

A JKO SPLITTING SCHEME FOR KANTOROVICH-FISHER-RAO GRADIENT FLOWS

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ABSTRACT. In this article we set up a splitting variant of the JKO scheme in order to handle gradient flows with respect to the Kantorovich-Fisher-Rao metric, recently introduced and defined on the space of positive Radon measure with varying masses. We perform successively a time step for the quadratic Wasserstein/Monge-Kantorovich distance, and then for the Hellinger/Fisher-Rao distance. Exploiting some inf-convolution structure of the metric we show convergence of the whole process for the standard class of energy functionals under suitable compactness assumptions, and investigate in details the case of internal energies. The interest is double: On the one hand we prove existence of weak solutions for a certain class of reaction-advection-diffusion equations, and on the other hand this process is constructive and well adapted to available numerical solvers.

1. INTRODUCTION

A new Optimal Transport distance on the space of positive Radon measures has been recently introduced independently by three different teams [12, 13, 22, 24, 25]. Contrarily to the classical Wasserstein-Monge-Kantorovich distances, which are restricted to the space of measures with fixed mass (typically probability measures), this new distance has the advantage of allowing for mass variations, can be computed between arbitrary measures, and does not require decay at infinity (such as finite moments). In [12, 13] the distance is called Wasserstein-Fisher-Rao and is introduced with imaging applications in mind. In [24, 25] the distance is referred to as the Hellinger-Kantorovich one, and was studied as a particular case of a larger class of Optimal Transport problems including primal/dual and static formulations. The second author introduced the same distance in [22], with applications to population dynamics and gradient flows in mind. In this paper we propose the name Kantorovich-Fisher-Rao for this metric (KFR in the sequel), taking into account all contributions.

On one side we aim here at understanding the local behavior of the KFR metric with respect to the by now classical quadratic Monge-Kantorovich/Wasserstein metric MK_2 and the Hellinger/Fisher-Rao metric FR . On the other side we want to use this information to prove existence of weak solutions to gradient flows while avoiding to look too closely into the geometry of the KFR space. Moreover our constructive approach is naturally adapted to available numerical schemes and Monge-Ampère solvers.

A possible way to formalize abstract gradient flow structures is to prove convergence of the corresponding Minimizing Movement scheme, as introduced by De Giorgi [14] and later developed by Jordan-Kinderlehrer-Otto for the MK_2 metric [18].

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Given a metric space (X, d) and a functional $F : X \rightarrow \mathbb{R}$, the JKO scheme with time-step $\tau > 0$ writes

$$(1.1) \quad x^{n+1} \in \operatorname{Argmin}_{x \in X} \left\{ \frac{1}{2\tau} d^2(x, x^n) + F(x) \right\}.$$

Letting $\tau \rightarrow 0$ one should expect to recover a weak solution of the gradient flow

$$(1.2) \quad \dot{x}(t) = -\operatorname{grad}_d F(x(t)).$$

Looking at (1.2), which is a differential equality between infinitesimal variations, we guess that only the local behavior of the metric d matters in (1.1).

The starting point of our analysis is therefore the local structure of the Kantorovich-Fisher-Rao metric, which endows the space of positive Radon measures $\rho \in \mathcal{M}^+$ with a formal Riemannian structure [22]. Based on some inf-convolution structure, our heuristic considerations will suggest that, infinitesimally, KFR should be the orthogonal sum of MK_2 and FR :

$$(1.3) \quad \text{KFR}^2 \approx \text{MK}_2^2 + \text{FR}^2.$$

More precisely we will show that in the tangent plane there holds

$$(1.4) \quad \|\operatorname{grad}_{\text{KFR}} \mathcal{F}(\rho)\|^2 = \|\operatorname{grad}_{\text{MK}} \mathcal{F}(\rho)\|^2 + \|\operatorname{grad}_{\text{FR}} \mathcal{F}(\rho)\|^2,$$

at least formally for reasonable functionals \mathcal{F} . The notion of metric gradients and tangent norms appearing in (1.4) will be precised in section 2. This naturally leads to a splitting approach for KFR Minimizing Movements: we successively run a time step for MK_2 , leading to the diffusion term in the associated PDE, and then a second step for FR , leading to the reaction term in the PDE. Formula (1.4) also indicates that the energy dissipation $D(t) = -\frac{dF}{dt} = |x'|^2 = |\operatorname{grad} F|^2$ will be correctly approximated in (1.2). One elementary Monge-Kantorovich JKO step is now well known, see for instance [34] and references therein. On the other hand the Fisher-Rao metric enjoys a Riemannian structure that can be recast, up to a change of variable, into a Hilbert setting, and therefore the reaction step should be easy to handle numerically.

