# Time fractional gradient flows: Theory and numerics

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# Outline

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# Motivation

- Fractional derivatives and integrals are powerful tools to describe memory and hereditary properties of materials.
- Fractional partial differential equations (FPDEs) are emerging as a new powerful tool for modeling many difficult complex systems, i.e., systems with overlapping microscopic and macroscopic scales or systems with long-range time memory and long-range spatial interactions.
- In "classical" diffusion

$$\partial_t u - \Delta u = 0$$

  the mean squared displacement in time scales as $t \sim \langle x^2(t) \rangle$.
- In the superdiffusive case $t^\alpha \sim \langle x^2(t) \rangle$ with $\alpha > 1$.
- In the subdiffusive case $\alpha \in (0, 1)$, thus giving rise to

$$D_t^\alpha u - \Delta u = 0,$$

  where $D_t^\alpha$ is the so-called Caputo derivative.
- This is usually used to model memory effects.

# (Fractional) heat equation

- The (time fractional) heat equation

$$D_t^\alpha u - \Delta u = f.$$

- Define the energy

$$\Phi_2(w) = \frac{1}{2} \int_\Omega |\nabla w|^2 \, \mathrm{d}x,$$

its derivative (in the $L^2$–sense) is

$$\langle D\Phi_2(w), \varphi \rangle = \int_\Omega \nabla w \nabla \varphi \, \mathrm{d}x = \langle -\Delta w, \varphi \rangle \, .$$

- The (time fractional) heat equation can be understood as

$$D_t^\alpha u + D\Phi_2(u) = f.$$

# (Fractional) parabolic $p$-Laplace problem

- More generally, for $p > 1$, consider

$$D_t^\alpha u - \nabla \cdot (|\nabla u|^{p-2} \nabla u) = f.$$

- Define

$$\Phi_p(w) = \frac{1}{p} \int_\Omega |\nabla w|^p \, \mathrm{d}x,$$

  then

$$\langle D\Phi_p(w), \varphi \rangle = \int_\Omega |\nabla w|^{p-2} \nabla w \nabla \varphi \, \mathrm{d}x.$$

- Our problem reads

$$D_t^\alpha u + D\Phi_p(u) = f.$$

▸ $p = 1$

# (Fractional) ODE with obstacles I

- Consider the motion of a particle inside a well. If the particle does not touch the walls then it moves by "its usual" law of motion:

$$u(t) \in (-1, 1) \quad \Longrightarrow \quad D_t^\alpha u(t) = f(t).$$

- If it touches one of the walls it gets reflected. Say it touches the right one. If

$$D_t^\alpha u \leq 0$$

the wall does not do anything, as the particle will move to the left anyways. If that is not the case, since right before it touches we had

$$D_t^\alpha u = f = f^+ - f^-$$

the reflection means

$$D_t^\alpha u = -f^-.$$

# (Fractional) ODE with obstacles II

- In short

$$\begin{cases} D_t^\alpha u(t) = -f^-(t), & u(t) = 1, \\ D_t^\alpha u(t) = f(t), & u(t) \in (-1,1), \\ D_t^\alpha u(t) = f^+(t), & u(t) = -1. \end{cases}$$

Subdifferential

# (Fractional) parabolic obstacle problems

- Define
$$\mathcal{K} = \{w \in \widetilde{H}^s(\Omega) : w \geq g \ a.e. \ \Omega\},$$
for some sufficiently nice $g$.
- Consider the problem given by the complementarity conditions
$$D_t^\alpha u + (-\Delta)^s u \geq f, \quad u \geq g, \quad (D_t^\alpha u + (-\Delta)^s u - f)(u - g) = 0.$$
- This is equivalent to the evolution variational inequality
$$\int_\Omega D_t^\alpha u(u - w)\,\mathrm{d}x + \langle(-\Delta)^s u, u - w\rangle \leq \int_\Omega f(u - w)\,\mathrm{d}x, \quad \forall w \in \mathcal{K}.$$

Subdifferential

# Problem statement

- Ambient space: Let $\mathcal{H}$ be a (separable) Hilbert space.
- Energy: $\Phi : \mathcal{H} \to \mathbb{R} \cup \{+\infty\}$ convex and l.s.c.
- Initial condition: $u_0 \in \mathcal{H}$.
- Right hand side: $f : [0, T] \to \mathcal{H}$.

We need to find $u : [0, T] \to \mathcal{H}$ such that

$$\begin{cases} D_t^\alpha u(t) + \partial\Phi(u(t)) \ni f(t), & t \in (0, T], \\ u(0) = u_0. \end{cases}$$

- Here $D_t^\alpha$ denotes the Caputo derivative, and $\partial\Phi(w)$ is the subdifferential of $\Phi$ at point $w$.
- $D_t^\alpha = \partial_t$ for $\alpha = 1$ and we get a classical gradient flow.
- If $f = 0$ this can be understood as steepest descent to find the minimum of $\Phi$.

Subdifferential

# Outline

# Energy solutions

$$\xi \in \partial\Phi(u) \quad \Longleftrightarrow \quad \Phi(u) - \Phi(w) \le \langle \xi, u - w \rangle$$

- Let us consider the classical case. We set $\alpha = 1$ to get

$$\begin{cases} u'(t) + \partial\Phi(u(t)) \ni f(t), \quad t \in (0, T], \\ u(0) = u_0. \end{cases}$$

## Definition (energy solution)

A function $u \in H^1(0, T; \mathcal{H})$ is an energy solution if $u(0) = u_0$ and

$$\langle u'(t), u(t) - w \rangle + \Phi(u(t)) - \Phi(w) \le \langle f(t), u(t) - w \rangle, \quad \forall w \in \mathcal{H}.$$

# Energy solutions: uniqueness

## Theorem (uniqueness[📘])

*Energy solutions are unique.*

## Proof.

If $u_1$ and $u_2$ are energy solutions,

$$\begin{aligned}
\langle u_1'(t), u_1(t) - w\rangle + \Phi(u_1(t)) - \Phi(w) &\le \langle f(t), u_1(t) - w\rangle, && w \leftarrow u_2,\\
\langle u_2'(t), u_2(t) - w\rangle + \Phi(u_2(t)) - \Phi(w) &\le \langle f(t), u_2(t) - w\rangle, && w \leftarrow u_1,
\end{aligned}$$

adding, we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_1(t) - u_2(t)\|^2 \le 0.$$

