Chair of Advanced Mathematics and Analytical Mechanics
Department of Mathematic
Technical University of Munich

SFB TRR 109 Discretization in Geometry and Dynamics

A BDF2-Approach for the Non-Linear Fokker-Planck Equation

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Joint work with Daniel Matthes (TUM)

Workshop: *"Entropies, the Geometry of Nonlinear Flows, and their Applications"*
Banff
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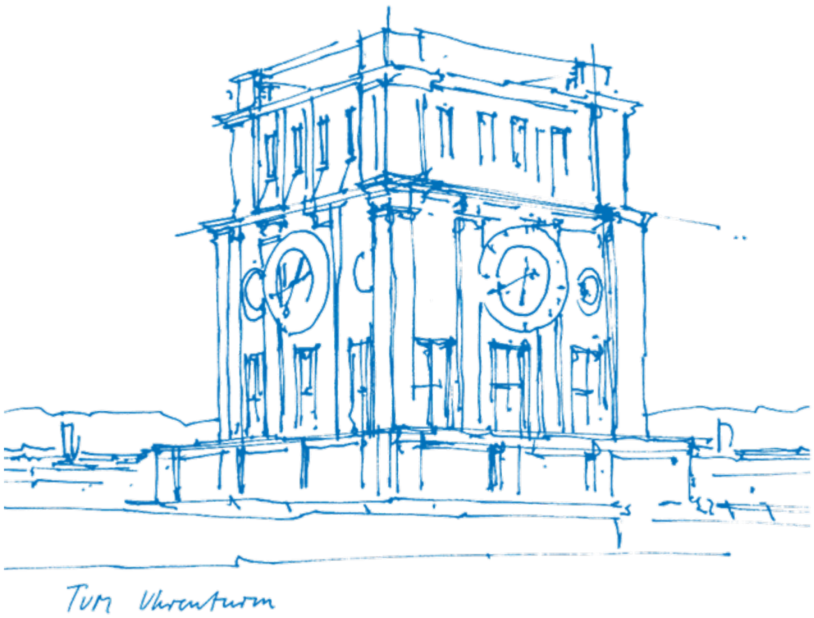
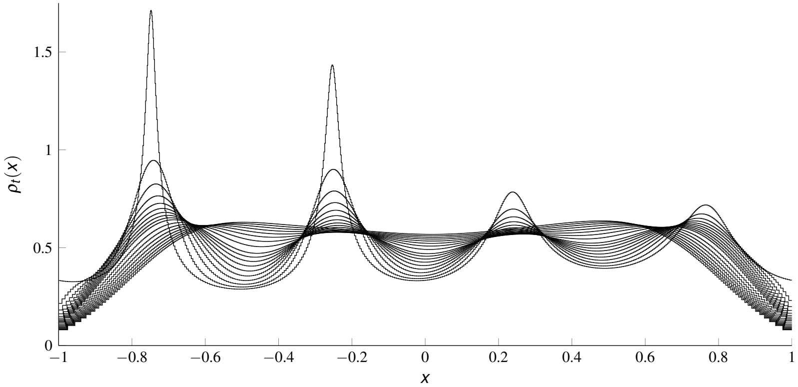


Outline

Non-Linear Fokker-Planck equation

$$\partial_t \rho_t = \Delta(\rho_t^m) + \operatorname{div}(\rho_t \nabla V) + \operatorname{div}(\rho_t \nabla (W * \rho_t))$$

no-flux BC $\qquad \rho(0) = \rho^0$



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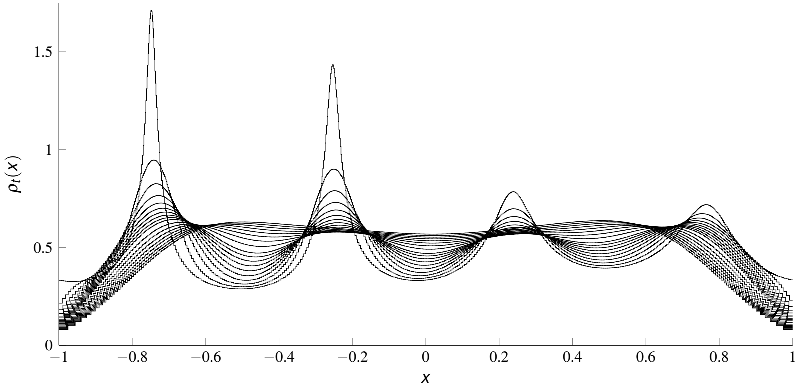

Goal: Construct solutions

- Inherit essential structural properties (mass preservation, positivity, energy dissipation,...)
- Develop Second Order Scheme (outperform Minimizing Movement Scheme)