Here we show that the classical estimates (energy monotonicity, total square distance, mass control, BV...) propagate along each MK_2 and FR substeps, and nicely fit together in the unified KFR framework. This allows us prove existence of weak solutions for a whole class of reaction-advection-diffusion PDEs associated with KFR gradient flows

$$\partial_t \rho = -\operatorname{grad}_{\text{KFR}} \mathcal{F}(\rho),$$

including e.g. the tumor growth model introduced in [31]. Moreover we retrieve a natural Energy Dissipation Inequality, which is well known [2] to completely characterize metric gradient flows.

Our splitting method has several interests: First we avoid a possibly delicate geometrical analysis of the KFR space, in particular we do not need to differentiate the squared KFR distance. This is usually required to derive the Euler-Lagrange equations in the JKO scheme, but might not be straightforward here (see Section 3 for discussions). Secondly, the approach leads to a new constructive existence proof for weak solutions to a class of PDEs, and can be implemented numerically (see [21] for an early application of this idea). For one elementary MK_2 step there are now many discretizations available, such as the semi-discrete scheme [28, 5], the augmented Lagrangian procedure [4], or the Entropic relaxation [32]. The Fisher-Rao minimizing step should not be difficult to implement, since the problem is convex with the good choice of variables.

The paper is structured as follows. In Section 2 we recall some basic facts on the three metrics involved: the quadratic Monge-Kantorovich MK_2 , the Fisher-Rao FR , and the Kantorovich-Fisher-Rao KFR distances. We highlight the three differential Riemannian structures and gradient flow interpretations. Section 3 details the local relation between the three metrics and in particular the inf-convolution. In section 4 we define the splitting minimizing movement scheme for the KFR distance and prove, under natural compactness assumptions, the convergence towards a weak solution of the expected PDE. As an example we investigate in section 5 the compactness hypothesis for the particular case of internal energies.

2. PRELIMINARIES

From now on we always assume that $\Omega \subset \mathbb{R}^d$ is a convex subset, possibly unbounded. In this section we recall some facts about the Wasserstein/Monge-Kantorovich and Hellinger/Fisher-Rao distances MK_2 , FR , and introduce the Kantorovich-Fisher-Rao distance KFR as recently defined independently in [22, 13, 24]. We also present the differential points of view for each of them, allowing to retrieve the three corresponding pseudo Riemannian structures and compute gradients of functionals with respect to the MK , FR , KFR metrics.

2.1. The quadratic Monge-Kantorovich distance MK_2 . We refer to [37] for an introduction and to [38] for a complete overview of the Wasserstein-Monge-Kantorovich distances.

Definition 2.1. *For any nonnegative Radon measures $\rho_0, \rho_1 \in \mathcal{M}_2^+$ with same mass $|\rho_0| = m = |\rho_1|$ and finite second moments, the quadratic Monge-Kantorovich distance is*

$$(2.1) \quad \text{MK}_2^2(\rho_0, \rho_1) = \min_{\gamma \in \Gamma[\rho_0, \rho_1]} \int_{\Omega \times \Omega} |x - y|^2 d\gamma(x, y),$$

where the admissible set of transference plans $\Gamma[\rho_0, \rho_1]$ consists in nonnegative measures $\gamma \in \mathcal{M}^+(\Omega \times \Omega)$ with mass $|\gamma| = m$ and prescribed marginals $\Pi_x(\gamma) = \rho_0(x)$ and $\Pi_y(\gamma) = \rho_1(y)$.

The minimizer is unique and is called an optimal plan. When ρ_0 does not charge small sets we have the characterization in terms of transport maps:

Theorem 1 (Brenier, Gangbo-McCann, [10, 16]). *With the same assumptions as in Definition 2.1, assume that ρ_0 does not give mass to \mathcal{H}^{d-1} sets. Then*

$$(2.2) \quad \text{MK}_2^2(\rho_0, \rho_1) = \min_{\rho_1 = \mathbf{t} \# \rho_0} \int_{\Omega} |x - \mathbf{t}(x)|^2 d\rho_0(x),$$

and the optimal transport map is unique $d\rho_0$ almost everywhere.

