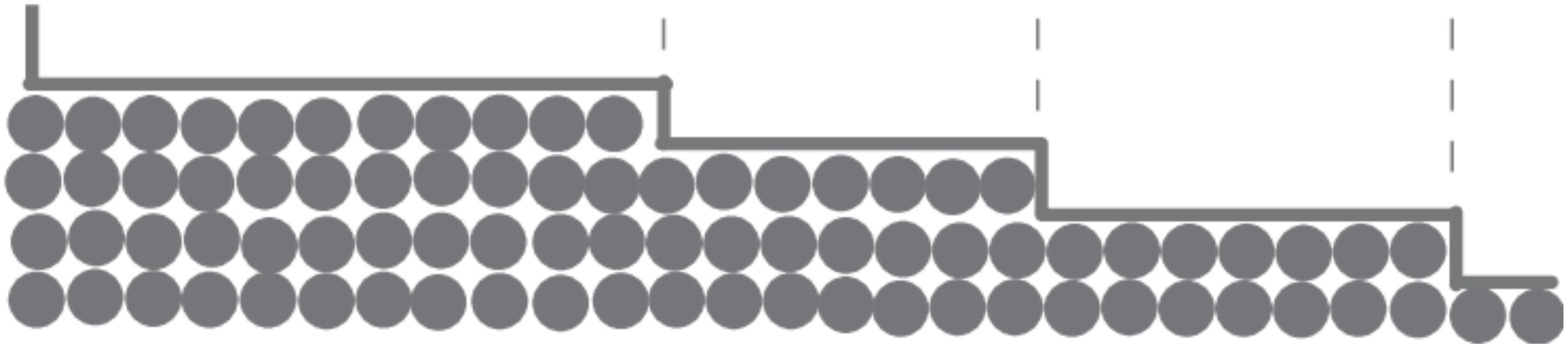 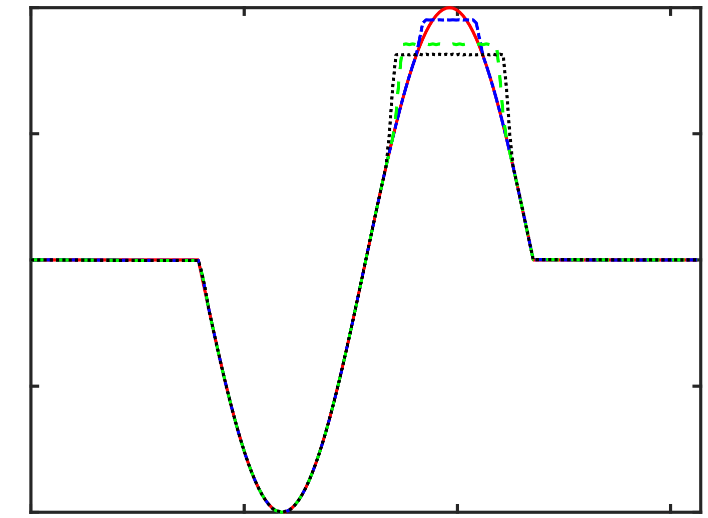

A Proximal-Gradient Algorithm for Crystal Surface Evolution

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joint with J.-G. Liu (Duke), J Lu (Duke), J. Marzuola (UNC), and L. Wang (Minnesota)

University of Massachusetts, Amherst, September 29th, 2020

Crystal surface evolution

- Evolution of a crystal near a fixed crystallographic plane of symmetry
- h(x,t) = height of crystal; facets on crystal = { x: ∇ h(x,t) = 0 }
- [Marzuola, Weare ’13]: continuum limit of kinetic Monte Carlo models

$$E(h) = \frac{1}{p}\int |\nabla h|^p, \ p \geq 1 \qquad \partial_t h = \Delta e^{-\Delta_p h}$$

- p=2, existence, uniqueness [Liu, Xu ’16-‘17, Xu ’18, Ambrose ’19,…]
- p=1, numerics via microscopic SOS system [Marzuola, Weare ’13]
  finite difference method [Liu, Lu, Margetis, Marzuola ’17]

Our goal:

leverage (very formal) gradient flow structure to design new numerical method

crystal growth PDE

$$\partial_t h = \Delta e^{-\Delta_1 h}$$

"gradient flow"

$$\partial_t h + \nabla \cdot \left(M(h) \nabla \frac{\partial \mathcal{E}}{\partial h} \right) = 0$$

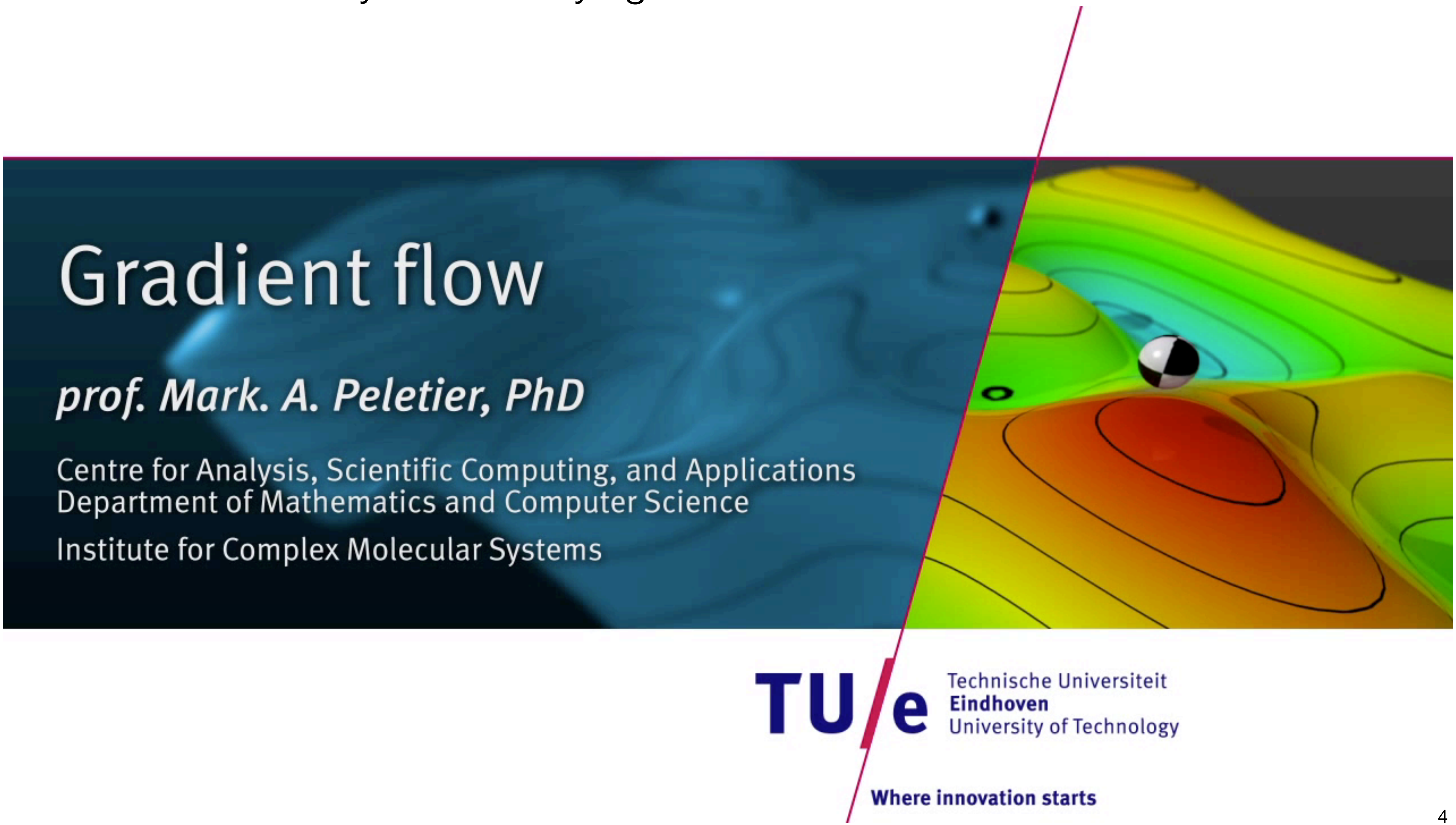
$$M(h) = e^{-\Delta_1 h}, \quad \mathcal{E}(h) = \|\nabla h\|_1$$

$$\frac{d}{dt} h(t) = -\nabla_M \mathcal{E}(h(t))$$

$$\nabla_M \mathcal{E}(h) = -\nabla \cdot \left(M(h) \nabla \frac{\partial \mathcal{E}}{\partial h} \right)$$