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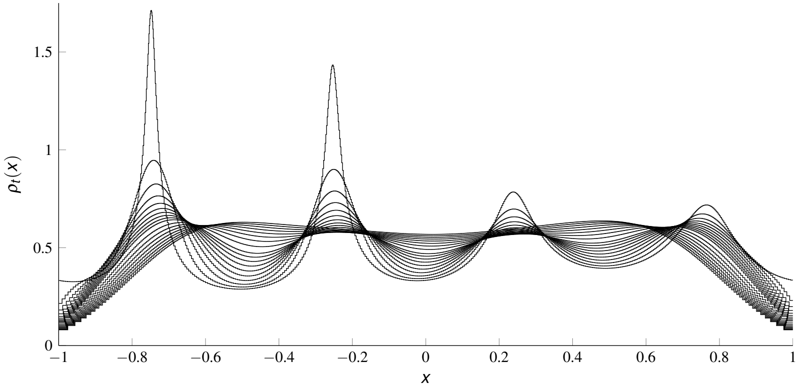

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Method: Semi-discretization in time

- Exploit the Gradient Flow structure

$$\text{(FP)} \begin{cases} \dot{\rho}_t & = -\nabla_{W_2} F(\rho_t) \\ \rho(0) & = \rho^0 \end{cases}$$

- Variational formulation of BDF2
- Geometry of $(\mathscr{P}_2(\Omega), W_2)$

Gradient Flow Structure

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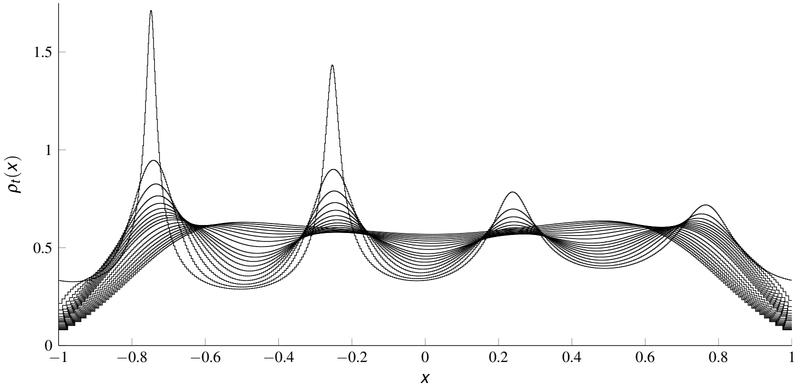

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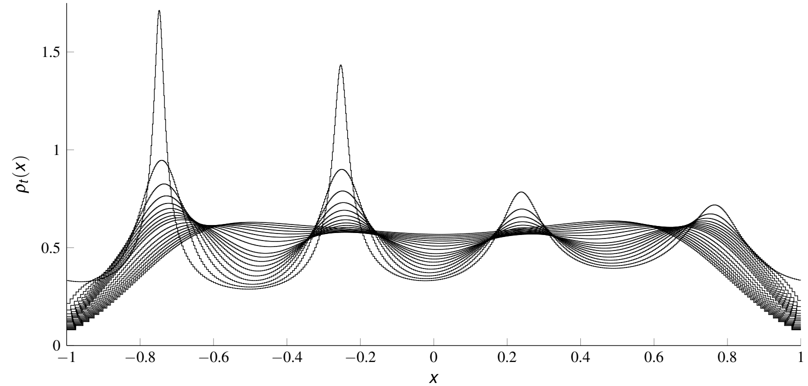
Diffusion + Confinement + Aggregation



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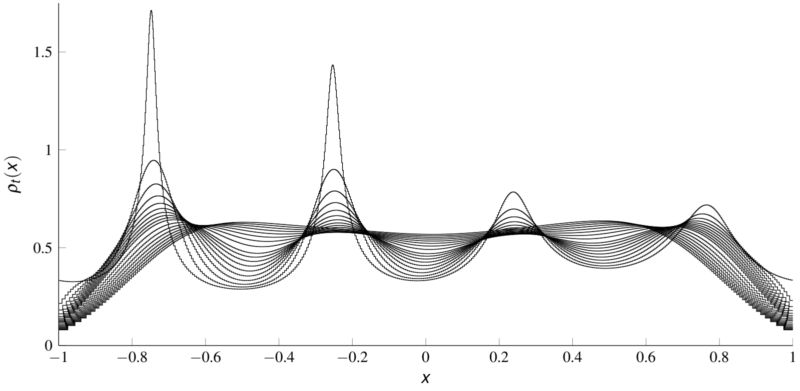

Dynamics: JKO'98, Otto'99, AGS'05

ρ_t solves the continuity equation

$$\partial_t \rho_t = -\mathrm{div}(\rho_t v_t), \quad \text{with} \quad v_t = -\nabla \frac{\delta F}{\delta \rho}(\rho_t),$$

where the energy functional F is given by

$$F(\rho) := \begin{cases} \int_\Omega \rho \log(\rho) + V\rho + \frac{1}{2}(W * \rho)\rho \, dx \\ \int_\Omega \frac{1}{m-1}\rho^m + V\rho + \frac{1}{2}(W * \rho)\rho \, dx \end{cases}$$