Since $u_1(0) = u_2(0) = u_0$ we conclude. □

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📘 Brézis 1973

# Energy solutions: existence I

- To show existence of solutions we employ a minimizing movements scheme[📘].
- Introduce a partition

$$\mathcal{P} = \{0 = t_0 < t_1 < \ldots < t_N = T\}, \quad \tau_n = t_n - t_{n-1}, \quad \boldsymbol{\tau} = \max_{n=1}^{N} \tau_n.$$

- We introduce approximations $U_n \approx u(t_n)$ via: set $F_n = \fint_{t_{n-1}}^{t_n} f \, \mathrm{d}t$, $U_0 = u_0$ and define

$$U_n = \operatorname*{argmin}_{w \in \mathcal{H}} \left[ \frac{1}{2\tau_n} \|w - U_{n-1}\|^2 + \Phi(w) - \langle F_n, w \rangle \right].$$

- Since we are in a Hilbert space this problem has a unique solution.
- The minimization problem is equivalent to (implicit Euler)

$$\frac{1}{\tau_n} (U_n - U_{n-1}) + \partial\Phi(U_n) \ni F_n$$

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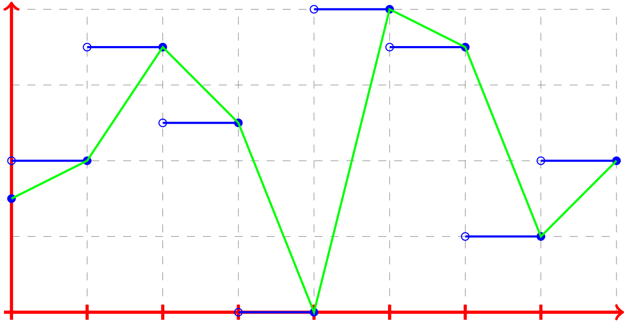
📘 De Giorgi

# Energy solutions: existence II



- The function $\bar{U}$ is piecewise constant

$$\bar{U}(t) = U_n, \quad t \in (t_{n-1}, t_n].$$

- The function $\widehat{U}$ is piecewise linear

$$\widehat{U}(t) = \frac{t_n - t}{\tau_n} U_{n-1} + \frac{t - t_{n-1}}{\tau_n} U_n, \quad t \in (t_{n-1}, t_n].$$

and its time derivative satisfies

$$\widehat{U}'(t) = \tau_n^{-1} \left( U_n - U_{n-1} \right).$$

# Energy solutions: existence III

- The minimizing movements scheme can then be written as

$$\left\langle \widehat{U}'(t), \bar{U}(t) - w \right\rangle + \Phi(\bar{U}(t)) - \Phi(w) \leq \left\langle \bar{F}(t), \bar{U}(t) - w \right\rangle, \quad \forall w \in \mathcal{H}.$$

- Setting $w = U_{n-1}$ we get

$$\tau_n \|\widehat{U}'\|^2 + \Phi(U_n) - \Phi(U_{n-1}) \leq \tau_n \|F_n\| \|\widehat{U}'\|,$$

which, provided $f \in L^2(0, T; \mathcal{H})$ and $\Phi(U_0) < +\infty$, gives

$$\widehat{U}' \in L^2(0, T; \mathcal{H})$$

uniformly in $\mathcal{P}$.

- The previous estimate "is enough" to pass to the limit $\boldsymbol{\tau} \to 0$ by compactness.

## Theorem (existence)

*If $f \in L^2(0, T; \mathcal{H})$ and $\Phi(u_0) < \infty$ the classical gradient flow has an energy solution.*

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Rothe 1930; Crandall, Ligett 1971; Brézis 1973; ...

# Classical gradient flows: the heart of the matter

To develop this theory we required:

- Uniqueness: The inequality

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_1 - u_2\|^2 \leq \langle (u_1 - u_2)', u_1 - u_2 \rangle \,.$$

- Existence: A minimizing movements scheme to obtain $\{U_n\}_{n=0}^{N}$.
- Existence: A suitable interpolation $\widehat{U}$ such that its derivative $\widehat{U}'$ is piecewise constant.

# Outline

# The Caputo derivative

- For sufficiently smooth functions

$$D_t^\alpha w(t) = I^{1-\alpha}[w'](t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} w'(s)\,\mathrm{d}s.$$

- Question: Can we define the Caputo derivative for rougher functions?
- Yes! There are several approaches[1]. We define it as follows[2]:

$$D_t^\alpha w(t) = \frac{\mathrm{d}}{\mathrm{d}t} I^{1-\alpha}[w(t) - w(0)\theta(t)]$$
$$= \frac{1}{\Gamma(1-\alpha)} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t (t-s)^{-\alpha} [w(t) - w(0)\theta(t)]\,\mathrm{d}s$$

  where $\theta$ is the Heaviside function.
- If $w \in L^1_{loc}([0,\infty))$, $⨍_0^t \|w(s) - w(0)\|\,\mathrm{d}s \to 0$, and $D_t^\alpha w \in L^1_{loc}([0,\infty))$ then

$$w(t) = w(0) + I^\alpha[D_t^\alpha w](t) = w(0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} D_t^\alpha w(s)\,\mathrm{d}s.$$

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[1] Marchaud 1927; Feng, Sutton 2020; ...

[2] Li and Liu, 2018, 2019

# The Caputo derivative

- Key inequality: For $\Psi : \mathcal{H} \to \mathbb{R}$ convex, we have

$$D_t^\alpha \Psi(w) \leq \langle \partial\Psi(w), D_t^\alpha w \rangle.$$

- This is the needed analogue of

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|w\|^2 \leq \langle w, w' \rangle \,,$$

when $\Psi(w) = \frac{1}{2}\|w\|^2$.

