

# Interface motions via Optimal transport

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# Examples of Interface motions

- Tumor growth (Hele-Shaw flow)
- Water and Oil in a container (Muskat problem)
- Melting and Freezing of Ice (Stefan problem)

# Main goals

Based on their energy dissipation structure, we hope to achieve:

- Formulation of interface motions via optimization schemes;
- Global well-posedness past topological changes;
- Analysis of interface motions from variational perspective...

# Hele-Shaw flow: Motion laws

A model problem:

$$\rho_t - \nabla \cdot (\nabla p \rho) + \nabla \cdot (\vec{v} \rho) = 0,$$

# Gradient flow formulation Maury, Roudneff-Chupin and Santambrogio, 2010

When  $\vec{v} = \nabla\Phi$ , this problem can be formulated as the gradient flow of the energy

$$E(\rho) = \int \Phi(x)\rho dx \quad \text{if } \rho \leq 1; \quad \text{otherwise } \infty,$$

in the 2-Wasserstein space

$$d^2(\rho_1, \rho_2) := \inf \left\{ \int_{\Omega \times \Omega} |x - y|^2 d\gamma, \gamma \in \Pi(\mu, \nu) \right\}$$

for probability measures supported in  $\Omega$ .

$$\rho_t - \nabla \cdot (\nabla p + \nabla \Phi \rho) = 0.$$

# Gradient flow: review

Gradient flow : “Steepest decent”

$$\frac{d\rho}{dt}(\cdot, t) = -\nabla E(\rho(\cdot, t))$$

Derivatives on both sides depend on the structure of the (Riemannian) metric space. We consider the space of probability measures with finite second moments, with the  $W_2$  distance

$$W_2^2(\rho_1, \rho_2) := \inf_{T \# \rho_1 = \rho_2} \int |x - T(x)|^2 d\rho_1,$$

among measure-preserving maps  $T$ .

The formal Riemannian structure on  $W_2$ -space, as well as the resulting discrete-time optimization scheme is introduced by Otto (1999). In this setting the gradient flow can be written as the continuity equation

$$\rho_t - \nabla \cdot (\nabla E \rho) = 0.$$

# Minimizing movement Jordan, Kinderlehrer, Otto (1998),

A discrete-time variational scheme (or JKO scheme): For each time  $t = k\tau$  the solution  $\rho_\tau^k := \rho(x, k\tau)$  solves

$$\rho_\tau^k := \operatorname{argmin}_\rho [E(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_\tau^{k-1})].$$

This is an iterative scheme, where  $\rho_\tau^k$  is generated based on the previous data  $\rho_\tau^{k-1}$ . The hope is to now send  $\tau \rightarrow 0$  to recover the original continuum limit.

Note that, as long as  $E$  is "semi-convex", for sufficiently small  $\tau$  the minimization is convex, and thus it presents a unique and stable minimizer.

# Backward Euler Scheme

In finite dimensions  $\mathbb{R}^n$ , if we replace  $W_2$  by Euclidean distance, then it corresponds to the Implicit Euler Scheme

$$x_\tau^k := \operatorname{argmin}\left[F(x) + \frac{1}{2\tau}|x - x^{k-1}|^2\right],$$

which converges to the finite dimensional gradient flow

$$\dot{x} = -\nabla F(x) \quad \text{in } \mathbb{R}^n$$

as  $\tau \rightarrow 0$ .



# Energy Dissipation inequality

The JKO scheme is a natural approximation to the PDE system with a formal gradient flow structure in  $W_2$  space. Its discrete-time solutions satisfy

$$E(\rho(\cdot, t)) - E(\rho(\cdot, s)) + \frac{1}{2\tau} \sum_{k=\frac{t}{\tau}}^{\frac{s}{\tau}} W_2^2(\rho^k, \rho^{k-1}) \leq 0.$$

or, by Benamou-Brennier formula,

$$E(\rho(\cdot, t)) - E(\rho(\cdot, s)) + \frac{\tau}{2} \sum_{k=\frac{t}{\tau}}^{\frac{s}{\tau}} \int \left| \frac{\nabla \varphi_k}{\tau} \right|^2 \rho_k dx \leq 0, \quad \nabla \varphi_k(x) = x - T_k(x).$$

## Energy dissipation inequality

In the continuum limit, the limit solution is thus endowed with the *energy dissipation inequality*

$$E(\rho(\cdot, t)) - E(\rho(\cdot, s)) + \frac{1}{2} \int_s^t \int |\vec{b}|^2 d\rho_\tau d\tau \leq 0,$$

Where  $\vec{b}$  is the velocity for the limit density  $\rho$ , or the limit of the discrete transport velocity  $\frac{\nabla\varphi_k}{\tau}$ . We expect then the continuum solution to solve

$$\rho_t - \nabla \cdot (\rho \vec{b}) = 0.$$

In the next slides we will show that  $\vec{b}$  corresponds to  $\nabla E = \nabla p + \nabla \Phi$ .