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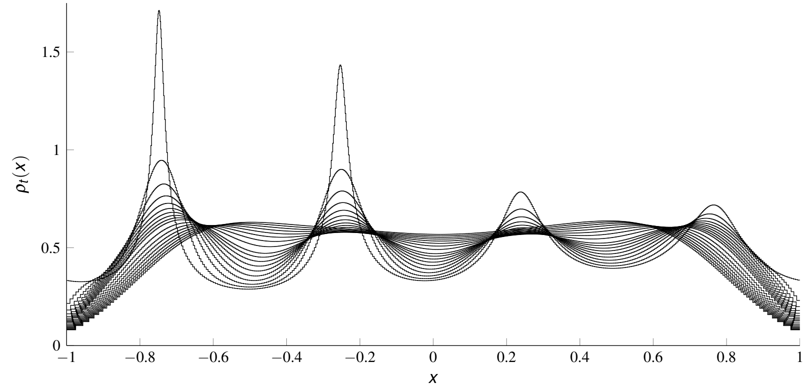

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L^2-Wasserstein space:

$(\mathscr{P}_2(\Omega), W_2)$ is the space of probability measures $\mathscr{P}_2(\Omega)$ equipped with

$$W_2^2(\mu,\nu) := \inf_{p \in \Gamma(\mu,\nu)} \int_{\Omega^2} |x-y|^2 \, \mathrm{d}p(x,y).$$

The set of transport plans $\Gamma(\mu,\nu)$ is defined by

$$\Gamma(\mu,\nu) := \{ p \in \mathscr{P}(\Omega^2) \mid \pi^1_{\#} p = \mu, \ \pi^2_{\#} p = \nu \}.$$

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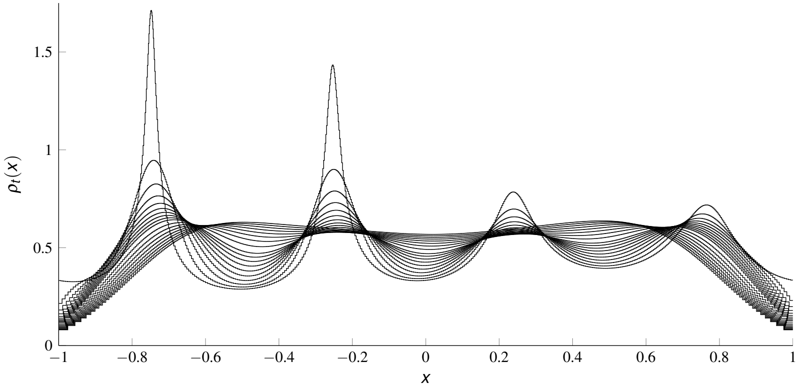

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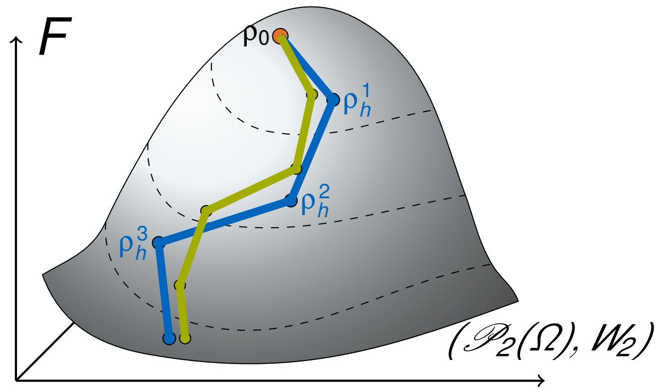
Brenier's Formula: If μ is regular there exits an OT-map t with $t_\# \mu = \nu$ such that

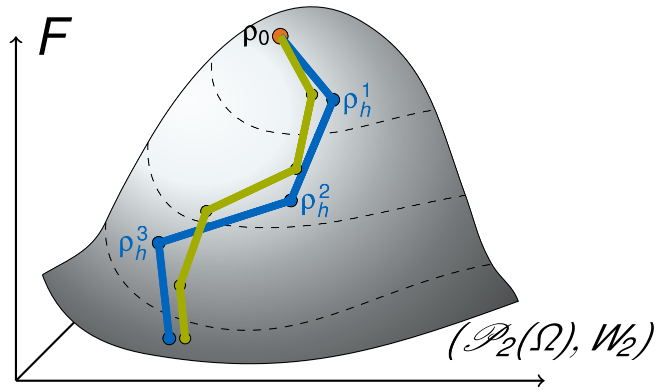
$$W_2^2(\mu,\nu) = \int_\Omega |x - t(x)|^2 \, d\mu(x)$$

