cdot \nu)\nu = -\frac{\partial_t \Pi}{|\nabla \Pi|} \frac{\nabla \Pi}{|\nabla \Pi|}, \quad \text{in general } v_\parallel \neq 0$$

$v_\parallel$ satisfies continuity eq. (with $n = \tau^{-1}$)

$$\nabla.(\tau^{-1} v_\parallel) = f, \quad f = -\partial_t \tau^{-1} - \nabla \cdot (\tau^{-1} v_\perp) \quad \text{known from above}$$

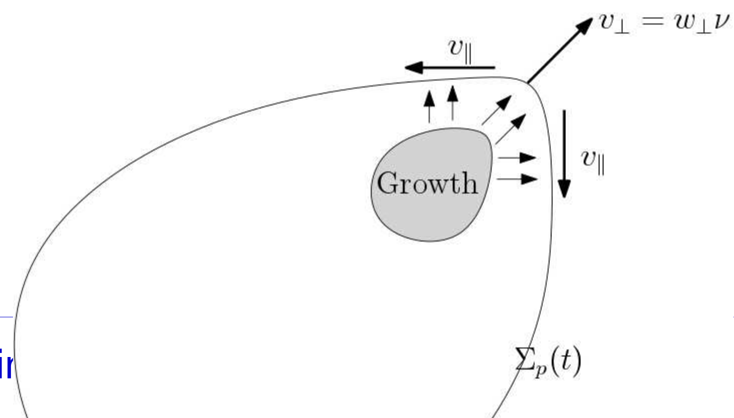
Lemma (solvability condition)

Suppose a tangent vector field A to Σ_p is such that $\nabla_\parallel \cdot A = f$

Then, f must satisfy the constraint $\int_{\Sigma_p} f(x) \frac{d\Sigma_p(x)}{|\nabla \Pi|} = 0$

Theorem: $f = -\partial_t \tau^{-1} - \nabla \cdot (\tau^{-1} v_\perp)$ satisfies this constraint

guarantees the existence of $v_\parallel$ satisfying the continuity eq.



$v_\parallel$ not unique: uniqueness requires additional rule

principle of minimal displacements

$v_\parallel$ minimizes kinetic energy $T[w_\parallel] = \int_{\Sigma_p} |w_\parallel(x)|^2 \, g(\tau(x)) \, \frac{d\Sigma_p(x)}{|\nabla \Pi|}$

with g appropriate weight (standard KE: $g(\tau) = \tau^{1-\frac{1}{d}}$)

among fields $w_\parallel$ s.t. $\nabla_\parallel \cdot (\tau^{-1} w_\parallel) = f$

$$v_\parallel = \text{arg}\min\{T[w_\parallel] \, , \; w_\parallel \text{ s.t. } \nabla_\parallel \cdot (\tau^{-1} w_\parallel) = f\}$$

Minimization problem has a unique solution

$$v_\parallel = -(g\tau)^{-1} \, \nabla_\parallel \theta$$

where $\theta =$ unique solution in $H_0^1(\Sigma_p)$ of

$$-\nabla_\parallel(\tau^{-2} g^{-1}(\tau) \nabla_\parallel \theta) = f \quad \text{on } \Sigma_p, \, \forall p$$

with $H_0^1(\Sigma_p) = \{\theta \in H^1(\Sigma_p) \, | \, \int_{\Sigma_p} \theta(x) \, \frac{d\Sigma_p(x)}{|\nabla \Pi|} = 0\}$

6. Determination of volumic growth

Summary of model

Equilibrium under non-overlapping constraint: at any time t

$$n(x,t) = \begin{cases} \tau^{-1}(x,t) & \text{if } x \in \Omega_N(t) \\ 0 & \text{otherwise} \end{cases}$$

$$\Omega_p(t) = \{x \,|\, 0 \leq \Pi(x,t) \leq p\}, \quad \Sigma_p(t) = \{x \,|\, \Pi(x,t) = p\}$$

$$\Pi(x,t) = \int_{0 \leq W(y,t) \leq W(x,t)} \tau^{-1}(y,t)\, dy$$

Movement: normal velocity to Σ_p (non-swapping condition)

$$v_\perp = -\frac{\partial_t \Pi}{|\nabla \Pi|} \frac{\nabla \Pi}{|\nabla \Pi|}$$

Movement: parallel velocity (minimal displacement rule):

$v_{||} = -(g\tau)^{-1} \nabla_{||}\theta$ and $\theta =$ unique (average zero) solution of

$$-\nabla_{||}(\tau^{-2} g^{-1}(\tau) \nabla_{||}\theta) = f \quad \text{on } \Sigma_p,\ \forall p$$

In practice, τ not given a priori. Depends on v instead

Determination of τ

Swelling rate $=$ Lagrangian quantity attached to each particle

$(\partial_t + v \cdot \nabla)\tau = q(x,t,\tau)$ with $q =$ swelling rate

$\Rightarrow$ nonlinear coupling between τ and v

v must be smooth enough to make sense of eq. for τ

Suppose V and $\tau_0 := \tau|_{t=0}$ are C^∞. Denote $\mathbb{R}^d_* = \mathbb{R}^d \setminus \{0\}$

Lemma: $\tau \in C^\infty(\mathbb{R}^d_* \times [0,T]) \Rightarrow v \in C^\infty(\mathbb{R}^d_* \times [0,T])$

Note: possible singularity at $x=0$ as $x=0$ critical for W

Conversely

$\tau \in C^\infty(\mathbb{R}^d_* \times [0,T]) \Rightarrow v \in C^\infty(\mathbb{R}^d_* \times [0,T])$ if characteristics issued from $x \neq 0$ do not reach $x=0$ or ∞ in finite time

Lemma: Assume $q(x,t,\tau) = \bar{q}(x,t)\tau$ and $\exists C>0$ s.t. $|\bar{q}| \leq C$, and $C^{-1} \leq \tau_0 \leq C$. Then, no characteristics issued from $x \neq 0$ reaches $x=0$ or ∞ in finite time

7. Conclusion and perspectives

New rule-based model for swelling materials

- non-overlapping / non-swapping / minimal displacements

$\neq$ from Darcy law and Hele-Shaw model:

- in HS / Darcy, $v_{\|} = 0$ at the domain boundary. Here $v_{\|} \neq 0$

Perspectives (modelling)

- contact interactions between nearby particles
- cell division
- fuzzy tumor boundary ($\approx$ finite temperature)
- coupling to chemical signaling or nutrient transport
- statistical description of particle sizes
- multiple particle species

Perspective (theory)

- existence / uniqueness
- derivation from micro model
- derivation from singular limits of other macro models