Gradient flows $\frac{d}{dt}h(t) = -\nabla_M \mathcal{E}(h(t))$

- h(t) evolves in the direction of steepest descent of $\mathcal{E}$, with respect to M
- ∇_M is induced by the underlying metric structure



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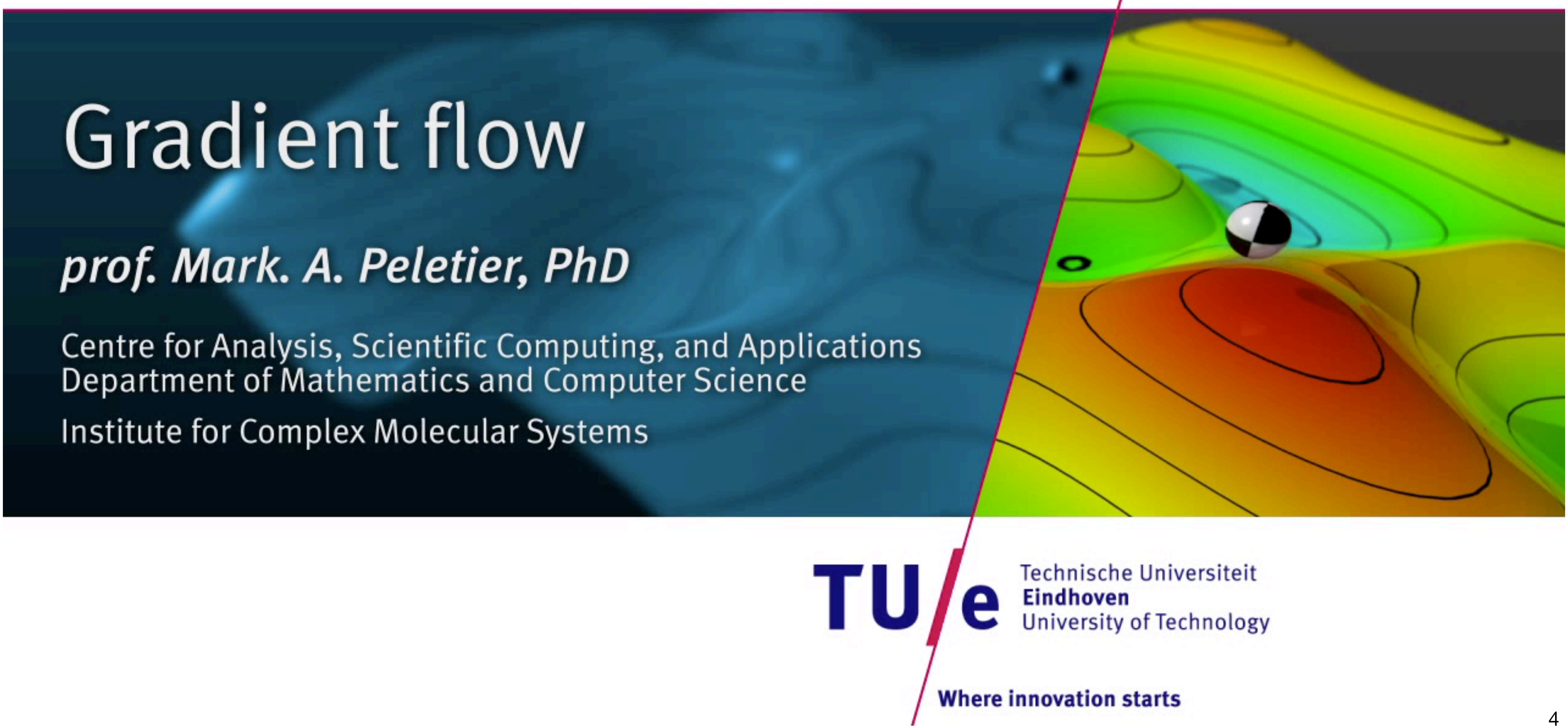

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Examples:

- M(h) = 1, H^{-1} gradient flow
- M(h) = h, W_2 gradient flow
- M(h) nonnegative, concave, weighted W_2 gradient flow
  [Carrillo, Lisini, Savaré, Slepčev '09, Dolbeault, Nazaret, Savaré '09, Lisini, Matthew, Savaré '19,…]
- $M(h) \in \mathrm{Lin}(\mathbb{R}^{l \times d}, \mathbb{R}^{l \times d})$, gradient system [Liero, Mielke '13]

Our mobility falls well outside existing, rigorous theory of GF structure.

Weighted H^{-1} GF perspective

[Otto '01,
Giga, Giga '10, …]

Suppose $M(h) \in L^1(\mathbb{T}^d)$ is nonnegative. Define $\Delta_h v = \nabla \cdot (M(h)\nabla v)$

- Weighted Hilbert space: $\|v\|^2_{H^1_h} = \int_{\mathbb{T}^d} M(h)|\nabla v|^2 = -\int_{\mathbb{T}^d} v\Delta_h v$
- Dual space: $\|\psi\|^2_{H^{-1}_h} = -\int_{\mathbb{T}^d} \psi\Delta_h^{-1}\psi$
- Subdifferential $\partial_{H^{-1}_h}\mathcal{E}$, gradient $\nabla_{H^{-1}_h}\mathcal{E}$

To go from here to a well-defined gradient flow, need to overcome obstacles:

- time derivative of h(t) with respect to $\|\cdot\|_{H^{-1}_{h(t)}}$
- M(h(t)) needs to remain integrable and nonnegative along the flow.

Then,

$$\partial_t h = -\nabla_{H^{-1}_h}\mathcal{E}(h) \iff \partial_t h + \Delta_h \frac{\partial E}{\partial h} = 0 \iff \partial_t h + \nabla \cdot \left(M(h)\nabla \frac{\partial E}{\partial h} \right) = 0$$

Weighted H-1 GF → Numerical Method

“gradient flow”

$$\partial_t h = -\nabla_{H_h^{-1}} \mathcal{E}(h)$$

$$M(h) = e^{-\Delta_1 h}, \quad \mathcal{E}(h) = \|\nabla h\|_1$$

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- how to interpret mobility?

Weighted H-1 GF → Numerical Method

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Weighted H⁻¹ GF -> Numerical Method

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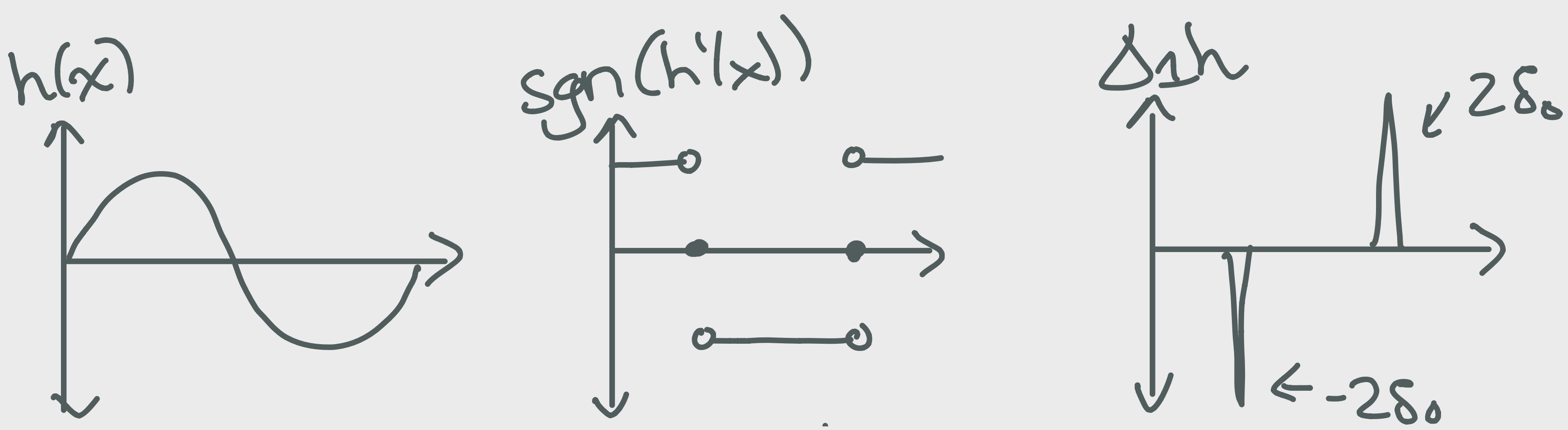
- how to interpret mobility?
- how to discretize in time?
- how to discretize in space?