Semi-discretization in time



Semi-discretization in time

$$\dot{x}_t = -\nabla F(x_t) \quad \underset{\text{Implicit Euler}}{\Rightarrow} \quad x_h^k - x_h^{k-1} = -h\nabla F(x_h^k)$$



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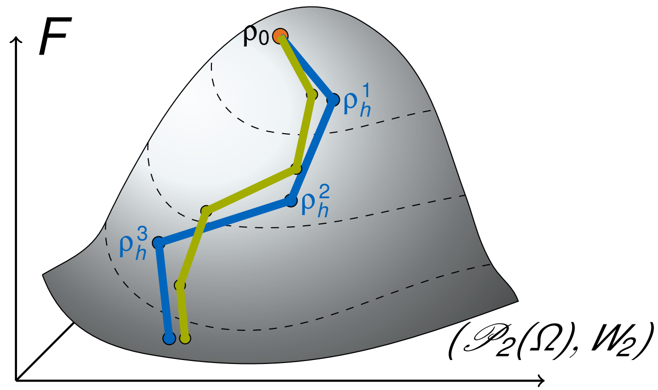
Variational Formulation: Minimizing Movement Scheme

Given a time step size h and ρ_h^0 define inductively

$$\rho_h^k \in \underset{\rho \in \mathscr{P}_2(\Omega)}{\operatorname{argmin}} \; \frac{1}{2h} W_2^2(\rho_h^{k-1}, \rho) + F(\rho)$$



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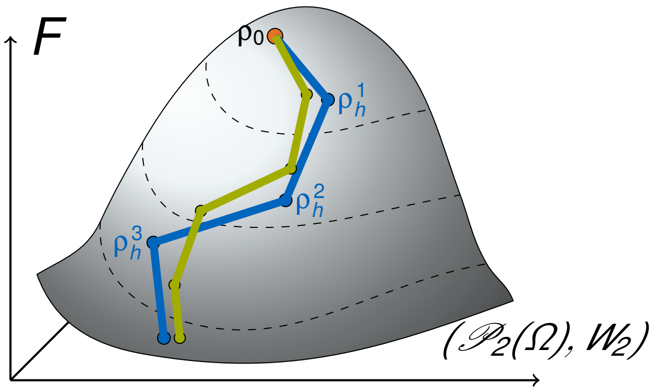

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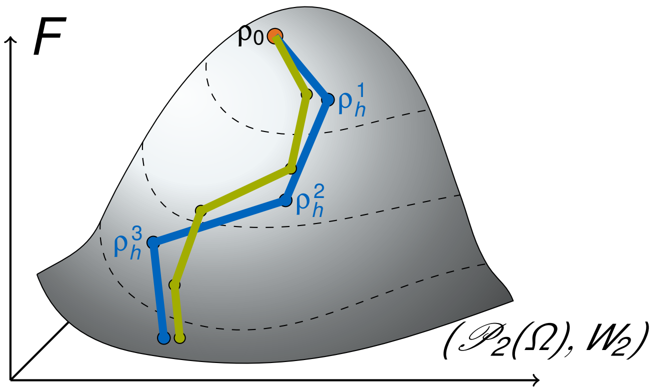

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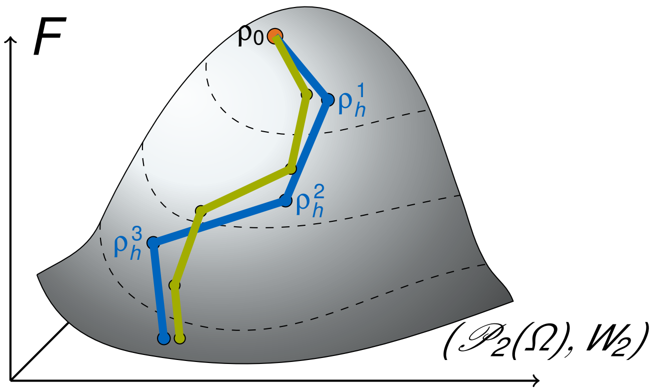

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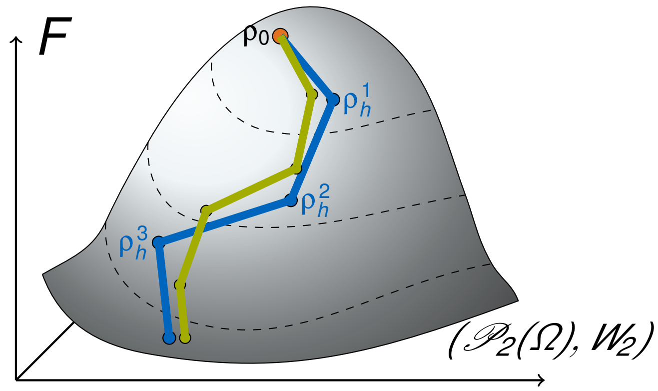