# Energy solutions

$$\xi \in \partial\Phi(u) \quad \Longleftrightarrow \quad \Phi(u) - \Phi(w) \le \langle \xi, u - w \rangle$$

$$\begin{cases} D_t^\alpha u(t) + \partial\Phi(u(t)) \ni f(t), & t \in (0, T], \\ u(0) = u_0. \end{cases}$$

## Definition (energy solution)

A function $u \in L^2(0, T; \mathcal{H})$ such that $D_t^\alpha u \in L^2(0, T; \mathcal{H})$ is an energy solution if

$$⨍_0^t \|u(s) - u_0\|^2 \, \mathrm{d}s \to 0$$

and

$$\langle D_t^\alpha u(t), u(t) - w \rangle + \Phi(u(t)) - \Phi(w) \le \langle f(t), u(t) - w \rangle, \quad \forall w \in \mathcal{H}.$$

# Energy solutions: uniqueness

## Theorem (uniqueness)

*Energy solutions are unique.*

## Proof.

Recall the key inequality

$$D_t^\alpha \Psi(w) \leq \langle \partial\Psi(w), D_t^\alpha w \rangle$$

and repeat the idea for the classical case:
If $u_1$ and $u_2$ are energy solutions,

$$\begin{aligned} \langle D_t^\alpha u_1(t), u_1(t) - w\rangle + \Phi(u_1(t)) - \Phi(w) &\leq \langle f(t), u_1(t) - w\rangle, && w \leftarrow u_2, \\ \langle D_t^\alpha u_2(t), u_2(t) - w\rangle + \Phi(u_2(t)) - \Phi(w) &\leq \langle f(t), u_2(t) - w\rangle, && w \leftarrow u_1, \end{aligned}$$

adding, we get

$$\langle D_t^\alpha (u_1(t) - u_2(t)), u_1(t) - u_2(t)\rangle \leq 0.$$

We set $\Psi(w) = \frac{1}{2}\|w\|^2$ in the key inequality. Since $u_1(0) = u_2(0) = u_0$

$$\Psi(u_1 - u_2)(t) = \cancelto{0}{\Psi(u_1 - u_2)(0)} + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} D_t^\alpha \Psi(u_1 - u_2)(s)\,\mathrm{d}s \leq 0.$$

□

# Energy solutions: existence I

- To define a fractional minimizing movements we need to find a discretization of the Caputo derivative.
- Starting from

$$w(t) = w(0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} D_t^\alpha w(s)\, \mathrm{d}s.$$

If $\mathcal{P}$ is a partition of $[0,T]$ and $D_t^\alpha w(s)$ is piecewise constant over this partition we obtain

$$\mathbf{W} = W_0 \mathbf{1} + \mathbf{K}_{\mathcal{P}} \mathbf{V}_\alpha,$$

where $\mathbf{V}_\alpha = \{D_t^\alpha w(t_n)\}_{n=1}^N \in \mathcal{H}^N$, $W_0 = w(0)$ and $\mathbf{W} = \{w(t_n)\}_{n=1}^N$.

# Energy solutions: existence II

- The matrix $\mathbf{K}_{\mathcal{P}}$ is lower triangular and nonsingular.
- We define the discrete Caputo derivative by inverting this matrix

$$D^{\alpha}_{\mathcal{P}}\mathbf{W} = \mathbf{V}_{\alpha} = \mathbf{K}_{\mathcal{P}}^{-1}\left(\mathbf{W} - W_0\mathbf{1}\right) \in \mathcal{H}^N$$

- If $\mathcal{P}$ is uniform, the matrix $\mathbf{K}_{\mathcal{P}}$ is Toeplitz. Matrix multiplication can be understood as convolution

$$\mathbf{W} = W_0\mathbf{1} + \mathbf{K}_{\mathcal{P}} \star \mathbf{V}_{\alpha},$$

and this discretization is usually called a deconvolution scheme

$$\mathbf{V}_{\alpha} = \mathbf{K}_{\mathcal{P}}^{-1} \star (\mathbf{W} - W_0\mathbf{1})$$

We will **NOT** assume that $\mathcal{P}$ is uniform!

# Energy solutions: existence III

## Theorem (properties of $\mathbf{K}_{\mathcal{P}}$)

*For any partition, all $n \in \{1, \ldots, N\}$, and all $i \in \{0, \ldots, n-1\}$,*

$$\mathbf{K}^{-1}_{\mathcal{P},nn} > 0, \quad \mathbf{K}^{-1}_{\mathcal{P},ni} < 0, \quad \mathbf{K}^{-1}_{\mathcal{P},ni} < \mathbf{K}^{-1}_{\mathcal{P},(n+1)i}$$

*where* $\mathbf{K}^{-1}_{\mathcal{P},n0} = -\sum_{j=1}^{n} \mathbf{K}^{-1}_{\mathcal{P},nj}$.

## Corollary (discrete key inequality)

*For any convex $\Psi$ and $\mathbf{W} \in \mathcal{H}^N$ set $\Psi(\mathbf{W}) = \{\Psi(W_n)\}_{n=1}^{N}$. Then,*

$$\left(D^{\alpha}_{\mathcal{P}} \Psi(\mathbf{W})\right)_n \leq \langle \partial\Psi(\mathbf{W})_n, (D^{\alpha}_{\mathcal{P}} \mathbf{W})_n \rangle.$$

## Proof.

$$\begin{aligned}\left(D^{\alpha}_{\mathcal{P}} \Psi(\mathbf{W})\right)_n &= \sum_{i=0}^{n-1} \mathbf{K}^{-1}_{\mathcal{P},ni} \left(\Psi(W_i) - \Psi(W_n)\right) \leq \left\langle \partial\Psi(W_n), \sum_{i=0}^{n-1} \mathbf{K}^{-1}_{\mathcal{P},ni} (W_i - W_n) \right\rangle \\ &= \langle \partial\Psi(\mathbf{W})_n, (D^{\alpha}_{\mathcal{P}} \mathbf{W})_n \rangle.\end{aligned}$$

□

# Energy solutions: existence IV

- We can now define a fractional minimizing movements scheme via:

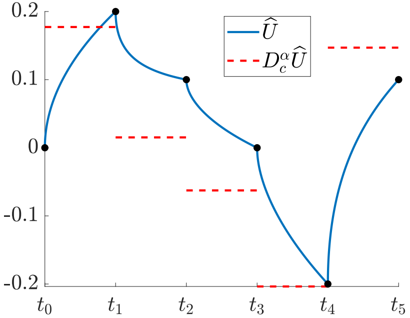
$$U_n = \operatorname*{argmin}_{w \in \mathcal{H}} \left[ \frac{1}{2} \sum_{i=0}^{n-1} (-\mathbf{K}_{\mathcal{P},ni}^{-1}) \|w - U_i\|^2 + \Phi(w) - \langle F_n, w \rangle \right].$$

- This is equivalent to

$$(D_{\mathcal{P}}^{\alpha} \mathbf{U})_n + \partial\Phi(U_n) \ni F_n.$$

- Question: What is the analogue of (the piecewise linear) $\widehat{U}$?