- the mobility $M(h) = e^{-\Delta_1 h}$ doesn't make sense, even for d=1

$$\Delta_1 h = \nabla \cdot \left(\frac{\nabla h}{|\nabla h|} \right) = \nabla \cdot \operatorname{sgn}(\nabla h)$$



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- the mobility $M(h) = e^{-\Delta_1 h}$ doesn't make sense, even for d=1
- previous work considered linearization of exponential [Giga, Giga '10,…]

$$e^x \approx 1 + x, \quad M(h) \approx 1 - \Delta_1 h$$

- we consider mollified mobility, which respects asymmetry of curvature

$$\varphi \in C_c^\infty(\mathbb{T}^d),\ \varphi \geq 0,\ \int_{\mathbb{T}^d} \varphi = 1,\ \varphi_\epsilon(x) := \varphi(x/\epsilon)/\epsilon^d,$$

$$M_\epsilon(h) := e^{-\varphi_\epsilon * \Delta_1 h}$$

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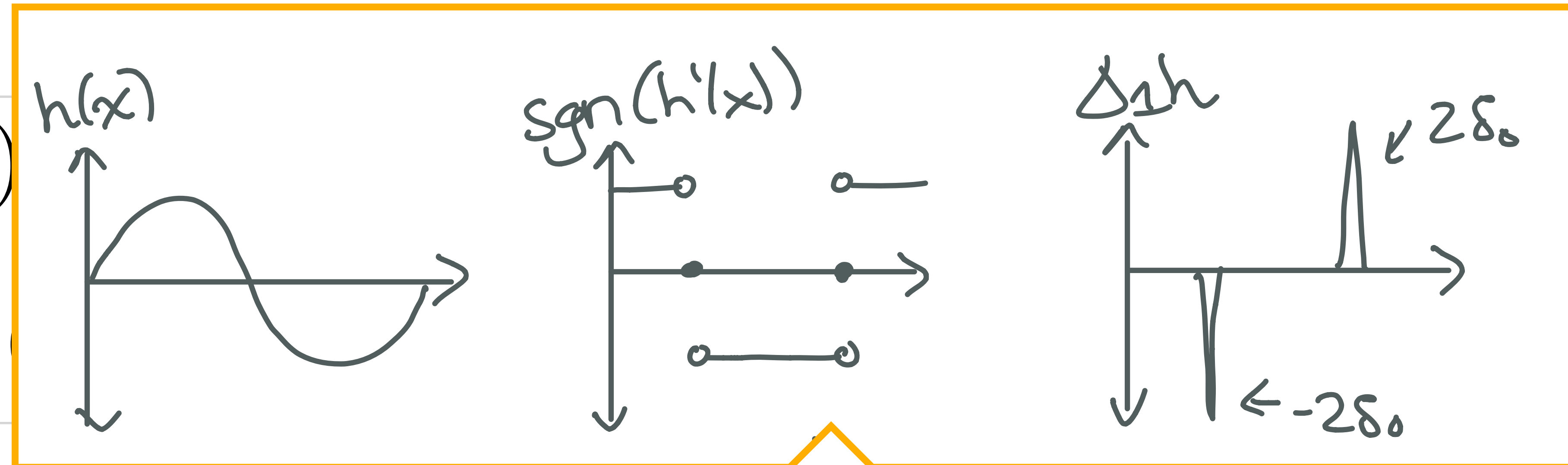

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- how to interpret mobility?
- how to discretize in time?
- how to discretize in space?

- we consider a semi-implicit scheme (c.f. [Murphy, Walkington '19] for PME)

$$h^{n+1} \in \arg\min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|^2_{H^{-1}_{h^n}}.$$

$$\frac{h^{n+1} - h^n}{\tau} = -\nabla \cdot \left(M(h^n) \nabla \frac{\partial \mathcal{E}}{\partial h^{n+1}} \right)$$

- for the TV energy E, if $h^n \in D(E)$ and $M(h^n)$ is integrable and nonnegative, there exists a unique solution h^{n+1} to our semi-implicit scheme

Weighted H-1 GF -> Numerical Method

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$$\Updownarrow$$

$$\frac{h^{n+1} - h^n}{\tau} = -\nabla \cdot \left(M(h^n) \nabla \frac{\partial \mathcal{E}}{\partial h^{n+1}} \right)$$

$$\frac{\partial E}{\partial h} = -\Delta_1 h$$

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- we want to solve

$$h^{n+1} \in \arg\min_h \underbrace{\mathcal{E}(h) + \frac{1}{2\tau}\|h - h^n\|^2_{H^{-1}_{h^n}}}.$$

$$\|\nabla h\|_1 + \frac{1}{2\tau}\|h - h^n\|^2_{H^{-1}_{h^n}} = f(Kh) + g(h)$$

$$f : \mathcal{Z} \to \mathbb{R} \text{ convex}, \ g : \mathcal{H} \to \mathbb{R} \text{ convex}, \ K : \mathcal{H} \to \mathcal{Z} \text{ bounded, linear}$$

- primal-dual algorithm! (c.f. [Laborde, Benamou, Carlier '16], [Carrillo, C., Wang, Wei '19],…)
- what is the role of the Hilbert spaces $\mathcal{Z}, \mathcal{H}$?

Weighted H-1 GF -> Numerical Method

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$$1$$

$$\|^2_{H^{-1}_{h^n}} .$$

Which Hilbert space?

1) $\mathcal{Z} = \mathcal{H} = L^2(\mathbb{R}^d)$

2) $\mathcal{Z} = L^2(\mathbb{R}^d)\ , \quad \mathcal{H} = \dot{H}^1(\mathbb{R}^d)$

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- [Jacobs, Léger, Li, Osher '19]
- Consider gradient descent of a smooth, convex function w/ unique min u_*.

$$F(u) = f(Ku) + g(u)$$

- Convergence rate:

$$F(u_n) \leq F(u^*) + 2L_{\mathcal{H}} \frac{\|u^* - u_0\|_{\mathcal{H}}^2}{n+4}$$

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- Nesterov:

$$\begin{aligned} F(u_n) &\leq \min_u \left[F(u) + 4L_{\mathcal{H}} \frac{\|u - u_0\|_{\mathcal{H}}^2}{(n+2)^2} \right] \\ &\leq \min_{\|u-u_0\|_{\mathcal{H}} \leq R} \left[F(u) + 4L_{\mathcal{H}} \frac{\|u - u_0\|_{\mathcal{H}}^2}{(n+2)^2} \right] \\ &\leq F(u_*) + 4L_{\mathcal{H}} \frac{R^2}{(n+2)^2} + \underbrace{\min_{\|u-u_0\|_{\mathcal{H}} \leq R} F(u) - F(u_*)}_{\delta_F(R)} \end{aligned}$$

Thus, one can get around $\|u_* - u_0\|_{\mathcal{H}} = +\infty$, as long as $\delta_F(R) \to 0$.