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Plan:

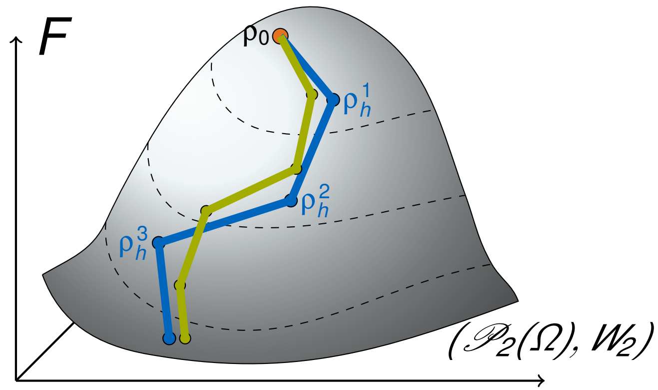
- Existence of $(\rho_h^k)_{k \in \mathbb{N}}$
- Euler-Lagrange Equations
- Estimates
- Convergence

Single Step Analysis

BDF2 Penalization:

$$\rho \mapsto \frac{1}{h} W_2^2(\mu,\rho) - \frac{1}{4h} W_2^2(\nu,\rho) + F(\rho)$$

Questions: Existence of Minimizer? Discrete Euler-Lagrange Equation?



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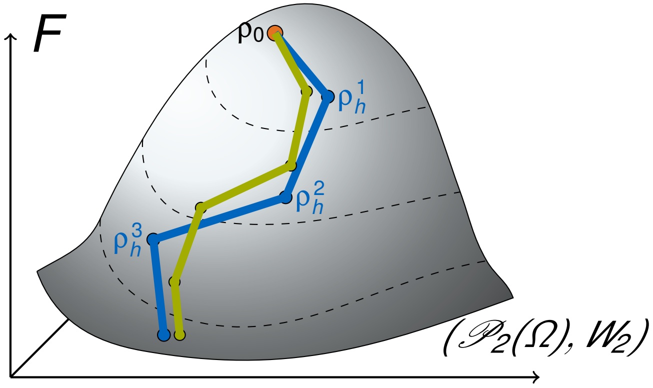

Theorem: Existence of Minimizer

For h small there exists an absolutely continuous minimizer $\rho_* \in \mathscr{P}_{2,ac}(\Omega)$.

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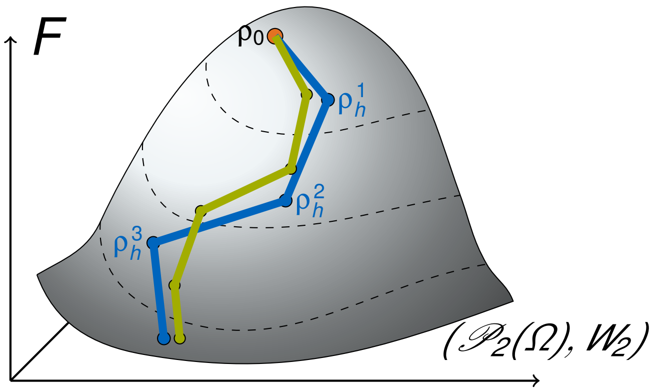

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Main observation: The map

$$\rho \mapsto 4W_2^2(\mu,\rho) - W_2^2(\nu,\rho)$$

is l.s.c. w.r.t. narrow convergence.

Single Step Analysis

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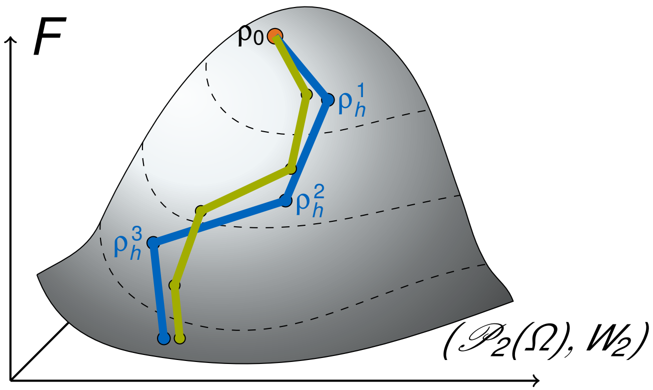

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Theorem: Discrete Euler-Lagrange equation