EDI rules out weak solutions of the limit problem with certain pathological behavior. On the other hand, this is not enough in general to guarantee uniqueness.

## Duality review

To identify the we recall the following duality formulation. Recall that

$$\varphi^c(y) := \inf_x \left[ \frac{|x - y|^2}{2} - \varphi(x) \right].$$

For absolutely continuous and compactly supported  $\rho, \nu$ ,

$$\frac{1}{2} W_2^2(\rho, \nu) = \sup \left[ \int \varphi d\rho + \int \varphi^c d\nu \right],$$

where the maximum is achieved by a  $c$ -concave function  $\varphi^*$ , and the optimal transport map  $T$  transporting  $\rho$  to  $\nu$  is given by  $x - T(x) = \nabla \varphi(x)$ .

## Optimal map and energy gradient

When the energy is  $E(\rho) = \int L(\rho(x), x) dx$ , our one-step minimization

$$\rho_1 = \operatorname{argmin}_{\rho} \left[ E(\rho, x) + \frac{W_2^2(\rho, \rho_0)}{2\tau} \right]$$

yields that

$$\partial_{\rho} L(\rho_1, x) + \frac{\varphi(x)}{\tau} = 0.$$

Hence the discrete velocity is given as  $\frac{x-T(x)}{\tau} = \frac{\nabla\varphi^*(x)}{\tau} = -\nabla(\partial_{\rho} L(\rho_1, x)) (= \nabla E)$ .

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Hence the discrete velocity is given as  $\frac{x-T(x)}{\tau} = \frac{\nabla\varphi^*(x)}{\tau} = -\nabla(\partial_{\rho} L(\rho_1, x)) (:= \nabla E)$ .

Our energy is not of this form, but can be understood as the limit of the Rényi entropy

$$E_m(\rho) := \frac{1}{m-1} \int \rho^m dx + \int \Phi(x) \rho dx, \text{ as } m \rightarrow \infty.$$

and for this equation  $\nabla E_m(\rho) = \nabla p_m + \nabla \Phi$ , where  $p_m = \frac{m}{m-1} \rho^{m-1}$ . "Thus" for our energy

$$\nabla E(\rho) = \nabla p + \nabla \Phi, \text{ where } p \text{ is positive where } \rho = 1,$$

# Characterizing the discrete velocity

$$\rho^* = \operatorname{argmin} E(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_0) \quad i=1,2.$$

Here

Lemma

$\rho^*$  minimizes  $\int F(x)\rho(x)dx$ , where  $F = \Phi + \frac{1}{\tau}\varphi$  over  $\rho \in K$ .

From this lemma we conclude that  $p := (\ell - F)_+$  for some  $\ell$ , satisfying  $\nabla p + \nabla \Phi = -\frac{1}{\tau} \nabla \varphi$ .

Now for any  $\rho \in K$ , let  $\rho_\varepsilon := (1 - \varepsilon)\rho^* + \varepsilon\rho$ , and let us denote  $\varphi_\varepsilon$  as the Kantorovich potential for the pair  $(\rho_\varepsilon, \rho_0)$ . Then due to the dual formulation, we have

$$W_2^2(\rho_\varepsilon, \rho_0) - W_2^2(\rho^*, \rho_0) \leq \int 2\varphi_\varepsilon(\rho_\varepsilon - \rho^*)(x)dx = \varepsilon \int 2\varphi_\varepsilon(\rho - \rho^*)dx.$$

Combining with the potential energy, and taking  $\varepsilon \rightarrow 0$  we have

$$\int (\Phi(x) + \frac{1}{\tau}\varphi)\rho dx \geq 0,$$

and thus  $\rho^*$  minimizes  $\int F(x)\rho(x)dx$  for  $\rho \in K$ , with  $F = \Phi + \frac{1}{\tau}\varphi$ .

□

# Convergence: compactness

- For time variable, the energy dissipation inequality readily delivers some equicontinuity for density.

$$E(\rho(\cdot, t)) - E(\rho(\cdot, s)) + \frac{\tau}{2} \sum_{k=\frac{t}{\tau}}^{\frac{s}{\tau}} \int |\nabla p_k + \nabla \Phi|^2 \rho_k dx \leq 0,$$

- EDI above also yields space compactness ( $H^1(d\rho)$ ) for the discrete velocity variable, and thus pressure gradient.
- To obtain the continuum equation, we would need to show  $p(\rho - 1) = 0$ . This can be shown by using a space-time compensated compactness type argument (Santambrogio, 2018)



# Stability and convexity of the energy

- Given that the free energy is  $\lambda$ -convex, the gradient flows satisfy the estimate

$$\frac{d}{dt}W_2^2(\rho^1, \rho^2) \leq -2\lambda W_2^2(\rho^1, \rho^2).$$

In our case this is true if  $D^2V \geq \lambda Id$ . This yields stability in  $W_2$  (or  $H^{-1}$ ) distance.