Which Hilbert space?

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- [Jacobs, Léger, Li, Osher '19]
- Analogous result holds for Chambolle-Pock's PDHG method (nonsmooth):

$$u_{n+1} = \arg\min_{u \in \mathcal{H}} \; g(u) + (u, K^T \bar{p}_n)_{\mathcal{H}} + \frac{1}{2\lambda}\|u - u_n\|^2_{\mathcal{H}},$$

$$p_{n+1} = \arg\max_{p \in \mathcal{Z}} -f^*(p) + (K u_{n+1}, p)_{\mathcal{Z}} - \frac{1}{2\sigma}\|(p - p_n)\|^2_{\mathcal{Z}},$$

$$\bar{p}_{n+1} = 2p_{n+1} - p_n.$$

for $u^N = \frac{1}{N}\sum_{n=1}^N u_n$ and $\lambda\sigma\|K^T K\|^2_{\mathcal{H}} < 1$, we have

$$F(u_N) \leq F(u_*) + C\frac{R}{N} + \underbrace{\min_{\|u-u_0\|_{\mathcal{H}} \leq R} F(u) - F(u_*)}_{\delta_F(R)}$$

Numerical method for crystal evolution

- Outer time iteration:

$$h^{n+1} = \mathrm{argmin}_h \mathcal{E}(h) + \frac{1}{2\tau}\|h - h^n\|^2_{H^{-1}_{h^n}}$$

- Inner time iteration: for $\lambda\sigma < 1$,

$$h^{(m+1)} = \left(\frac{\tau}{\lambda}\Delta_{h^n}\Delta + \mathrm{id}\right)^{-1}\left(\frac{\tau}{\lambda}\Delta_{h^n}\Delta h^{(m)} - \tau\Delta_{h^n}\nabla\cdot\phi^{(m)} + h^n\right)$$
$$\bar{h}^{(m+1)} = 2h^{(m+1)} - h^{(m)}$$
$$\phi^{(m+1)} = (\mathrm{id} + \sigma\partial F^*)^{-1}(\phi^{(m)} + \sigma\nabla\bar{h}^{(m+1)}) \ ,$$

$$(\mathrm{id} + \sigma\partial F^*)^{-1}(u(x)) = \min(|u(x)|, 1)\,\mathrm{sgn}(u(x)).$$

} discretize via finite difference method

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Benefits:

- avoids inverting 1-Laplacian
- freedom to choose λ large helps with computation of $h^{(m+1)}$

Convergence of PDHG

Theorem: [CMLLW '20] Let d=1. Suppose the PDHG algorithm is initialized with

$$h^{(0)} = h^n, \phi^{(0)} = 0,$$

Then for all δ>0, there exist $\tilde{M}$, λ, σ, so that

$$F(h^{(M)}) - F(h^{n+1}) \leq \delta, \quad \forall M \geq \tilde{M}, \qquad F(h) = \mathcal{E}(h) + \frac{1}{2\tau}\|h - h^n\|^2_{H^{-1}_{h^n}}$$

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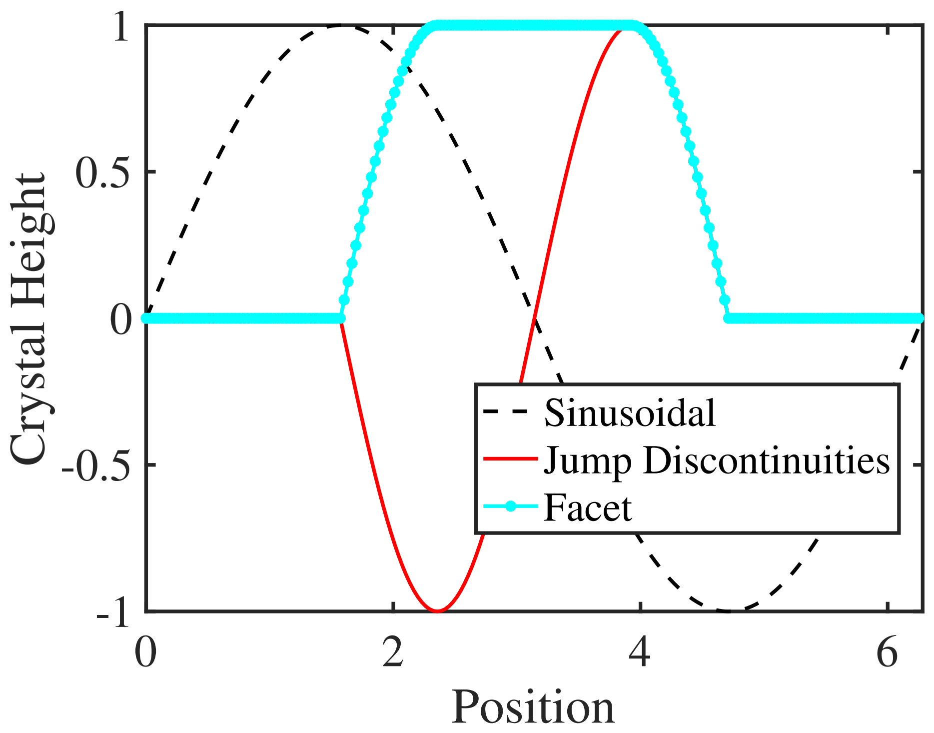
Remarks:

- Extends to general M(h) provided that $M(h^n)$ and $1/M(h^{n+1})$ integrable [c.f. Cancés, Gallouët, and Todeschi '19]
- We require d=1 to conclude $\|h^n\|_\infty \leq \mathcal{E}(h^n) < +\infty$. Higher integrability of $1/M(h^{n+1})$ would be required to weaken this assumption.
- If one has $\nabla h^n \in BV$, quantitative estimates: $\tilde{M} \sim \delta^{-2}$, $\lambda \sim \delta^{-1}$, $\sigma \sim \delta$
- Key step: $\delta_F(R) = \min_{\|h^n - h\|_{\dot{H}^1} \leq R} F(h) - F(h^{n+1}) \xrightarrow{R \to +\infty} 0$

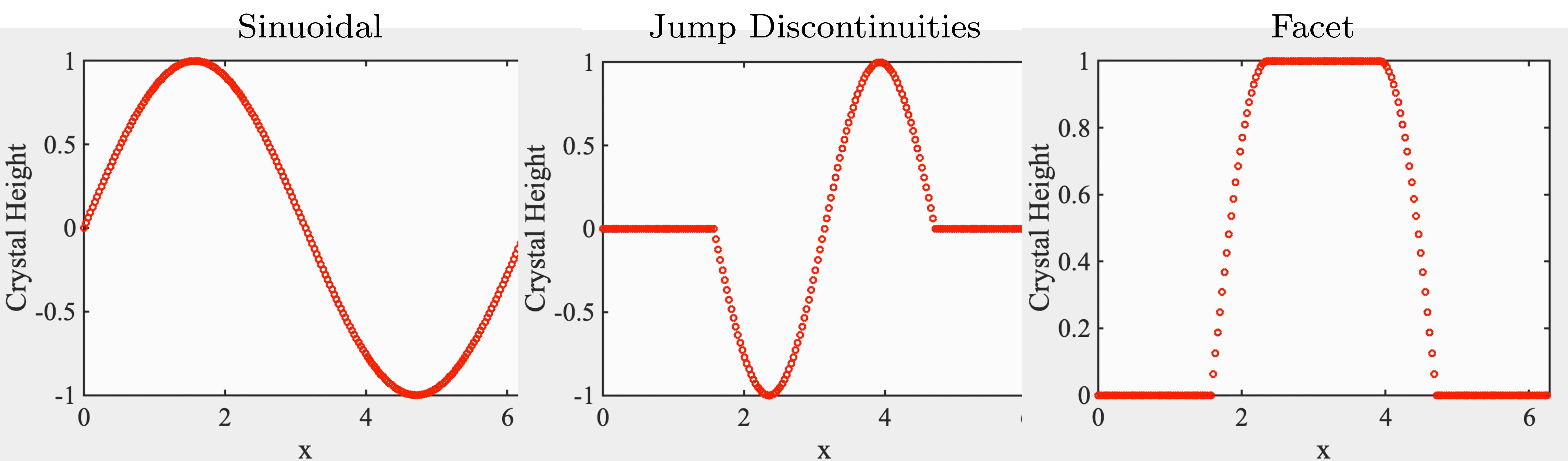
Numerical Results: dynamics



Observations:

- facet formation at local maxima
- pinning at local minima

Nx = 200, Nt = 10, σ = 0.0005, λ = 500, ε =0.04



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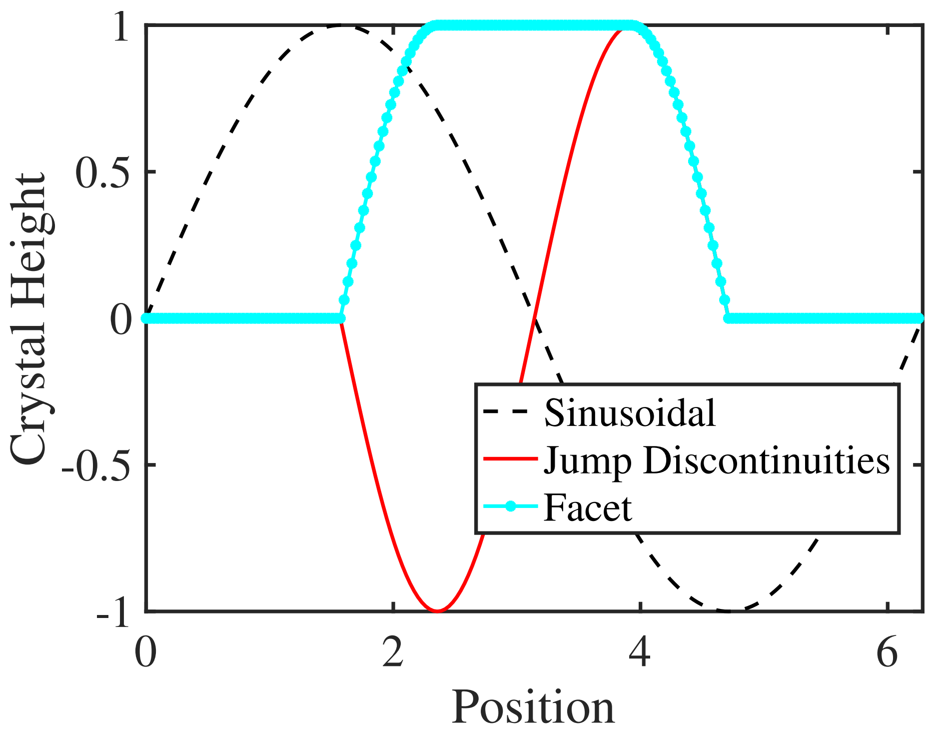

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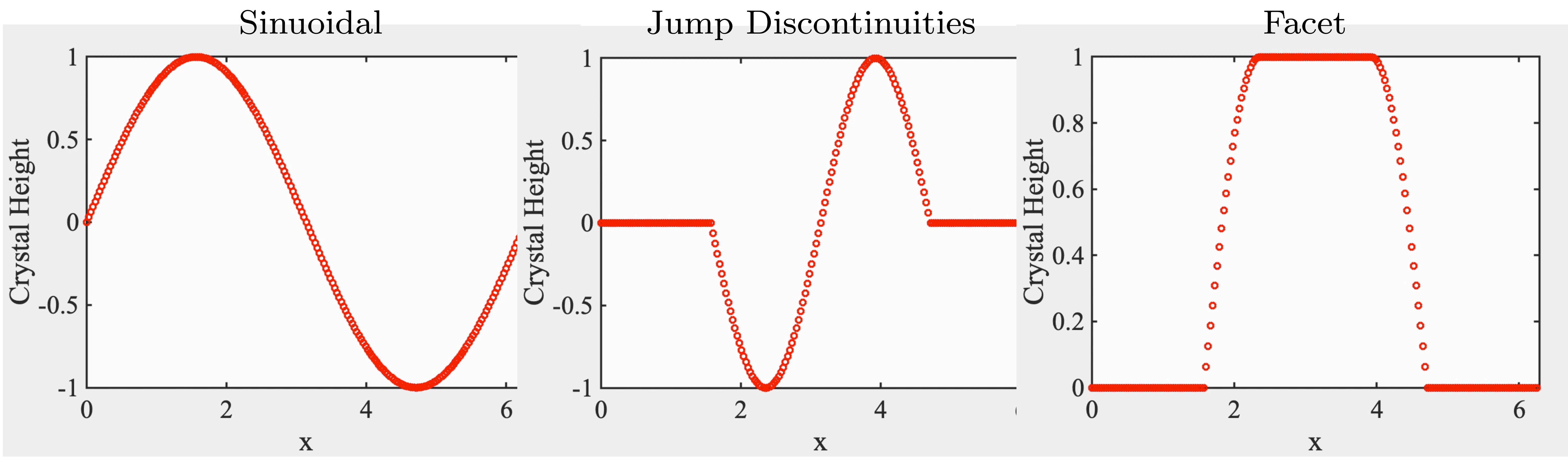

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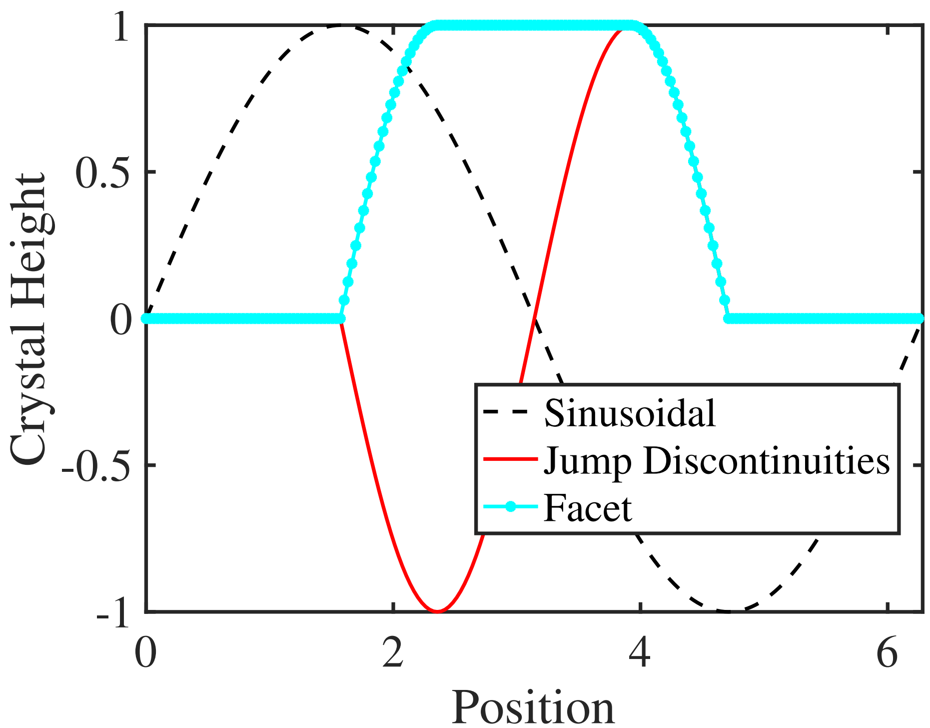