Let t and s be the OT-maps between ρ_* and μ or ρ_* and ν, respectively, then $\forall \xi \in C_c^\infty(\Omega, \mathbb{R}^d)$:

$$0 = \frac{1}{h}\int_\Omega \langle \xi(x), \frac{3}{2}x - 2t(x) + \frac{1}{2}s(x)\rangle \rho_*(x)\,dx$$
$$- \int_\Omega \operatorname{div}(\xi)\rho_*^m - \langle \xi, \nabla V + \nabla W * \rho_*\rangle \rho_*\,dx.$$

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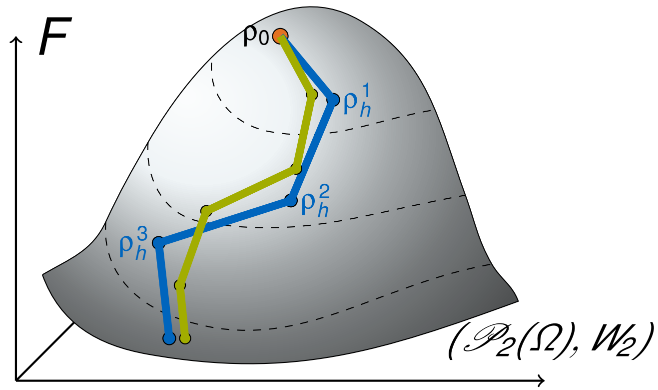

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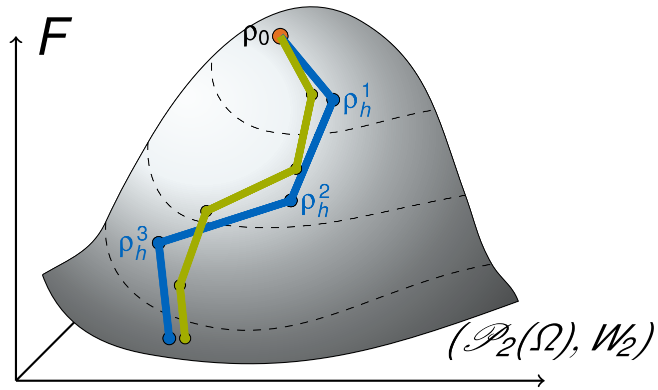

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Idea of proof: Variation by (CE)

$$\text{(CE)} \quad \begin{cases} \partial_s \rho_s + \operatorname{div}(\xi \rho_s) = 0 \\ \rho_0 = \rho_* \end{cases}$$

and use the differential calculus in $(\mathscr{P}_2(\Omega), W_2)$.

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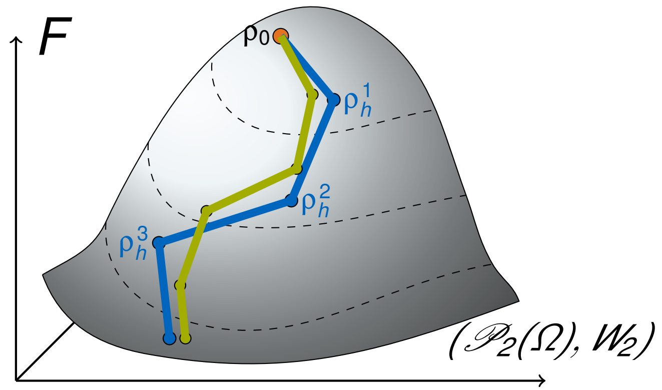
Estimates

Discrete Solution $(\rho_h^k)_{k\in\mathbb{N}}$ **and pc-interpolation** $\overline{\rho}_h(t)$**:**

$$\rho_h^k \in \operatorname*{argmin}_{\rho\in\mathscr{P}_2(\Omega)} \frac{1}{h}W_2^2(\rho_h^{k\text{-}1},\rho) - \frac{1}{4h}W_2^2(\rho_h^{k\text{-}2},\rho) + F(\rho)$$

$$\overline{\rho}_h(0) = \rho_0, \qquad \overline{\rho}_h(t) = \rho_h^k \quad \text{for } t\in((k-1)h, kh]$$



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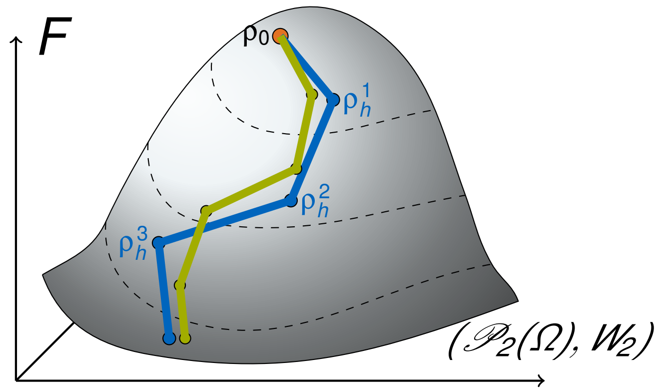

Theorem: Intrinsic Bounds (A-stability)