- We will discuss a proof of  $L^1$  contraction, which yields  $L^1$ - stability between discrete solutions with different total mass. Here the convexity of  $E$  is also used.

# $L^1$ contraction and comparison principle.

Let us consider the one step minimization

$$\rho_i^* = \operatorname{argmin} E(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_i) \quad i=1,2.$$

Here  $\rho_1$  and  $\rho_2$  may have different total mass.

We are interested in proving the following theorem

## Theorem

*Jacobs-K-Tong, 2021*

$$\|(\rho_1^* - \rho_2^*)_+\|_{L^1} \leq \|(\rho_1 - \rho_2)_+\|_{L^1}.$$

*In particular, if  $\rho_1 \leq \rho_2$ , then the order is preserved with the scheme.*

Such result is well-known for the continuum equation, and is rather useful in obtaining stability properties of solutions. The proof generalizes that of K-Yao (2012), addressed for a specific energy.

# $L^1$ contraction: Key Lemma

Let  $T_i$  be a map such that for any  $x$ ,  $T_i(y)$  minimize  $\frac{|x-y|^2}{2\tau} + q_i(x)$  over all  $x$ .  
When  $\varphi_i = -q_i$  is the Kantorovich potential for  $W_2(\rho_i, \nu)$ ,  $T_i$  is the optimal map from  $\nu$  to  $\rho$ .

## Lemma

*If  $q_1, q_2$  are continuous and  $V := \{q_1 < q_2\}$ , then  $T_2^{-1}(V) \subset T_1^{-1}(V)$ .*

# $L^1$ contraction: Strictly convex energy

Let us approximate our singular energy by a strictly convex integral energy, for instance,

$$E_{m,\varepsilon}(\rho, x) := \int (\rho^m + \varepsilon\rho^2) + \int \Phi\rho dx.$$

Recall that  $\varphi(x) \in -\partial_\rho L(\rho, x)$ . Thus if  $L$  is strictly convex then  $\rho_1(x) > \rho_2(x)$  if and only if  $-\varphi_1(x) < -\varphi_2(x)$ .

# $L^1$ contraction: Proof

Let  $\varphi_i$  be the Kantorovich potential for  $\rho_i^*$ . Then  $\rho_i^* = (T_i)_\# \rho_i$  and

$$V = \{-\varphi_2 < -\varphi_1\} = \{\rho_2 < \rho_1\}.$$

Recall also that from the previous lemma  $T_1^{-1}(V) \subset T_2^{-1}(V)$ . Thus

$$\begin{aligned} \int (\rho_1^*(x) - \rho_2^*(x))_+ dx &= \int (\rho_1^*(x) - \rho_2^*(x)) \chi_V dx \\ &= \int \rho_1 \chi_{T_1^{-1}(V)} - \int \rho_2 \chi_{T_2^{-1}(V)} \\ &= \int (\rho_1 - \rho_2) \chi_{T_1^{-1}(V)} + \int \rho_2 [\chi_{T_1^{-1}(V)} - \chi_{T_2^{-1}(V)}] \\ &\leq \int (\rho_1 - \rho_2)_+ dx. \end{aligned}$$

- The proof presents the usage of dual variable in nonlocal way, in contrast to the usual proof of comparison principle or  $L^1$ -contraction. This is natural due to the nonlocality of the  $W_2$ -distance.
- $L^1$  contraction hints that we could control the gradient of the density in  $L^1$  norm (i.e. in  $BV$  norm), but it is unclear how to directly obtain this. For our specific problem, the  $BV$  norm can be controlled when the initial density is in  $BV$ , but with a very different proof De Philippis-Meszaros-Santambrogio-Velichkov, 2016.

# Convergence result

## Theorem

- *MRS 2010* Along a subsequence the discrete solutions  $\rho^\tau$  converge to  $\rho$  in  $L_t^\infty L_x^1$ , and  $p^\tau$  converges to  $p$  weakly in  $L_t^2 H_x^1$ . Moreover,  $0 \leq \rho \leq 1$ ,  $p \geq 0$  and

$$\rho_t - \nabla \cdot ((\nabla p + \nabla \Phi)\rho) = 0, \quad p(1 - \rho) = 0.$$

- *Alexander-K-Yao 2014* When  $\rho_0 = \chi_A$ , and if  $\Delta \Phi \geq 0$ , then  $\rho(\cdot, t) = \chi_{A(t)}$ , corresponding to the classical Hele-Shaw flow.

The global-time regularity of the interface  $\partial A(t)$  remains open in general. Regularity analysis usually requires PDE approach.