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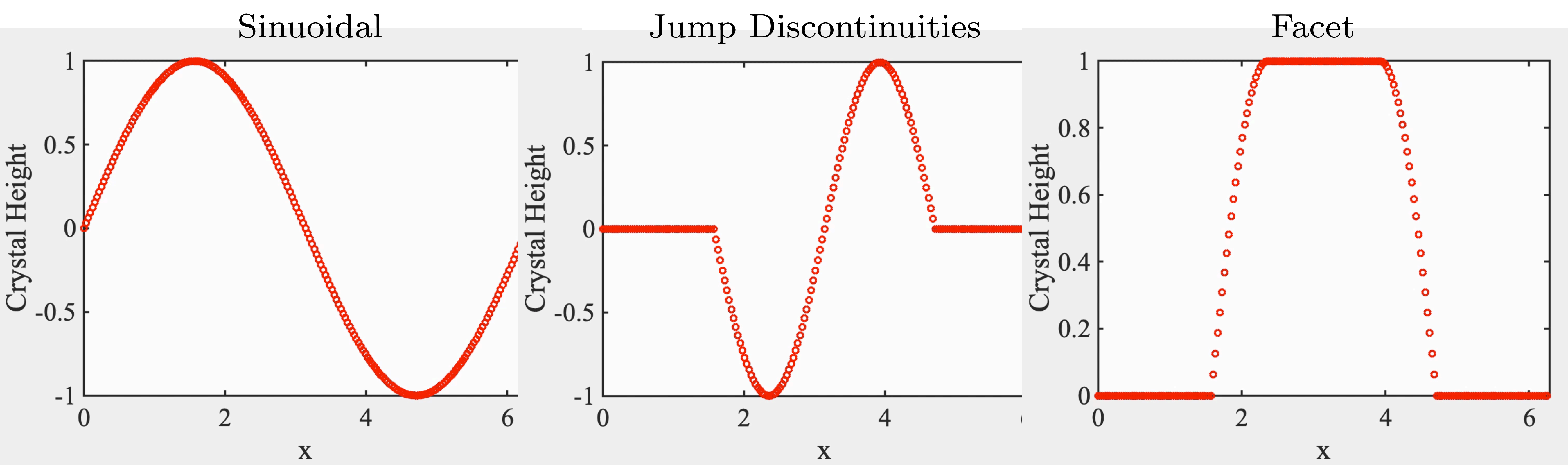

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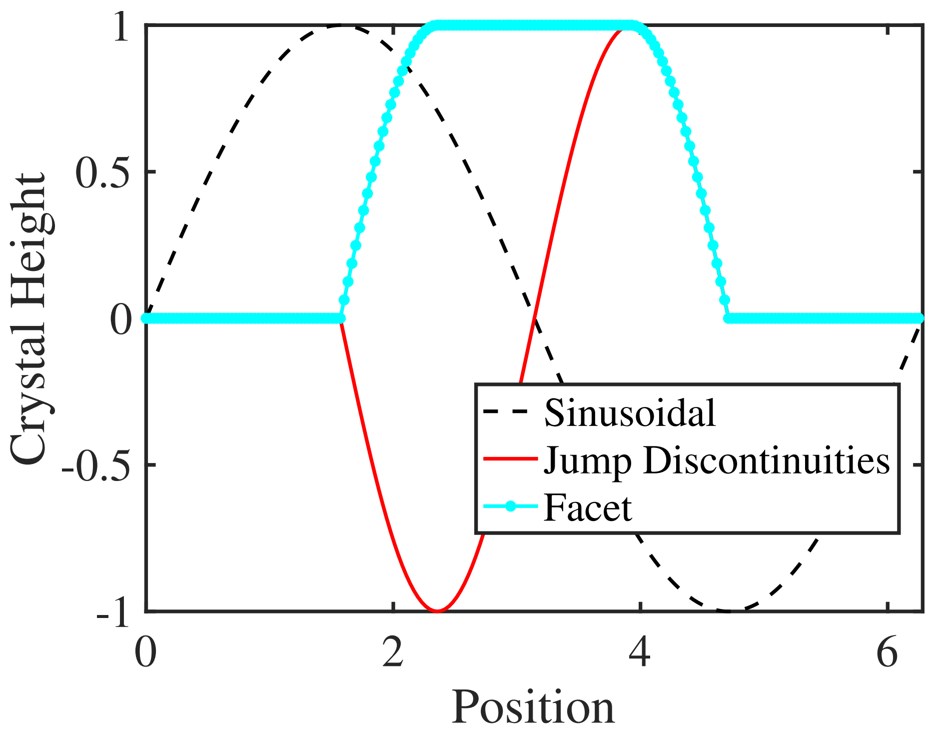

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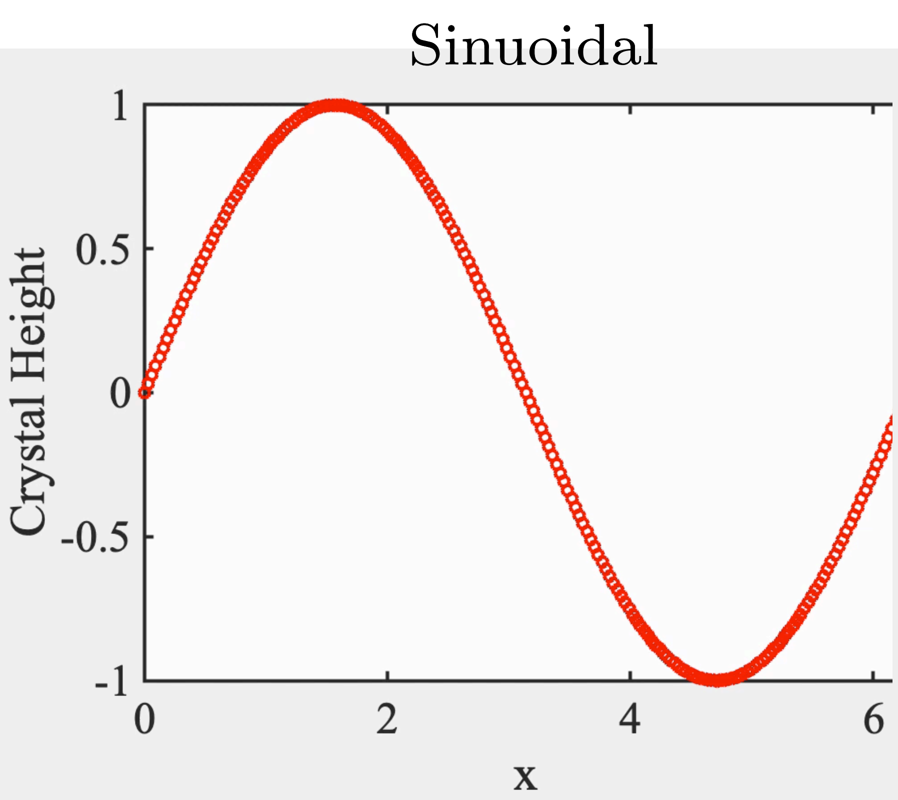