# Energy solutions: existence V




- Define $\{\varphi_i\}_{i=1}^N$ as functions with $(D_{\mathcal{P}}^\alpha \boldsymbol{\varphi}_i)_j = \delta_{i,j}$. Then

$$\widehat{U}(t) = \sum_{i=0}^{n} U_i \varphi_i(t).$$

- The minimizing movements becomes

$$\left\langle D_t^\alpha \widehat{U}(t), \bar{U}(t) - w \right\rangle + \Phi(\bar{U}(t)) - \Phi(w) \leq \left\langle \bar{F}, \bar{U}(t) - w \right\rangle, \quad \forall w \in \mathcal{H}.$$

# Energy solutions: existence VI

- Judicious choices of $w$ and some algebra yield

$$\|D_t^\alpha \widehat{U}\|^2_{L^2(0,T;\mathcal{H})} \lesssim \Phi(U_0) + \sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \|\bar{F}(s)\|^2 \,\mathrm{d}s < \infty.$$

- As expected, we must require $\Phi(u_0) < \infty$. What about the other quantity?

## Proposition (continuity)

For any partition $\mathcal{P}$

$$\sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \|\bar{F}(s)\|^2 \,\mathrm{d}s \lesssim \sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \|f(s)\|^2 \,\mathrm{d}s.$$

## Proof.

For $\alpha \in (0,1)$, the weight $\omega(s) = |s|^{\alpha-1} \in A_2$. □

# Energy solutions: existence VII

- We have enough estimates to pass to the limit.

## Theorem (existence[1])

*Assume that* $\Phi(u_0) < \infty$ *and*

$$\sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1}\|f(s)\|^2 \,\mathrm{d}s < \infty,$$

*then the fractional gradient flow problem has an energy solution which, moreover, satisfies* $u \in C^{0,\alpha/2}([0,T];\mathcal{H})$.

- Recall that in the classical gradient flow ($\alpha = 1$) an energy solution satisfies $u \in H^1(0,T;\mathcal{H}) \hookrightarrow C^{0,1/2}([0,T];\mathcal{H})$.

[1] Li, AJS 2021

# Outline

# A posteriori error estimate I

- Recall that the discrete solution is obtained via

$$\frac{1}{\tau_n}\left(U_n - U_{n-1}\right) + \partial\Phi(U_n) \ni F_n,$$

which is equivalent to

$$\left\langle \frac{1}{\tau_n}\left(U_n - U_{n-1}\right), U_n - w \right\rangle + \Phi(U_n) - \Phi(w) \leq \left\langle F_n, U_n - w \right\rangle, \quad \forall w \in \mathcal{H}.$$

- Set $w = U_{n-1}$ and define the quantity

$$\mathcal{E}_n = \left\langle F_n - \frac{1}{\tau_n}\left(U_n - U_{n-1}\right), \frac{1}{\tau_n}\left(U_n - U_{n-1}\right) \right\rangle - \frac{\Phi(U_n) - \Phi(U_{n-1})}{\tau_n} \geq 0$$

Nochetto, Savaré, Verdi 2000

# A posteriori error estimate II

- Recall that

$$\left\langle \widehat{U}'(t), \bar{U}(t) - w \right\rangle + \Phi(\bar{U}(t)) - \Phi(w) \le \left\langle \bar{F}(t), \bar{U}(t) - w \right\rangle, \quad \forall w \in \mathcal{H}.$$

- Using that $\Phi$ is convex and that $\widehat{U}(t)$ is a convex combination of $U_n$ and $U_{n-1}$ we get

$$\left\langle \widehat{U}'(t), \widehat{U}(t) - w \right\rangle + \Phi(\widehat{U}(t)) - \Phi(w) \le \left\langle \bar{F}(t), \widehat{U}(t) - w \right\rangle + (t_n - t)\bar{\mathcal{E}}.$$

- Combining with the continuous problem we get the a posteriori error estimate

$$\|u - \widehat{U}\|_{L^\infty(0,T;\mathcal{H})} \lesssim \|f - \bar{F}\|_{L^2(0,T;\mathcal{H})} + \left( \sum_{n=1}^{N} \tau_n^2 \mathcal{E}_n \right)^{1/2}.$$

# A priori error estimate

- A simple calculation reveals that

$$\sum_{n=1}^{N} \tau_n \mathcal{E}_n \lesssim \Phi(U_0) + \|\bar{F}\|^2_{L^2(0,T;\mathcal{H})}$$

- So that provided $\Phi(u_0) < \infty$ we get the a priori estimate

$$\|u - \widehat{U}\|_{L^\infty(0,T;\mathcal{H})} \lesssim \boldsymbol{\tau}^{1/2}.$$

- This is optimal with respect to the regularity $u \in C^{0,1/2}([0,T];\mathcal{H})$.

Nochetto, Savaré, Verdi 2000

# Error analysis: the heart of the matter

- A positive quantity $\mathcal{E}_n$ that depends only on the computed approximations.
- The function $\widehat{U}$ solves a perturbed gradient flow, where $\mathcal{E}_n$ is the perturbation.
- The fact that our interpolant $\widehat{U}$ is a convex combination of the computed approximations.