## Long time behavior: general challenges

- One can show that the long time limit of the discrete-time solutions always is a critical point of the energy. If there is only one critical point below the initial free energy, the solution converges to this critical point  $\rho_\infty$ .
- To obtain a rate of convergence, energy difference must bound the velocity from below. This step usually involves some functional/rearrangement inequality. This amounts to some version of local convexity property of the energy.

More precisely, we have from the minimizing movement

$$\frac{1}{2\tau} W_2^2(\rho_k, \rho_{k+1}) \leq E(\rho_k) - E(\rho_{k+1}).$$

So **if** we can also obtain

$$E(\rho_k) - E(\rho_\infty) \leq C \frac{1}{\tau^2} W_2^2(\rho_{k+1}, \rho_k) = C \int \left| \frac{\nabla \varphi}{\tau} \right|^2 dx.$$

Then we can conclude an exponential convergence.

Relevant literature: Otto-Villani (2000), Carrillo et al. (2001), Feldman (2019), Craig-K-Yao (2020), ...



The discrete-time scheme can be modified to address variations of the density-constrained model. We discuss one of the variations which exhibit interesting irregularity on the interface.

# Tumor growth model with Nutrients

One can consider replacing the drift term in our problem with a source term. A particular model describing tumor growth driven by nutrients is:

$$\begin{cases} \rho_t - \nabla \cdot (\rho \nabla p) = (n - \mu)\rho; \\ n_t - D\Delta n = -n\rho; \\ 0 \leq \rho \leq 1, p(1 - \rho) = 0. \end{cases}$$

In this system,  $\rho$  denotes the cell population density and  $n$  denotes the concentration of nutrients.  $\mu > 0$  denotes the death rate of the cells.

[Kitsunezaki 96, Quiros-Perthame-Vazquez 13, Maury-R. Chupin- Santambrogio 14, Jacobs-K-Tong 22]

# Minimizing movements

$$\rho_{k+1} = \operatorname{argmin}[E(\rho) + \frac{1}{2\tau} W_2^2(\rho, (1 + n_k - \mu)\rho_k)],$$

$$n_{k+1} = e^{\tau D\Delta}(n_k(1 - \tau\rho_{k+1})),$$

where  $E(\rho) = 0$  if  $\rho \leq 1$ , otherwise  $\infty$ .

Convergence to the continuum as  $\tau \rightarrow 0$  can be obtained as before.

Interestingly:

- Uniqueness of the weak solutions can be obtained, as well as stability in  $L^1$ .  
[Quiros-Perthame-Vazquez, Jacobs-K-Tong]

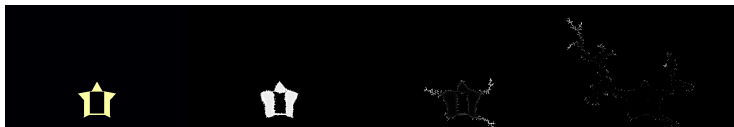
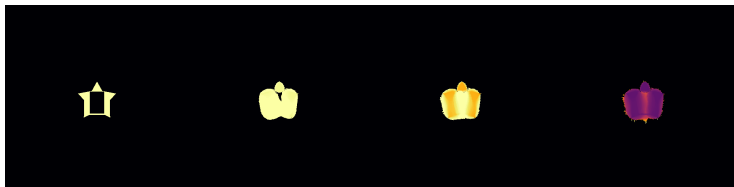
- Irregular growth of the tumor zone is observed when either  $\mu > 0$  or  $D > 0$ .  
[Kitsunezaki, Maury- R. Chupin-Santambrogio, Perthame-Tang-Vauchlet, Jacobs-Lee]

The formation and scale of the irregularity remains to be understood.

- This irregularity disappears when  $\mu, D \rightarrow 0$  for fixed time frame Jacobs-K-Tong 22, Lelmi-K preprint. .

# Numerical Simulations Thanks to Wonjun Lee

From top to bottom:  $(\mu, D) = (0.2, 0)$ ,  $(0, 10^{-6})$ ,  $(0.3, 10^{-5})$ .  $n(\cdot, 0) = 1$ .



Thank you!

## Lecture II

### Muskat problem with surface tension: an example of multi-density problem

## Density constraint with multiple species

It is natural to discuss two or more population groups or different types of cells, each with different desired velocity. In general very little is known about global well-posedness of competitive multi-species problems, due to the possibility of *mixing*.

One particular example we will discuss is the Muskat problem [Muskat (1934)] introduced to model the interface between water and oil in tar sands. In general the problem models flow of incompressible and immiscible fluids in porous media.



## Setting of the problem

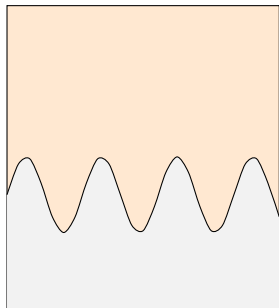


Figure: Two fluids in a container

- Two **incompressible, immiscible** fluids that fills up a container.
- They are represented by **characteristic functions**  $\rho_1$  and  $\rho_2$ .
- Sharp **interface** with Mobility constants  $b_1$  and  $b_2$ .