We recall the definition of pushforwards by maps $\mathbf{t} : \Omega \rightarrow \Omega$

$$\rho_1 = \mathbf{t} \# \rho_0 \quad \Leftrightarrow \quad \int_{\Omega} \phi(y) d\rho_1(y) = \int_{\Omega} \phi(\mathbf{t}(x)) d\rho_0(x) \quad \text{for all } \phi \in \mathcal{C}_c(\Omega).$$

As first pointed out by Benamou and Brenier [3] we also have the following dynamic representation of the Wasserstein distance:

Theorem 2 (Benamou-Brenier formula, [2, 3]). *There holds*

$$(2.3) \quad \text{MK}_2^2(\rho_0, \rho_1) = \min_{(\rho, \mathbf{v}) \in \mathcal{A}_{\text{MK}}[\rho_0, \rho_1]} \int_0^1 \int_{\Omega} |\mathbf{v}_t|^2 d\rho_t dt,$$

where the admissible set $\mathcal{A}_{\text{MK}}[\rho_0, \rho_1]$ consists in curves $(0, 1) \ni t \mapsto (\rho_t, \mathbf{v}_t) \in \mathbb{R}^+ \times \mathbb{R}^d$ such that $t \mapsto \rho_t$ is narrowly continuous with endpoints $\rho_t(0) = \rho_0$, $\rho_t(1) = \rho_1$ and solving the continuity equation

$$\partial_t \rho_t + \operatorname{div}(\rho_t \mathbf{v}_t) = 0$$

in the sense of distributions $\mathcal{D}'((0, 1) \times \Omega)$.

In (2.3) a minimizing curve $t \mapsto \rho_t$ is a geodesics, with constant metric speed $\|\mathbf{v}_t\|_{L^2(d\rho_t)}^2 = cst = \text{MK}_2^2(\rho_0, \rho_1)$. Note that we allow here for any arbitrary mass $|\rho_0| = m = |\rho_1| > 0$, and that the distance scales as $\text{MK}_2^2(\alpha\rho_0, \alpha\rho_1) = \alpha\text{MK}_2^2(\rho_0, \rho_1)$. This is apparent in all three formulations (2.1)(2.2)(2.3), which are linear in γ , ρ_0 , ρ_1 , and ρ_t respectively.

As is now well-known from the works of Otto [30], we can view the set of measures with fixed mass as a pseudo-Riemannian manifold, endowing the tangent plane

$$T_\rho \mathcal{M}_{\text{MK}}^+ = \{\partial_t \rho = -\operatorname{div}(\rho \mathbf{v}) \quad \text{evaluated at } t = 0\}$$

with the metrics

$$\|\partial_t \rho\|_{T_\rho \mathcal{M}_{\text{MK}}^+}^2 = \inf \left\{ \|\mathbf{v}\|_{L^2(d\rho)}^2 : \partial_t \rho = -\operatorname{div}(\rho \mathbf{v}) \right\}.$$

It is easy to see formally that, among all possible velocities \mathbf{v} representing the same tangent vector $\partial_t \rho = -\operatorname{div}(\rho \mathbf{v})$, there is a unique one with minimal $L^2(d\rho)$ norm. A back of the envelope computation shows that this particular velocity is necessarily potential, $\mathbf{v} = \nabla p$ for a pressure function p uniquely defined up to constants (see the proof of Proposition 2.2 below for a sketchy argument). As a consequence we always choose to represent

$$\|\partial_t \rho\|_{T_\rho \mathcal{M}_{\text{MK}}^+}^2 = \|\nabla p\|_{L^2(d\rho)}^2 \quad \text{with the identification } \partial_t \rho = -\operatorname{div}(\rho \nabla p).$$

Here we remained formal and refer again to [37, 38] for details. Now metric gradients $\operatorname{grad}_{\text{MK}}$ can be computed by the chain rule as follows: If $\partial_t \rho_t = -\operatorname{div}(\rho_t \nabla p_t)$ is a “ \mathcal{C}^1 ” curve passing through $\rho_t(0) = \rho$ with arbitrary initial velocity $\zeta = \partial_t \rho(0) = -\operatorname{div}(\rho \nabla p)$ then for functionals $\mathcal{F}(\rho) = \int_\Omega F(\rho(x), x) dx$

$$\begin{aligned} \langle \operatorname{grad}_{\text{MK}} \mathcal{F}(\rho), \zeta \rangle_{T_\rho \mathcal{M}_{\text{MK}}^+} &= \frac{d}{dt} \mathcal{F}(\rho_t) \Big|_{t=0} = \frac{d}{dt} \left(\int_\Omega F(\rho_t(x), x) dx \right) \Big|_{t=0} \\ &= \int_\Omega F'(\rho) \times \{-\operatorname{div}(\rho \nabla p)\} = \int_\Omega \nabla F'(\rho) \cdot \nabla p \, d\rho \\ &= \langle \nabla F'(\rho), \nabla p \rangle_{L^2(d\rho)}, \end{aligned}$$