Step size independent bounds $\forall\, kh \le T$:

$$F(\rho_h^k) \le C \quad \text{(internal energy)}$$

$$\sum_{n=1}^{k} \frac{W_2^2(\rho_h^n,\rho_h^{n-1})}{h} \le C \quad \text{(kinetic energy)}$$

$$W_2^2(\delta_0,\rho_h^k) \le C \quad (W_2\text{-bounded})$$

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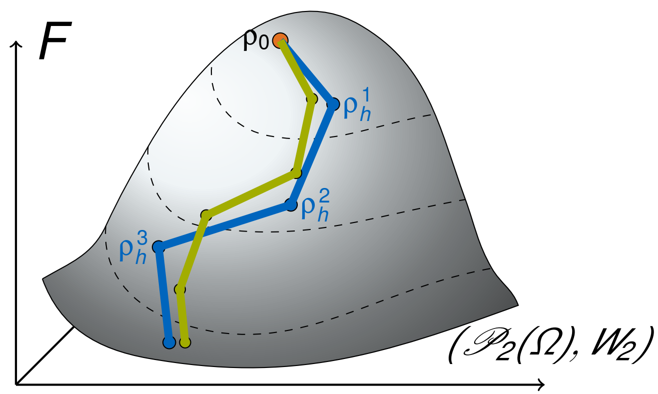

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$$W_2^2(\delta_0,\rho_h^k) \le C \quad (W_2\text{-bounded})$$

Theorem: $BV(\Omega)$-estimates

Step size independent bounds $\forall\ kh \le T$:

$$\operatorname{Var}((\rho_h^k)^m,\Omega) \le \frac{C}{h}\left(h + W_2(\rho_h^k,\rho_h^{k\text{-}1}) + W_2(\rho_h^k,\rho_h^{k\text{-}2})\right)$$

$$\|\bar{\rho}_h^m\|_{L^2(0,T,BV(\Omega))} \le C$$

Intrinsic Bounds (A-stability)

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Use that $W_2^2(\rho, \mu) \leq 2W_2^2(\rho, \nu) + 2W_2^2(\nu, \mu)$. Summing up yields

$$F(\rho_h^k) + \sum_{n=1}^{k} \frac{1}{4h} W_2^2(\rho_h^n, \rho_h^{n-1}) \leq F(\rho_h^0).$$

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Taking the supremum over all $\xi \in C^\infty(\Omega,\mathbb{R}^d)$ with $\|\xi\|_\infty \le 1$ yields the claim.

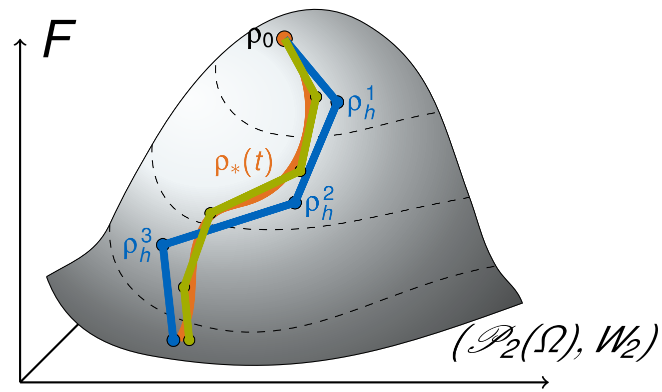
BDF2: Main Theorem

Main Result [P. '18]

Let $h \searrow 0$. Then

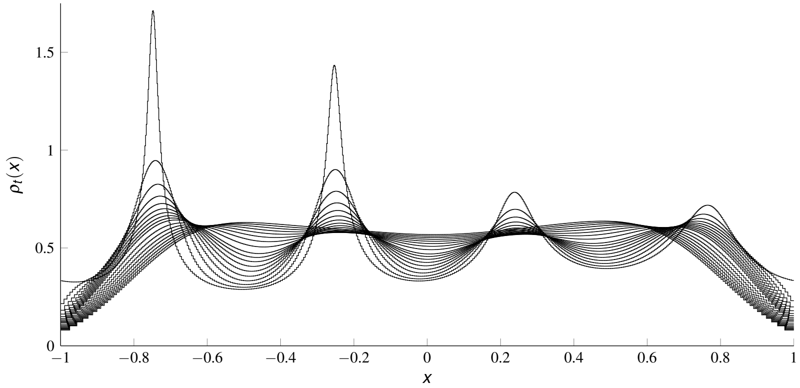
- $\bar{\rho}_h(t) \rightharpoonup \rho_*(t)$ narrowly, $\forall t > 0$
- $\bar{\rho}_h \to \rho_*$ in $L^m(0, T; L^m_{\mathrm{loc}}(\Omega))$

and ρ_* is a weak solution of the FP equation.