# Muskat problem

The equations are

$$(\rho_i)_t + b_i \nabla \cdot ((\nabla p + \nabla \Phi_i) \rho_i) = 0, \quad \rho_i \in \{0, 1\}.$$

The pressure variable  $p$  is generated by the constraint  $\rho_1 + \rho_2 = 1$ . The potentials are

$$\Phi_i = g_i x \cdot e_d, \quad g_i > 0,$$

where  $g_i$ 's correspond to the specific gravity of each fluid.

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$$\Phi_i = g_i x \cdot e_d, \quad g_i > 0,$$

where  $g_i$ 's correspond to the specific gravity of each fluid.

The problem can then be formally given as the gradient flow of the free energy

$$E_\infty(\boldsymbol{\rho}) = \int \Phi_1 \rho_1 dx + \int \Phi_2 \rho_2 dx \quad \text{if } \rho_1 + \rho_2 \leq 1, \quad \text{otherwise } \infty.$$

in  $W_2 \times W_2$ , with the metric  $W_2(\boldsymbol{\rho}, \boldsymbol{\mu}) := b_1^{-1} W_2(\rho_1, \mu_1) + b_2^{-1} W_2(\rho_2, \mu_2)$ .

# Literature

One can consider the problem where the interface between  $\rho_1$  and  $\rho_2$  is a graph, "close" to the equilibrium hypersurface  $\{x : x \cdot e_d = 0\}$ , and in **stable** setting, where the heavy fluid sits below the light fluid. Most of the existing results discuss local and global well-posedness of classical (strong) solutions in this setting.

We are interested in constructing a global-time weak solution that allows topological singularities. For the original model, this is an open problem even in stable setting, due to potential mixing.

Technically the problem lies in the lack of compactness to carry the problem from the discrete-time scheme to the continuum, to obtain a weak solution of the PDE system.

# Minimizing movement and compactness

Consider the approximate problem

$$(\rho_1^k, \rho_2^k) = \operatorname{argmin} \int (\rho_1 + \rho_2)^m dx + (\text{potential part}) + b_1^{-1} W_2(\rho_1, \rho_1^{k-1}) + b_2^{-1} W_2(\rho_2, \rho_2^{k-1}).$$

The corresponding EDI will yield information for  $\rho_1 + \rho_2$  and for the Kantorovich potential, which will be given a different form in the support of  $\rho_1$  and  $\rho_2$ . Thus we fall short of enough compactness to track evolution of the separate densities  $\rho_1$  and  $\rho_2$ .

# Muskat problem with surface tension

To prevent micro-sopic mixing of the densities, we introduce the surface tension energy into the problem:

$$\mathcal{E}(\rho) := E_\infty(\rho) + E_s^\varepsilon(\rho),$$

where  $E_s^\varepsilon$  is a relaxation of the capillary energy

$$E_s(\rho) = \sigma \text{Per}(\Gamma)$$

where  $\Gamma$  is the interface separating two characteristic functions  $\rho_1$  and  $\rho_2$ .

The corresponding gradient flow in this setting yields the Muskat problem with surface tension. While the capillary regularizes the interface in small scales, the interface still could develop topological singularities.

In our variational scheme, we would like to avoid the singular energy  $E_s(\boldsymbol{\rho}) = \text{Per}(\Gamma)$ , which requires  $\rho_i \in \{0, 1\}$ . This is to avoid

- numerical challenges associated with the nonconvex constraint, and
- for the challenge in analysis with the multi-phase fluid (e.g. water, oil, honey) scenario in mind.

# Relaxation of the Capillary energy: the heat content

Here we adopt the nonlocal energy

$$E_s^\varepsilon(\rho) := \sigma \frac{1}{\sqrt{\varepsilon}} \int (G_\varepsilon * \rho_1) d\rho_2$$

where  $G_\varepsilon$  denotes the heat kernel at time  $\varepsilon$ , namely  $G_\varepsilon(x) := (2\pi\varepsilon)^{-d/2} e^{-\frac{|x|^2}{2\varepsilon}}$ .



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where  $G_\varepsilon$  denotes the heat kernel at time  $\varepsilon$ , namely  $G_\varepsilon(x) := (2\pi\varepsilon)^{-d/2} e^{-\frac{|x|^2}{2\varepsilon}}$ .

Note that under the constraint  $\rho_1 + \rho_2 = 1$ , each density needs to segregate from each other to keep the energy small. In particular the energy approximates the perimeter when the densities are segregated, otherwise it blows up to infinity as  $\varepsilon \rightarrow 0$ .