where $F'(\rho) = \frac{\delta F}{\delta \rho}$ stands for the standard first variation with respect to ρ . For the classical case $\mathcal{F}(\rho) = \int_\Omega \{U(\rho) + \Psi\rho + \frac{1}{2}\rho K \star \rho\}$ considered here this means $F'(\rho) = U'(\rho) + \Psi(x) + K \star \rho$. This shows that one should identify gradients

$$(2.4) \quad \operatorname{grad}_{\text{MK}} \mathcal{F}(\rho) = -\operatorname{div}(\rho \nabla F'(\rho))$$

through the $L^2(d\rho)$ action in the tangent plane, and as a consequence the Monge-Kantorovich gradients flows read

$$(2.5) \quad \partial_t \rho = -\operatorname{grad}_{\text{MK}} \mathcal{F}(\rho) \quad \Leftrightarrow \quad \partial_t \rho = \operatorname{div}(\rho F'(\rho)).$$

2.2. The Fisher-Rao distance FR. The classical Hellinger-Kakutani distance [17, 19], or Fisher-Rao metric, was first introduced for probability measures and is well known in statistics and information theory for its connections with the Kullback's divergence and Fisher information [8]. It can be extended to arbitrary nonnegative measures as

Definition 2.2. *The Fisher-Rao distance between measures $\rho_0, \rho_1 \in \mathcal{M}^+$ is given by*

(2.6)

$$\text{FR}^2(\rho_0, \rho_1) = \min_{(\rho_t, r_t) \in \mathcal{A}_{\text{FR}}[\rho_0, \rho_1]} \int_0^1 \int_{\Omega} |r_t(x)|^2 d\rho_t(x) dt = 4 \int_{\Omega} \left| \sqrt{\frac{d\rho_0}{d\lambda}} - \sqrt{\frac{d\rho_1}{d\lambda}} \right|^2 d\lambda.$$

The admissible set $\mathcal{A}_{\text{FR}}[\rho_0, \rho_1]$ consists in curves $[0, 1] \ni t \mapsto (\rho_t, r_t) \in \mathbb{R}^+ \times \mathbb{R}$ such that $t \mapsto \rho_t \in \mathcal{C}_w([0, 1]; \mathcal{M}^+)$ is weakly continuous with endpoints $\rho_t(0) = \rho_0, \rho_t(1) = \rho_1$, and

$$\partial_t \rho_t = \rho_t r_t$$

in the sense of distributions $\mathcal{D}'((0, 1) \times \Omega)$.

In the last explicit formula λ is any reference measure such that ρ_0, ρ_1 are both absolutely continuous with respect to λ , with Radon-Nikodym derivatives $\frac{d\rho_i}{d\lambda}$. By 1-homogeneity this expression does not depend on the choice of λ , and the normalizing factor 4 is chosen so that the metric for the pivot space in the first dynamic formulation is exactly $L^2(d\rho_t)$ (and not some other multiple $\beta \|r_t\|_{L^2(d\rho_t)}^2$).

One can check that the minimum in the first definition is attained along the geodesics

$$\rho_t = [(1-t)\sqrt{\rho_0} + t\sqrt{\rho_1}]^2 \quad \text{and} \quad r_t := 2 \frac{\sqrt{\rho_1} - \sqrt{\rho_0}}{\sqrt{\rho_t}} \in L^2(d\rho_t).$$

Moreover this optimal curve $\partial_t \rho_t = \rho_t r_t$ has constant metric speed $\|r_t\|_{L^2(d\rho_t)}^2 = 4 \int_{\Omega} |\sqrt{\rho_1} - \sqrt{\rho_0}|^2 = \text{FR}^2(\rho_0, \rho_1)$, which should be expected for geodesics.

More importantly, the first Lagrangian formulation in (2.6) suggests to view the metric space $(\mathcal{M}^+, \text{FR})$ as a Riemannian manifold, endowing the tangent plane

$$T_{\rho} \mathcal{M}_{\text{FR}}^+ = \left\{ \partial_t \rho_t = \rho_t r_t \quad \text{evaluated at } t=0 \right\}$$

with the metrics

$$\|\partial_t \rho\|_{T_{\rho} \mathcal{M}_{\text{FR}}^+}^2 = \|r\|_{L^2(d\rho)}^2 \quad \text{with the identification } \partial_t \rho = \rho r.$$