Proof:

- Compactness:
  Aubin-Lions Lemma for Banach-spaces RS'03
- Weak Formulation:
  Sum discrete Euler-Lagrange eq. JKO'98

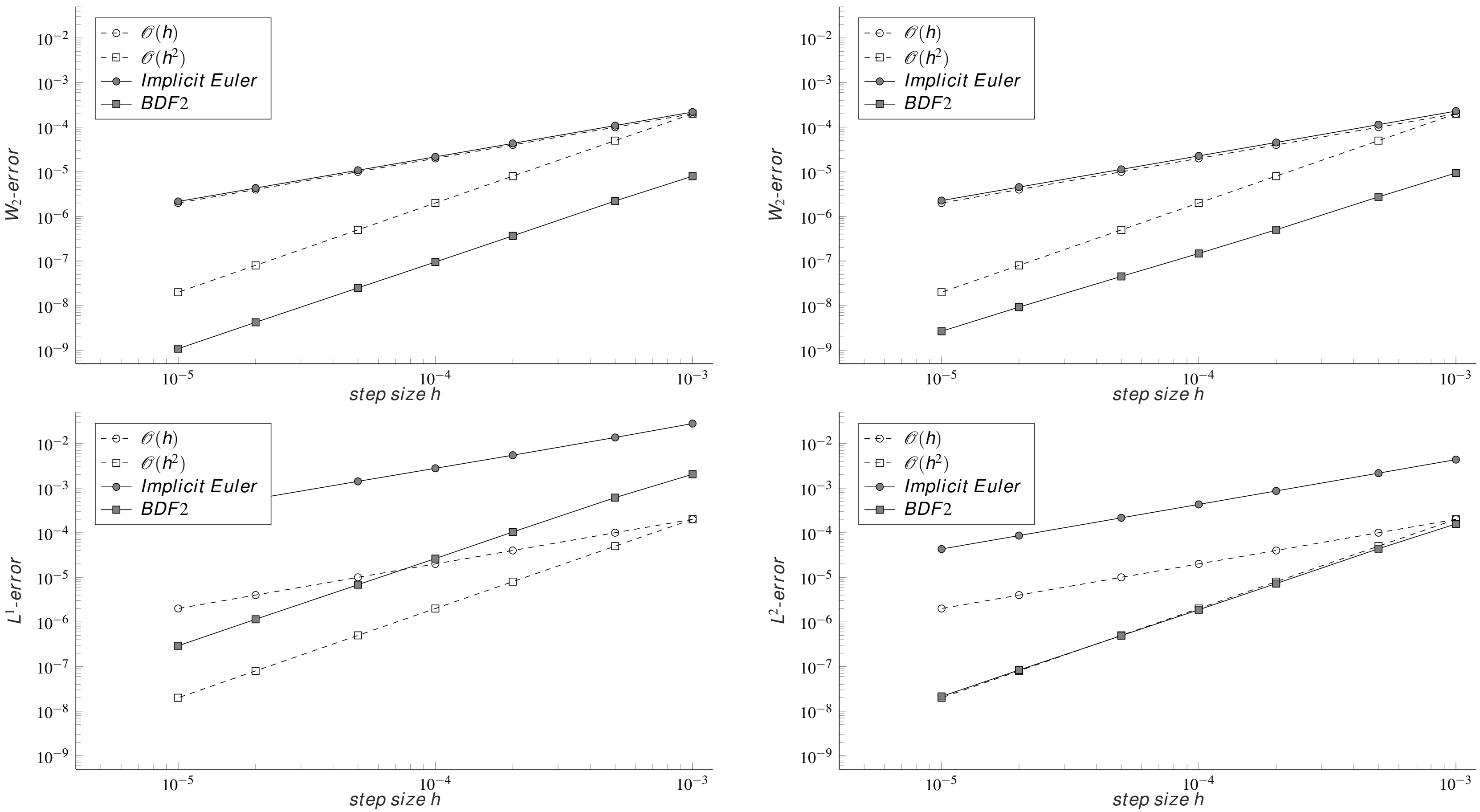


Numerics

m = 1 | **m = 2**

W_2-error:

L^m-error:



Conclusion

Pros

- Well-posedness and convergence of BDF2:
  - No convexity assumptions (contrary to MP'18)
  - Solely differential calculus in $(\mathscr{P}_2(\Omega), W_2)$
  - Application to other PDEs?
- Numerically better convergence than MMS
- New ansatz for spacial discretization

Cons

- No extension to BDFk schemes
- No analytical convergence rate
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Thank you for your attention!

D. Matthes, S. Plazotta *A Variational Formulation of the BDF2 Method for Metric Gradient Flows*, arXiv preprint arXiv:1711.02935 (2018)

S. Plazotta *A BDF2-Approach for the Non-linear Fokker-Planck Equation*, arXiv preprint arXiv:1801.09603 (2018)