# Motivation: Merriman-Bence-Osher scheme

The MBO scheme (MBO 1992) iteratively produces sequence of characteristic functions  $\chi^n := \chi_{A_n}$ , defined by

$$A_n = \{x : (G_\varepsilon * \chi^{n-1})(x) > \frac{1}{2}\}.$$

As  $\varepsilon \rightarrow 0$ , the sequence of sets  $\chi(n\varepsilon) := \chi^n$  converges to the evolution  $(\chi_{A(t)})_{t>0}$  by mean curvature.

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◦ The Mean curvature flow is formally a gradient flow with respect to the surface length  $Per(\partial\chi_t)$  and with  $L^2$ -type "distance". Does MBO scheme has a gradient flow structure?

## MBO scheme as minimizing movement

This question was addressed by Esedoglu-Otto (2015). They show that the *MBO* scheme can be formulated as  $\chi^n$  minimizing

$$\frac{1}{2\varepsilon}d^2(u, \chi^{n-1}) + E_\varepsilon(u), \quad E_\varepsilon(u) := \varepsilon^{-1/2} \int (G_\varepsilon * u)(1 - u)dx, \quad 0 \leq u \leq 1,$$

which is a discrete-time gradient flow for the energy  $E_h$  with a  $L^2$ -type “distance”  $d$ .

The scheme can generalize to approximate multi-phase evolution, with different mobility weights.

# Our discrete-time scheme

Our discrete-time scheme is given by in the probability density space,

$$\rho_k := \operatorname{argmin} \mathcal{E}^\varepsilon(\rho) + \frac{1}{2\tau} [(b_1)^{-1} W_2^2(\rho_1, \rho_{k-1}^1 + (b_2)^{-1} W_2^2(\rho_2, \rho_{k-1}^2)],$$

where

$$\mathcal{E}^\varepsilon(\rho) = \int \Phi_1 \rho_1 + \int \Phi_2 \rho_2 + E_s^\varepsilon(\rho) \quad \text{if } \rho_1 + \rho_2 = 1, \text{ otherwise } + \infty.$$

Let us denote the resulting density pair by  $\rho^\varepsilon = (\rho_1^\varepsilon, \rho_2^\varepsilon)$ .

## The $\varepsilon$ -problem and discrete segregation

The energy  $E_s^\varepsilon$  is strictly concave on the set  $\{\rho_1 + \rho_2 = 1\}$ , since (in the torus)

$$\int (G_\varepsilon * \rho)(1 - \rho) = \int G_\varepsilon * \rho - \int (G_\varepsilon * \rho)\rho = \hat{u}(0) - \int \sqrt{\varepsilon} \hat{G}_1(\xi \sqrt{\varepsilon}) |\hat{u}|^2(\xi) d\xi.$$

Using this feature, we can show that the discrete-time solutions of the  $\varepsilon$ -problem are segregated.

### Proposition

*Minimizers  $(\rho_1^\varepsilon, \rho_2^\varepsilon)$  of the minimizing movement with energy  $\mathcal{E}^\varepsilon$  form a partition in the domain, that is  $\rho_i^\varepsilon \in \{0, 1\}$  and  $\rho_1^\varepsilon \rho_2^\varepsilon = 0$ .*

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$E_s^\varepsilon$  also satisfies “ $D^2 E_s^\varepsilon \geq O(-\frac{1}{\varepsilon^3})$ ”, which yields the uniqueness of the continuum limit. However the convergence is not strong enough to rule out small-scale (beyond  $\sqrt{\varepsilon}$ ) mixing for the continuum density pair.

# Main result [Jacobs-K-Mészáros (2019)]

Let us choose  $\tau \rightarrow 0$  as  $\varepsilon \rightarrow 0$ . Then for any  $T > 0$  the following holds along a subsequence:

## Theorem

- (a) *The discrete-time density pair  $(\rho_1^\varepsilon, \rho_2^\varepsilon)$  strongly converges to a pair of characteristic functions  $(\rho_1, \rho_2)$  in  $L^1([0, T] \times \Omega)$ .*
- (b) *The pressure gradient for the discrete-time  $\varepsilon$ -problem, that is the correction for the velocity fields due to the constraint  $\rho_1 + \rho_2 = 1$ , converges to a pressure gradient  $\nabla p$ , weak-\* in  $L^2([0, T], (C^1)^*(\Omega))$ .*

The main compactness is the *BV* bound for  $G_\varepsilon * \rho_i^\varepsilon$ , due to the surface energy  $\frac{1}{\sqrt{\varepsilon}} \int [G_\varepsilon * \rho_i^\varepsilon (1 - \rho_i^\varepsilon)]$ . The pressure gradient converges to the limit pressure plus a surface measure, which we will explain later for a simpler setting.