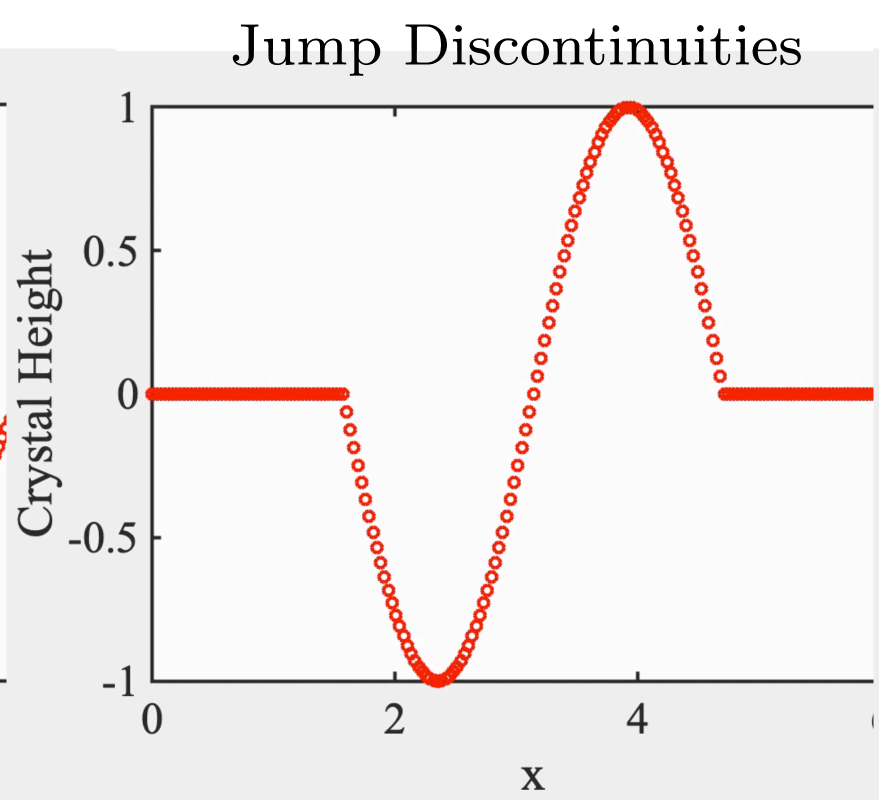

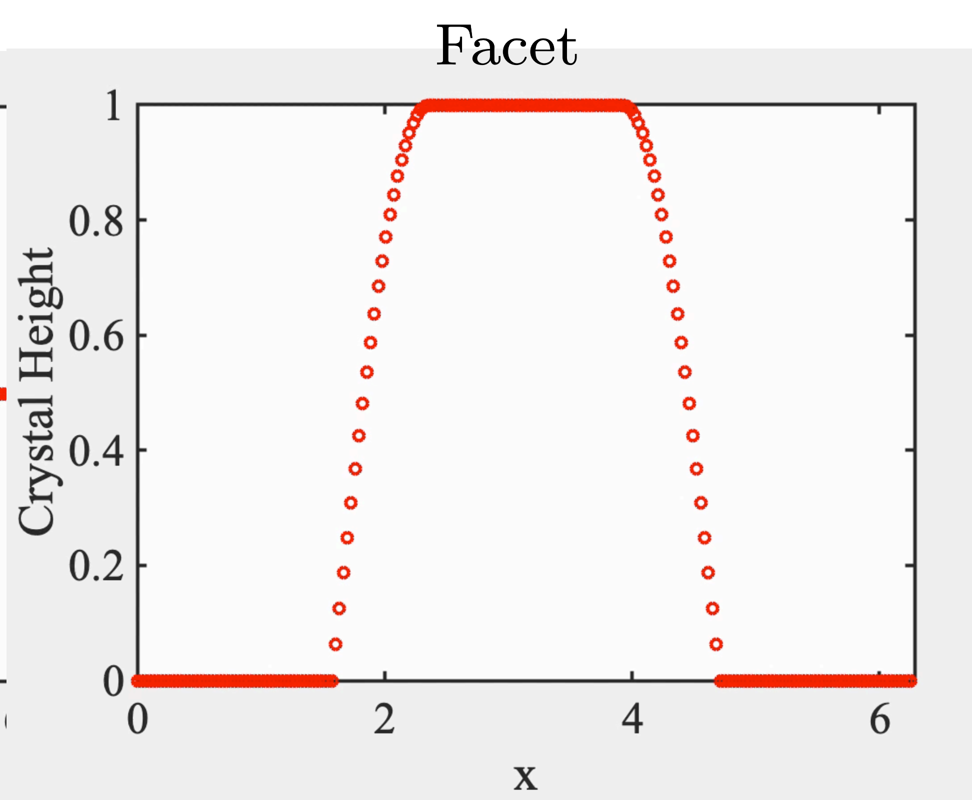

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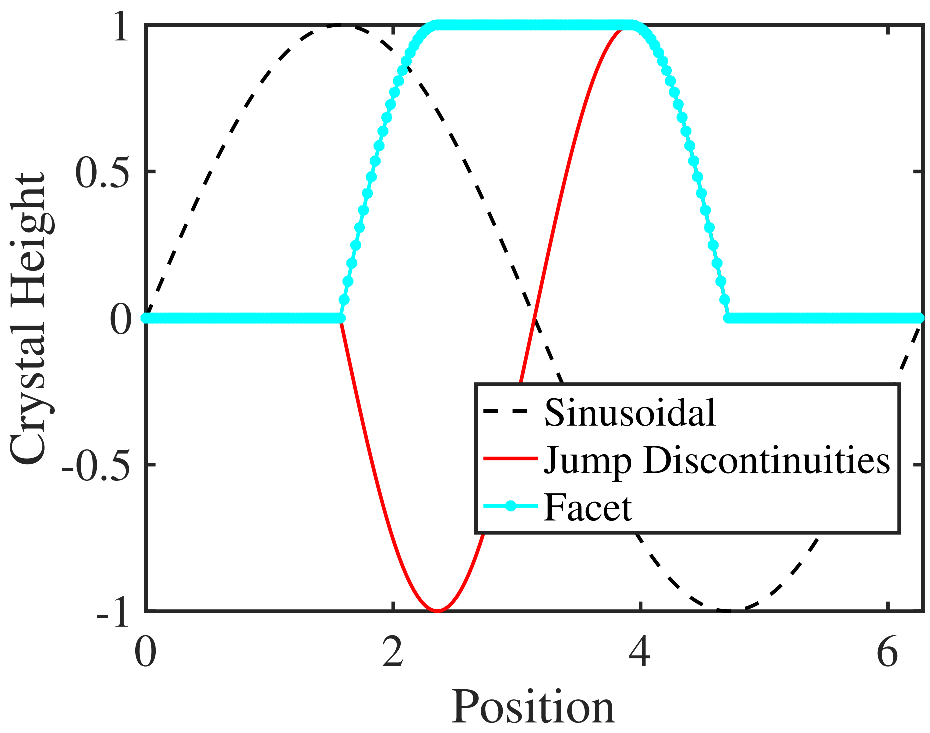