# Outline

# A posteriori error analysis I

- Recall that our minimizing movements scheme reads

$$(D^\alpha_{\mathcal{P}} \mathbf{U})_n + \partial\Phi(U_n) \ni F_n,$$

and that this can be rewritten as

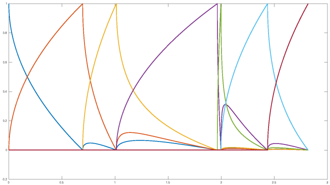
$$\left\langle D^\alpha_t \widehat{U}(t), \bar{U}(t) - w \right\rangle + \Phi(\bar{U}(t)) - \Phi(w) \le \left\langle \bar{F}(t), \bar{U}(t) - w \right\rangle, \quad \forall w \in \mathcal{H}.$$

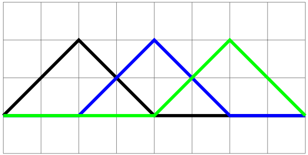
- We define

$$\mathcal{E}_\alpha(t) = \left\langle D^\alpha_t \widehat{U}(t) - \bar{F}(t), \widehat{U}(t) - \bar{U}(t) \right\rangle + \Phi(\widehat{U}(t)) - \Phi(\bar{U}(t)) \ge 0,$$

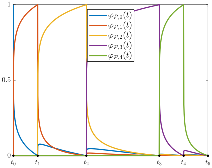
which depends only on the discrete solutions, and is thus computable.

# A posteriori error analysis II

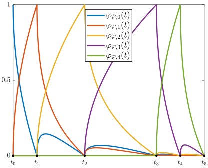




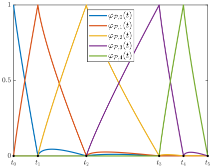
$\alpha = 0.1$




$\alpha = 0.5$




$\alpha = 0.9$



# A posteriori error analysis III

- The functions $\{\varphi_i\}$ used to define $\widehat{U}$ are all nonnegative, and $\sum_i \varphi_i = 1$.
- The value of the interpolant $\widehat{U}(t)$ is a convex combination of $\{U_i\}_{i=0}^n$ with $t \in (t_{n-1}, t_n]$.
- The interpolant $\widehat{U}$ satisfies, for every $w \in \mathcal{H}$,

$$\left\langle D_t^\alpha \widehat{U}(t), \widehat{U}(t) - w \right\rangle + \Phi(\widehat{U}(t)) - \Phi(w) \leq \left\langle \bar{F}(t), \widehat{U}(t) - w \right\rangle + \mathcal{E}_\alpha(t),$$

where, again, the quantity $\mathcal{E}_\alpha$ is a perturbation.

# A posteriori error analysis IV

## Theorem (a posteriori error estimate[1])

*Assume that* $\Phi(u_0) < \infty$. *For every* $\mathcal{P}$ *we have*

$$\|u - \widehat{U}\|_{L^\infty(0,T;\mathcal{H})} \lesssim \sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \|f - \bar{F}\|(s)\,\mathrm{d}s + \left( \sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \mathcal{E}_\alpha(s)\,\mathrm{d}s \right)^{1/2}.$$

## Proof.

Combine the inequalities that $u$ and $\widehat{U}$ satisfy to get

$$\left\langle D_t^\alpha (u - \widehat{U}), u - \widehat{U} \right\rangle \le \left\langle f - \bar{F}, u - \widehat{U} \right\rangle + \mathcal{E}_\alpha(t).$$

Use the discrete key inequality. □

[1] Li, AJS 2021

# A priori error analysis I

- Recall

$$\mathcal{E}_\alpha(t) = \left\langle D_t^\alpha \widehat{U}(t) - \bar{F}(t), \widehat{U}(t) - \bar{U} \right\rangle + \Phi(\widehat{U}(t)) - \Phi(\bar{U}(t)).$$

- Since there is a bound for $D_t^\alpha \widehat{U}$, and $\widehat{U}(t_n) = \bar{U}(t_n) = U_n$

$$\sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \|\widehat{U} - \bar{U}\|^2(s)\,\mathrm{d}s \lesssim \boldsymbol{\tau}^{2\alpha}.$$

- Since $\widehat{U}(t)$ is a convex combination of $\{U_i\}_{i=0}^n$ with $t \in (t_{n-1}, t_n]$

$$\Phi(\widehat{U}(t)) - \Phi(\bar{U}(t)) \le \sum_{i=1}^n \Phi(U_i)\varphi_i(t) - \Phi(\bar{U}(t)),$$

which implies

$$\sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \left( \Phi(\widehat{U}(s)) - \Phi(\bar{U}(s)) \right) \mathrm{d}s \lesssim \boldsymbol{\tau}^{\alpha}.$$

# A priori error analysis II

### Theorem (a priori error estimate)

*Assume that* $\Phi(u_0) < \infty$ *and that*

$$\sup_{t\in[0,T]} \int_0^t (t-s)^{\alpha-1} \|f(s)\|^2 \,\mathrm{d}s < \infty.$$

*Then, for every* $\mathcal{P}$*, we have*

$$\|u - \widehat{U}\|_{L^\infty(0,T;\mathcal{H})} \lesssim \boldsymbol{\tau}^{\alpha/2}.$$

- Recall that energy solutions satisfy $u \in C^{0,\alpha/2}([0,T];\mathcal{H})$ so this is optimal.

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# Outline

# A linear example I

- Consider, on $\Omega = (0,1)$,

$$D_t^\alpha u - \Delta u = 0, \qquad u(x,0) = u_0(x),$$

  supplemented with homogeneous Dirichlet boundary conditions. The exact solution is

$$u(t) = \sum_{k=0}^{\infty} u_{0,k} E_\alpha(-\lambda_k t^\alpha)\varphi_k(x), \qquad u_{0,k} = \int_\Omega u_0(x)\varphi_k(x)\,\mathrm{d}x,$$

  where $E_\alpha$ is the Mittag–Leffler function, and $\{(\lambda_k, \varphi_k)\}_{k=1}^{\infty}$ are the eigenpairs of the Dirichlet Laplacian.
- Set $T = 1$. Spectral discretization in space with $m = 100$ modes, and uniform $\mathcal{P}$.
- We measure

$$e_{end} = \|u(T) - U_N\|_{L^2(\Omega)}, \qquad e_{inf} = \max_n \|u(t_n) - U_n\|_{L^2(\Omega)}.$$

# A linear example II

- Set

$$u_{0,k} = k^{-1.5+\delta}, \qquad \delta \ll 1,$$

so that $u_0 \in D(\Phi) = H_0^1(\Omega)$, but $u_0 \notin D(\partial\Phi) = H^2(\Omega) \cap H_0^1(\Omega)$.