# Main result continued

## Theorem

$(\rho_1, \rho_2, p)$  is a weak solution of the Muskat problem with surface tension, which can be summarized as (more classical form to be present later for one phase problem)

$$\begin{cases} (\rho_i)_t - \nabla \cdot (\rho_i(\nabla p + \nabla \Phi_i)) = 0, & \rho_i \in \{0, 1\}, \\ p = \kappa & \text{on } \partial\{\rho_1 = 1\} = \partial\{\rho_2 = 1\}. \end{cases}$$

under the energy convergence assumption

$$(EC) \quad \lim_{\varepsilon, \tau \rightarrow 0} \int_0^T E_s(\rho^\varepsilon) dt = \int_0^T E_S(\rho) dt.$$

## Main result continued

We thus have a variational approximation for global-time weak solutions of Muskat problems with surface tension, where the sharp interface is present in the scheme.

The inequality  $\geq$  in (EC) always holds. Our assumption thus says that the perimeter of  $\varepsilon$ -interface is not lost in the limit  $\varepsilon \rightarrow 0$ . For instance it rules out the possibility that different parts of the fluid region merge into each other and instantly remove a sizable part of its boundary.

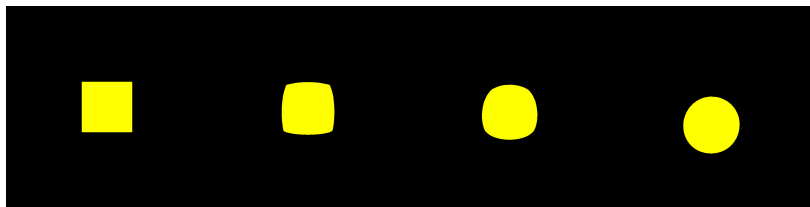
# On energy convergence assumption

We expect ( $EC$ ) to be true, and it would be a significant advance to remove this assumption for curvature driven flows. Luckhause-Sturzenhecker, Almgren-Taylor-Wang, Laux-Otto, Laux-Simon...

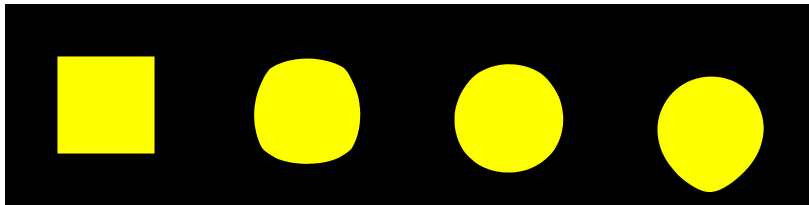
Alternative, weaker, notion of solutions based on varifolds has been proposed that does not require this assumption for Mullins-Sekarka and Stefan problems [Luckhaus (1993), Röger (2005), Chambolle-Laux (2019)] . It is likely that this notion will apply also for our problem.

# Numerical simulations Thanks to Matt Jacobs

All figures are snapshots of numerical simulations by Matt Jacobs. Two fluids are in a cylinder, with yellow being the heavier one.



Next we increase the mass in yellow fluid, which results in a different stationary state:



## Long time behavior with low energy

One could possibly ask, if the solution starts with its free energy close enough to the minimum value, and if the minimum is strict, whether it would converge to the global equilibrium. This is a reasonable question given the gradient flow structure, and an interesting question since low energy still allow various topological configurations.

For the discrete-time solution of the problem, one can make use of the minimization structure (almost-minimal surface) to obtain regularity for the interface. One can use this regularity to classify the set of critical points, and then to obtain long-time behavior of low energy solutions (Wallace, preprint). The question remains open for continuum solutions.

## Alternative kernels

As we mentioned before, one is not able to track individual velocities for the gradient flow of the approximate energy, (ignoring potential energy),

$$E_s^\varepsilon(\rho) := \int (K_\varepsilon * \rho_2) d\rho_1$$

with the particular choice of the rescaled heat kernel  $G_\varepsilon$ . Formally, the continuum PDE for the  $\varepsilon$ -problem will be written as

$$(\rho_1)_t - \nabla \cdot (\nabla p + \nabla(K_\varepsilon * \rho_2)\rho_1) = 0.$$

The potential velocity field then will have its divergence  $\Delta(K_\varepsilon * \rho_2)$  change its sign in  $\sqrt{\varepsilon}$ -scale, which in view of the first lecture, could potentially the set  $\{\rho_1 = 1\}$  to dissolve. This could explain the difficulty in rigorously addressing the continuum limit of the  $\varepsilon$ -problem.

# An alternative kernel and Chemotaxis K-Mellet-Wu 2022

Keller-Segel model describes movement of organisms in response to self-generated chemicals.

Here we consider the following model in  $\Omega \times [0, \infty)$ :

$$\begin{cases} \rho_t - \mu \Delta \rho - \nabla \cdot ((\nabla p + \varepsilon^{-1} \nabla \phi) \rho) = 0, & 0 \leq \rho \leq 1; \\ \sigma \phi - \varepsilon^2 \Delta \phi = \rho, & \sigma > 0. \end{cases}$$

Note that  $\phi$  can be written as  $K_\varepsilon * \rho$ , where  $K_\varepsilon(x, y)$  is not of the form  $K_\varepsilon(|x - y|)$ . Here  $\sigma$  denotes the degradation of the chemical.