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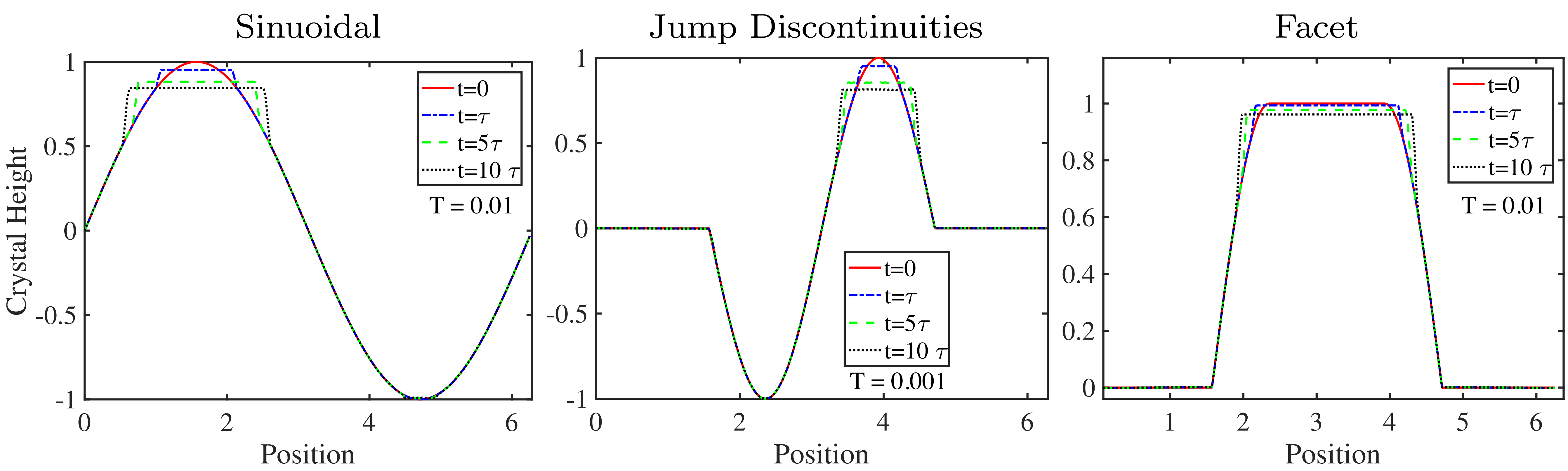
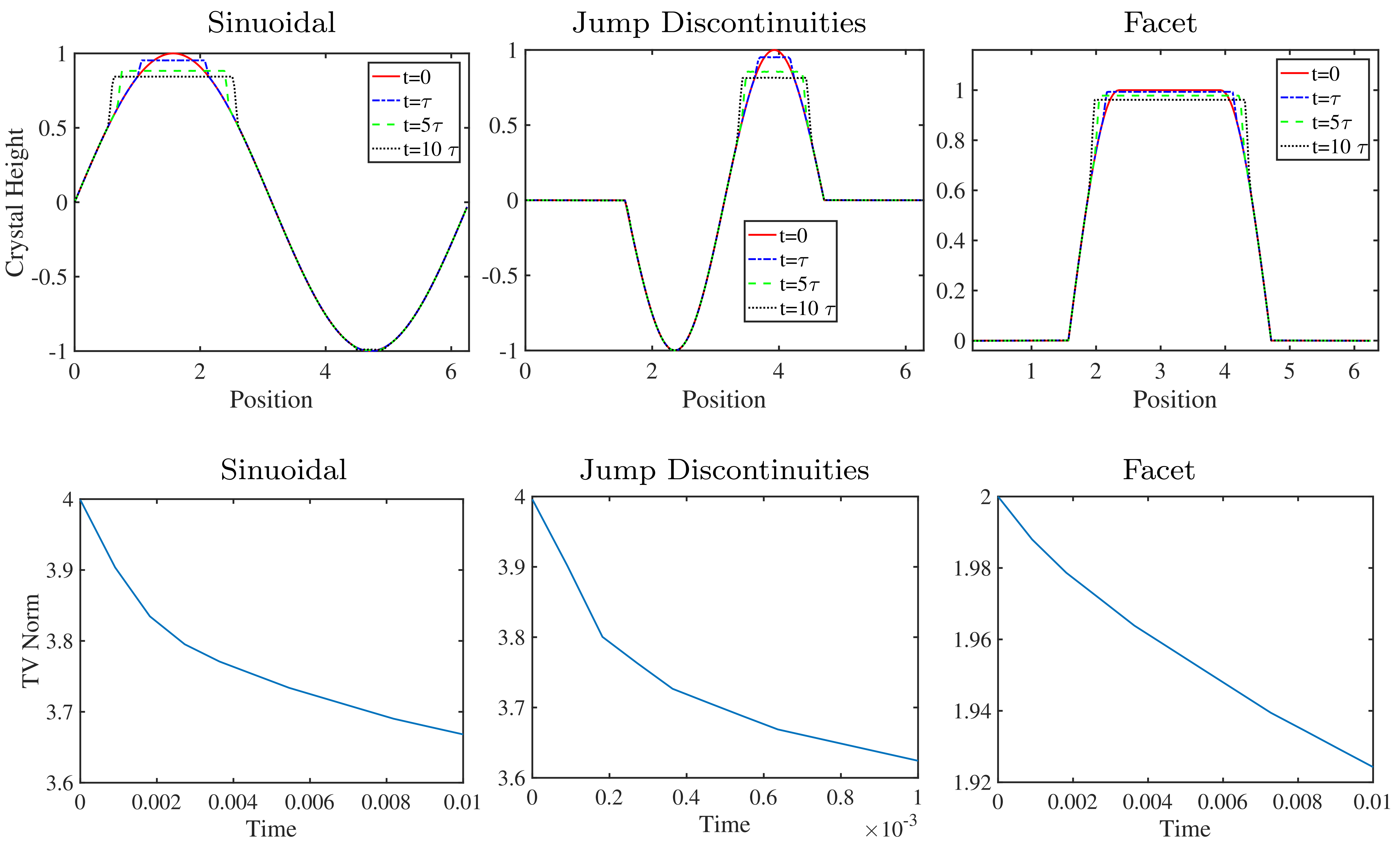
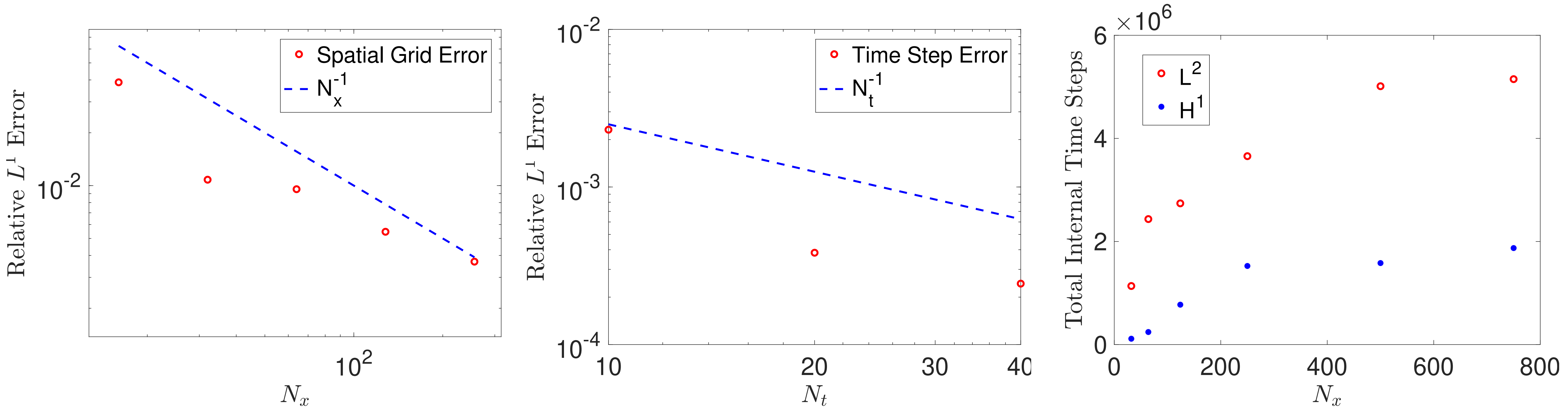


Numerical Results: energy decrease



Numerical Results: convergence



Observations:

- Error vs Nx: slightly sublinear convergence (low spatial regularity)
- Error vs Nt: first order (semi-implicit Euler)
- Internal time steps vs Nt: importance of selecting correct Hilbert space

sinusoidal, (Nx = 200), (Nt = 10), σ = 0.0005, λ = 500, ε =0.05, T = 10^{-4}

Open questions

crystal growth PDE

$$\partial_t h = \Delta e^{-\Delta_1 h}$$

→

“gradient flow”

$$\partial_t h = -\nabla_{H_h^{-1}} \mathcal{E}(h)$$

$$M_\epsilon(h) = e^{-\varphi_\epsilon * \Delta_1 h}, \ \mathcal{E}(h) = \|\nabla h\|_1$$

↓

discrete time scheme

$$h^{n+1} = \mathrm{argmin}_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|^2_{H^{-1}_{h^n}}$$

→

PDHG scheme

$$h^{(m+1)} = \left(\frac{\tau}{\lambda}\Delta_{h^n}\Delta + \mathrm{id}\right)^{-1} \left(\frac{\tau}{\lambda}\Delta_{h^n}\Delta h^{(m)} - \tau\Delta_{h^n}\nabla\cdot\phi^{(m)} + h^n\right)$$

$$\bar{h}^{(m+1)} = 2h^{(m+1)} - h^{(m)}$$

$$\phi^{(m+1)} = (\mathrm{id} + \sigma\partial F^*)^{-1}(\phi^{(m)} + \sigma\nabla\bar{h}^{(m+1)}) ,$$

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Today: Convergence of PDHG,
E TV energy, gen M(h), d=1

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- Convergence as $\tau \to 0$?
- Convergence as $\tau, \varepsilon \to 0$?

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Today: Convergence of PDHG, E TV energy, gen M(h), d=1

Open questions

crystal growth PDE

$$\partial_t h = \Delta e^{-\Delta_1 h}$$

- Appropriate notion of weak solution?
- Better time discretization/GF formulation to prove existence of wider class of weak solutions? numerics?

"gradient flow"

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Thank you!