$\alpha = 0.3$

| $\tau$ | $e_{\text{inf}}$ | rate | $e_{\text{end}}$ | rate |
|---|---|---|---|---|
| 5.00e-02 | 1.09e-02 | — | 1.71e-03 | — |
| 2.50e-02 | 9.74e-03 | 0.166 | 9.03e-04 | 0.921 |
| 1.25e-02 | 8.72e-03 | 0.159 | 4.70e-04 | 0.940 |
| 6.25e-03 | 7.84e-03 | 0.153 | 2.43e-04 | 0.954 |
| 3.13e-03 | 7.07e-03 | 0.150 | 1.25e-04 | 0.964 |
| 1.56e-03 | 6.37e-03 | 0.149 | 6.35e-05 | 0.971 |
| 7.81e-04 | 5.75e-03 | 0.149 | 3.23e-05 | 0.977 |
| 3.91e-04 | 5.18e-03 | 0.150 | 1.63e-05 | 0.982 |
| 1.95e-04 | 4.67e-03 | 0.150 | 8.25e-06 | 0.985 |
| 9.77e-05 | 4.21e-03 | 0.150 | 4.16e-06 | 0.988 |

$\alpha = 0.7$

| $\tau$ | $e_{\text{inf}}$ | rate | $e_{\text{end}}$ | rate |
|---|---|---|---|---|
| 5.00e-02 | 2.72e-02 | — | 5.97e-03 | — |
| 2.50e-02 | 2.13e-02 | 0.350 | 3.03e-03 | 0.979 |
| 1.25e-02 | 1.67e-02 | 0.350 | 1.53e-03 | 0.988 |
| 6.25e-03 | 1.31e-02 | 0.350 | 7.68e-04 | 0.993 |
| 3.13e-03 | 1.03e-02 | 0.350 | 3.85e-04 | 0.996 |
| 1.56e-03 | 8.08e-03 | 0.350 | 1.93e-04 | 0.997 |
| 7.81e-04 | 6.34e-03 | 0.350 | 9.65e-05 | 0.998 |
| 3.91e-04 | 4.98e-03 | 0.350 | 4.83e-05 | 0.999 |
| 1.95e-04 | 3.90e-03 | 0.350 | 2.41e-05 | 0.999 |
| 9.77e-05 | 3.06e-03 | 0.351 | 1.21e-05 | 1.000 |

- Convergence rate of $\mathcal{O}(\tau^{\alpha/2})$, as predicted by our theory.

# A linear example III

- Set

$$u_{0,k} = k^{-2.5+\delta}, \qquad \delta \ll 1,$$

so that $u_0 \in D(\partial\Phi) = H^2(\Omega) \cap H_0^1(\Omega)$.

$\alpha = 0.3$

| $\tau$ | $e_{\text{inf}}$ | rate | $e_{\text{end}}$ | rate |
|---|---|---|---|---|
| 5.00e-02 | 8.44e-03 | — | 1.64e-03 | — |
| 2.50e-02 | 6.88e-03 | 0.296 | 8.66e-04 | 0.919 |
| 1.25e-02 | 5.57e-03 | 0.305 | 4.52e-04 | 0.939 |
| 6.25e-03 | 4.50e-03 | 0.308 | 2.33e-04 | 0.953 |
| 3.13e-03 | 3.63e-03 | 0.307 | 1.20e-04 | 0.963 |
| 1.56e-03 | 2.94e-03 | 0.305 | 6.11e-05 | 0.971 |
| 7.81e-04 | 2.38e-03 | 0.303 | 3.10e-05 | 0.977 |
| 3.91e-04 | 1.93e-03 | 0.302 | 1.57e-05 | 0.981 |
| 1.95e-04 | 1.57e-03 | 0.301 | 7.94e-06 | 0.985 |
| 9.77e-05 | 1.27e-03 | 0.301 | 4.00e-06 | 0.988 |

$\alpha = 0.7$

| $\tau$ | $e_{\text{inf}}$ | rate | $e_{\text{end}}$ | rate |
|---|---|---|---|---|
| 5.00e-02 | 1.05e-02 | — | 5.81e-03 | — |
| 2.50e-02 | 6.48e-03 | 0.702 | 2.95e-03 | 0.977 |
| 1.25e-02 | 3.99e-03 | 0.701 | 1.49e-03 | 0.987 |
| 6.25e-03 | 2.45e-03 | 0.700 | 7.49e-04 | 0.992 |
| 3.13e-03 | 1.51e-03 | 0.700 | 3.76e-04 | 0.995 |
| 1.56e-03 | 9.30e-04 | 0.700 | 1.88e-04 | 0.997 |
| 7.81e-04 | 5.73e-04 | 0.700 | 9.42e-05 | 0.998 |
| 3.91e-04 | 3.52e-04 | 0.700 | 4.71e-05 | 0.999 |
| 1.95e-04 | 2.17e-04 | 0.700 | 2.36e-05 | 0.999 |
| 9.77e-05 | 1.34e-04 | 0.700 | 1.18e-05 | 1.000 |

- Convergence rate of $\mathcal{O}(\tau^\alpha)$. We have a theory that includes this case!

# A (fractional) parabolic obstacle problem I

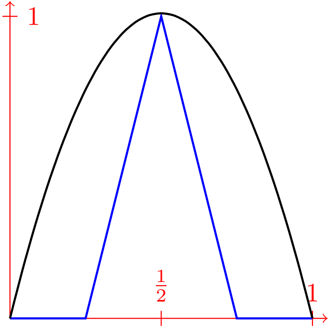
- Consider, in $\Omega = (0,1)$,

$$D_t^\alpha u + (-\Delta)^s u \geq f, \quad u \geq g, \quad (D_t^\alpha u + (-\Delta)^s u - f)(u-g) = 0.$$

supplemented with periodic boundary conditions.