One can consider this problem as a gradient flow of the free energy

$$E(\rho) = \mu \int \rho \ln \rho + \varepsilon^{-1} \int K_\varepsilon * \rho (1 - \rho) dx \text{ if } \rho \leq 1, \text{ otherwise } \infty.$$



# Chemotaxis to Hele-Shaw with surface tension

In the limit  $\varepsilon \rightarrow 0$  we obtain the Hele-Shaw flow with surface tension, namely

$$(HS) \quad \begin{cases} \rho_t - \nabla \cdot (\rho \nabla p) = 0, & \rho \in \{0, 1\}, \\ p = 4\sigma^{-3/2}\kappa & \text{on } \partial\{\rho = 1\}, \end{cases}$$

when one starts with an initial data  $\rho_0 \in \{0, 1\}$ .

We can show this both at the discrete level and for continuum:

$$\rho_t - \mu \Delta \rho - \nabla \cdot (\nabla(p + \varepsilon^{-1}\phi)\rho) = 0 \longrightarrow (HS).$$

Compared to the previous interaction drift, the velocity field  $-\nabla\phi$  is fully attractive, namely

$$\Delta\phi = \varepsilon^{-2}(1 - \sigma\phi) > 0 \quad \text{in } \{\rho = 1\}.$$

Based on this fact we can show that patch solutions stay as patches on both discrete-time and on PDE level:

## Patch solutions and convergence of the pressure variable

For patch solutions  $\rho = \chi_{A(t)}$ , one can write the evolution of  $A(t)$  for the equation  $\rho_t - \nabla \cdot (\nabla(p + \phi_\varepsilon)\rho) = 0$  as

$$\begin{cases} -\Delta p &= \varepsilon^{-1} \Delta \phi_\varepsilon \text{ in } A(t); & p = 0 \text{ on } \partial A(t); \\ V &= -\nabla(p - \varepsilon^{-1} \phi_\varepsilon) \cdot \nu \text{ on } \partial A(t). \end{cases}$$

This can be written with the modified pressure variable  $q := p + \varepsilon^{-1} \rho(\frac{1}{2\sigma} - \phi_\varepsilon)$ ,

$$\begin{cases} \Delta q &= 0 \text{ in } A(t); & q = \varepsilon^{-1}(\frac{1}{2\sigma} - \phi_\varepsilon) \text{ on } \partial A(t); \\ V &= -\nabla q \cdot \nu \text{ on } \partial A(t). \end{cases}$$

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From which we can recognize the classical Hele-Shaw problem with surface tension

$$\begin{cases} \Delta q = 0 \text{ in } A(t); & q = \frac{\kappa}{4\sigma^{3/2}} \text{ on } \partial A(t); \\ V = -\nabla q \cdot \nu \text{ on } \partial A(t). \end{cases}$$

## Boundary condition and contact angle K-Mellet-Wu

We also show that if we impose the Robin boundary condition  $\alpha\phi + \beta\varepsilon\nabla\phi \cdot n = 0$  on  $\partial\Omega$ , then in the limit  $\varepsilon \rightarrow 0$  it appears as the contact angle condition at the triple junction:

$$\cos\theta = -\min\left(1, \frac{2\alpha}{\alpha + \sqrt{\sigma}\beta}\right) \quad \text{on } \partial\{\rho = 1\} \cap \partial\Omega.$$

In particular, for  $\alpha > \sqrt{\sigma}\beta$ ,  $\cos\theta = -1$  and so  $\theta = \pi$  and we will have tangential touch at the triple junction.

Adjusting  $\alpha$  and  $\beta$  amounts to modifying the kernel  $G_\varepsilon$ . This is nice since it is difficult to consider imposing the angle condition directly on the density.

## Gradient flow in bounded domains: boundary data

In general it remains an interesting question to ask whether one can address boundary conditions other than no-flux condition.

Altering the metric to allow transport to and from the domain boundary: Figalli-Gigli, 2010 for heat equation with Dirichlet boundary data.

$$\tilde{W}^2(\mu, \nu) = \inf_{\gamma} \int_{\bar{\Omega} \times \bar{\Omega}} |x - y|^2 d\gamma(x, y), \quad \pi_x \gamma = \mu, \quad \pi_y \gamma = \nu.$$

# Preview

On Friday's lecture, we will introduce a different transportation problem between measures, where the transport is carried out by brownian motion, namely the "Optimal Skorokhod problem".

Here the stopping time of the brownian motion will be used for optimizing the transportation cost (It is a stochastic optimal control problem). We will discuss how this problem connects to the Stefan problem, a classical problem describing melting and freezing of ice and water.

Thank you for your attention!