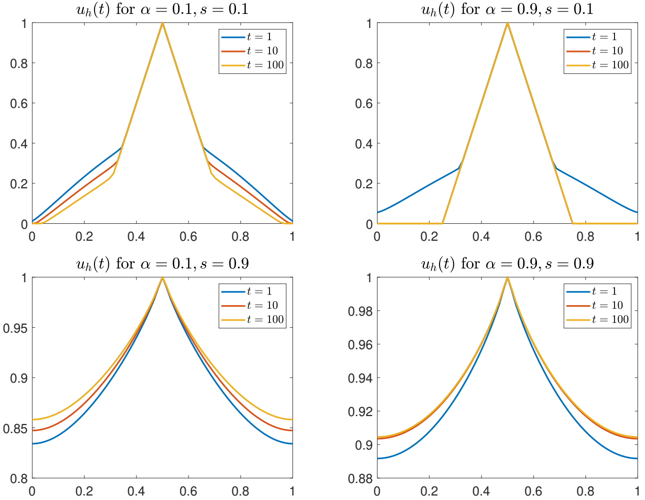
- We set

$$g(x) = \left(1 - 4|x - \tfrac{1}{2}|\right)_+, \quad u_0(x) = \sin(\pi x), \quad f(x,t) = -\frac{1}{2}$$



# A (fractional) parabolic obstacle problem II

- Collocation method with $M = 64$ nodes, $\tau = 2e-6$.
- Snapshots of discrete solutions of the time fractional parabolic obstacle problem for $\alpha = 0.1, 0.9,\ s = 0.1, 0.9$.



# The (fractional) Allen-Cahn equation I

- Consider, in $\Omega = (0,1)^2$,

$$D_c^\alpha u + (-\Delta)^s u + g(u) = f, \qquad u(x,0) = u_0(x),$$

  supplemented by periodic boundary conditions.

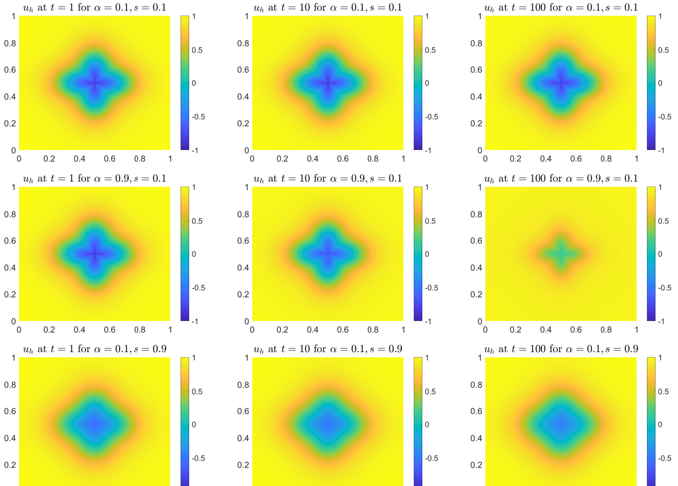
- Here

$$g(r) = G'(r), \qquad G(r) = \begin{cases} (r-1)^2, & r > 1, \\ \frac{1}{4}\left(1 - r^2\right)^2, & |r| \le 1, \\ (r+1)^2, & r < -1. \end{cases}$$

- The energy is NOT convex, but a Lipschitz perturbation of a convex one. We have a theory for this case.

# The (fractional) Allen-Cahn equation II

- Set
$$u_0(x) = \tanh\left(\frac{1}{\sqrt{2}\varepsilon_0}(2r - \frac{5}{16} - \frac{\cos(\theta)}{16})\right),$$
where $(r, \theta)$ are polar coordinates centered at $(\frac{1}{2}, \frac{1}{2})$.
- Collocation method with $M = 64$ nodes and $\tau = 2e-6$.



# The (fractional) Allen-Cahn equation III

$\alpha = 0.3$

| $\tau$ | $e_{\text{inf}}$ | rate | $e_{\text{end}}$ | rate |
|---|---|---|---|---|
| 2.50e-03 | 9.11e-04 | - | 3.11e-04 | - |
| 1.25e-03 | 7.29e-04 | 0.321 | 1.72e-04 | 0.859 |
| 6.25e-04 | 5.81e-04 | 0.328 | 9.23e-05 | 0.894 |
| 3.13e-04 | 4.60e-04 | 0.336 | 4.88e-05 | 0.919 |
| 1.56e-04 | 3.65e-04 | 0.336 | 2.55e-05 | 0.938 |
| 7.81e-05 | 2.92e-04 | 0.320 | 1.32e-05 | 0.951 |
| 3.91e-05 | 2.39e-04 | 0.287 | 6.77e-06 | 0.961 |
| 1.95e-05 | 2.02e-04 | 0.244 | 3.46e-06 | 0.969 |
| 9.77e-06 | 1.76e-04 | 0.203 | 1.76e-06 | 0.975 |

$\alpha = 0.7$

| $\tau$ | $e_{\text{inf}}$ | rate | $e_{\text{end}}$ | rate |
|---|---|---|---|---|
| 2.50e-03 | 7.24e-04 | - | 3.84e-04 | - |
| 1.25e-03 | 5.42e-04 | 0.416 | 1.97e-04 | 0.961 |
| 6.25e-04 | 4.04e-04 | 0.426 | 1.00e-04 | 0.977 |
| 3.13e-04 | 3.04e-04 | 0.411 | 5.06e-05 | 0.987 |
| 1.56e-04 | 2.33e-04 | 0.386 | 2.54e-05 | 0.992 |
| 7.81e-05 | 1.82e-04 | 0.355 | 1.28e-05 | 0.995 |
| 3.91e-05 | 1.45e-04 | 0.326 | 6.39e-06 | 0.997 |
| 1.95e-05 | 1.16e-04 | 0.322 | 3.20e-06 | 0.998 |
| 9.77e-06 | 9.01e-05 | 0.365 | 1.60e-06 | 0.999 |

- The rates for $e_{inf}$ are close to $\mathcal{O}(\tau^{\alpha/2})$ predicted in our theory.

# Time adaptivity I

- Consider the linear example with $\alpha = 0.5$, and $u_0 \in H_0^1(\Omega) \setminus H^2(\Omega)$.
- Given $\varepsilon > 0$, choose the time steps $\tau_n$ to equidistribute the error:

$$\max_{t \in (t_{n-1}, t_n]} \mathcal{E}_\alpha(t) \lesssim \varepsilon^2,$$

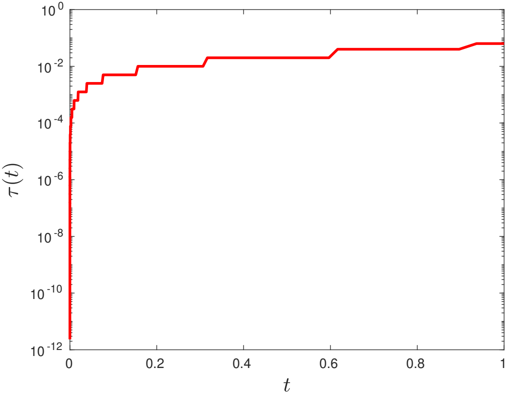
  then we can guarantee that

$$\|u - \widehat{U}\|_{L^\infty(0,T;L^2(\Omega))} \lesssim \varepsilon.$$

- Choose $\varepsilon = 1e - 2$.
- The adaptive solver requires $N = \#\mathcal{P} - 1 = 455$ time intervals with minimal timestep $\tau_{\min} \approx 2.3e - 12$ and maximal timestep $\tau_{\max} \approx 6.3e - 2$.
- In comparison, for a similar tolerance we must set $\tau_n = 2.44e - 5$ so that $N = 40960$.

There is a "*clear*" advantage in choosing the time step adaptively!

# Time adaptivity II




- The step size $\tau_n$ is very small at the beginning $\rightarrow$ the singularity of the solution at $t = 0$.
- For $t > 0$ the solution is smooth, so we can take larger time steps.

# Outline

# Conclusions I

- A discretization of the Caputo derivative that possesses suitable properties.
- Existence and uniqueness of energy solutions to fractional gradient flows.
- A posteriori error analysis.
- A priori error estimates without additional regularity assumptions. The estimates seem optimal given the available regularity.

# Conclusions II

Not discussed but we also have:

- Extension to the case of $\Phi$ being $\lambda$–convex, or we have a Lipschitz perturbations of a convex function: Fractional reaction diffusion, Fractional Allen-Cahn, ...
- Improved convergence rates for some special cases: linear equations, smooth energies, ...
- Asymptotic behavior of the solution. If $f = 0$ and $\Phi$ is uniformly convex with parameter $\mu > 0$, then

$$\Phi(u(t)) - \Phi_{\min} \leq (\Phi(u_0) - \Phi_{\min})\, E_\alpha(-2\mu t^\alpha)$$
$$\|u(t) - u_{\min}\|_{\mathcal{H}} \leq \|u_0 - u_{\min}\|_{\mathcal{H}} E_\alpha(-\mu t^\alpha).$$

- Asymptotic behavior of the solution. If $f = 0$ and $\Phi$ is merely convex, then

$$\Phi(u(t)) - \Phi_{\min} \lesssim t^{-\alpha/2}$$
$$\Phi(U_n) - \Phi_{\min} \lesssim t_n^{-\alpha/2}.$$

# Future work

- Some of the experiments show a rate of $\mathcal{O}(\tau^\alpha)$? Why? We have partial answers.
- Replace $\partial\Phi$ by a maximal monotone operator.
- Evolution in Banach spaces.
- Space discretization.

THANK YOU!

# (Fractional) ODE with obstacles III

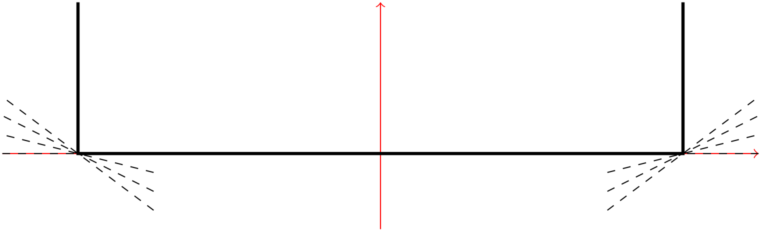
Define

$$\Phi(w) = \begin{cases} 0, & w \in [-1, 1], \\ +\infty, & w \notin [-1, 1]. \end{cases}$$

Then this problem can be succintly written as

$$D_t^\alpha u + \partial\Phi(u) \ni f,$$

where $\partial\Phi(w)$ denotes the subdifferential.



Back

# (Fractional) parabolic obstacle problems II

- Define

$$\Phi^s(w) = \frac{1}{2}|w|^2_{H^s(\mathbb{R}^d)} + \begin{cases} 0, & w \in \mathcal{K}, \\ +\infty, & w \notin \mathcal{K}. \end{cases}$$

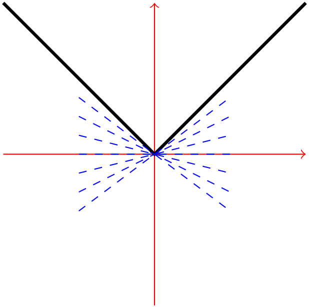
- The evolution variational inequality

$$\int_\Omega D_t^\alpha u(u-w)\,\mathrm{d}x + \langle (-\Delta)^s u, u-w \rangle \leq \int_\Omega f(u-w)\,\mathrm{d}x, \quad \forall w \in \mathcal{K}.$$

can be written as

$$D_t^\alpha u + \partial \Phi^s(u) \ni f.$$

# The subdifferential of a convex function



- A convex function $\Phi$ is not necessarily differentiable.
- However, by convexity, it can be touched from below by planes.
- The subdifferential $\partial\Phi(w)$ is the collection of slopes of the planes that touch from below at $w$

$$\xi \in \partial\Phi(w) \quad \iff \quad \Phi(w) - \Phi(v) \leq \langle \xi, w - v \rangle \,.$$

# (Fractional) TV flow

- Why $p > 1$? Consider the equation

$$D_t^\alpha u - \nabla\cdot\left(\frac{\nabla u}{|\nabla u|}\right) = f.$$

- Define

$$\Phi_1(w) = |Dw|(\Omega),$$

  where for $w \in BV(\Omega)$ we denote by $|Dw|$ its total variation (a Radon measure). This functional is not differentiable.

- The previous equation must be understood as follows: Find $u$ and $\mathbf{z}$ such that

$$\int_\Omega D_t^\alpha u w \, \mathrm{d}x + \int_\Omega \mathbf{z} \cdot Dw = \int_\Omega f w \, \mathrm{d}x, \quad \forall w \in BV(\Omega) \cap L^2(\Omega),$$

  and

$$\int_\Omega (\mathbf{q} - \mathbf{z}) \cdot Du \leq 0, \quad \forall \mathbf{q} \in \ldots$$