Metric gradients grad_{FR} can then be computed by the chain rule as follows. If $\partial_t \rho_t = \rho_t r_t$ is a “ \mathcal{C}^1 ” curve passing through $\rho_t(0) = \rho$ with arbitrary initial velocity $\zeta = \partial_t \rho = \rho r$ then for functionals $\mathcal{F}(\rho) = \int_{\Omega} F(\rho(x), x) dx$ we can compute

$$\begin{aligned} \langle \text{grad } \mathcal{F}(\rho), \zeta \rangle_{T_{\rho} \mathcal{M}_{\text{FR}}^+} &= \frac{d}{dt} \mathcal{F}(\rho_t) \Big|_{t=0} = \frac{d}{dt} \left(\int_{\Omega} F(\rho_t(x), x) dx \right) \Big|_{t=0} \\ &= \int_{\Omega} F'(\rho) \rho r = \langle F'(\rho), r \rangle_{L^2(d\rho)}, \end{aligned}$$

where $F'(\rho) = \frac{\delta F}{\delta \rho}$ as before. This shows that

$$(2.7) \quad \text{grad}_{\text{FR}} \mathcal{F}(\rho) = \rho F'(\rho)$$

with identification through the $L^2(d\rho)$ action in the tangent plane, and as a consequence gradients flows with respect to the Hellinger-Fisher-Rao metrics read

$$(2.8) \quad \partial_t \rho = -\operatorname{grad}_{\text{FR}} \mathcal{F}(\rho) \quad \leftrightarrow \quad \partial_t \rho = -\rho F'(\rho).$$

2.3. The Fisher-Rao-Hellinger-Wasserstein-Kantorovich distance KFR.

As introduced in [13], we have

Definition 2.3. *The Fisher-Rao-Hellinger-Kantorovich-Wasserstein distance between measures $\rho_0, \rho_1 \in \mathcal{M}^+(\Omega)$ is*

$$(2.9) \quad \text{KFR}^2(\rho_0, \rho_1) = \inf_{(\rho, \mathbf{v}, r) \in \mathcal{A}_{\text{KFR}}[\rho_0, \rho_1]} \int_0^1 \int_{\Omega} (|\mathbf{v}_t(x)|^2 + |r_t(x)|^2) d\rho_t(x) dt$$

The admissible set $\mathcal{A}_{\text{KFR}}[\rho_0, \rho_1]$ is the set of curves $[0, 1] \ni t \mapsto (\rho_t, \mathbf{v}_t, r_t) \in \mathbb{R}^+ \times \mathbb{R}^d \times \mathbb{R}$ such that $t \mapsto \rho_t \in \mathcal{C}_w([0, 1]; \mathcal{M}^+)$ is weakly continuous (for the narrow convergence of measures) with endpoints $\rho_t(0) = \rho_0, \rho_t(1) = \rho_1$, and the velocity and reaction $\mathbf{v}, r \in L^2(0, 1; L^2(d\rho_t))$ solve the continuity equation with source

$$\partial_t \rho_t + \operatorname{div}(\rho_t \mathbf{v}_t) = \rho_t r_t.$$

Comparing (2.9) with (2.3) and (2.6), this dynamic formulation *à la Benamou-Brenier* [3] shows that the KFR distance can be viewed as an inf-convolution of the Monge-Kantorovich and Fisher-Rao distances MK_2, FR . By the results of [13, 12, 24] the infimum in the definition is always a minimum, and the corresponding minimizing curves $t \mapsto \rho_t$ are of course called geodesics. As shown in [22, 13, 24] geodesics need not be unique, see also the brief discussion in section 4. Interestingly, there are other possible formulations of the distance in terms of static unbalanced optimal transportation, primal-dual characterizations with relaxed marginals, lifting to probability measures on a cone over Ω , and duality with subsolutions of Hamilton-Jacobi equations. See also [24, 25] as well as [33] for a related version with mass penalization. As an immediate consequence of the definition 2.9 we have a first interplay between the distances KFR, MK_2 , FR:

Proposition 2.1. *Let $\rho_0, \rho_1 \in \mathcal{M}_2^+$ such that $|\rho_0| = |\rho_1|$. Then*

$$\text{KFR}^2(\rho_0, \rho_1) \leq \text{MK}_2^2(\rho_0, \rho_1).$$

Similarly for all $\mu_0, \mu_1 \in \mathcal{M}^+$ (with possibly different masses) there holds

$$\text{KFR}^2(\mu_0, \mu_1) \leq \text{FR}^2(\mu_0, \mu_1).$$

Proof. If $|\rho_0| = |\rho_1|$ then the optimal Monge-Kantorovich geodesics $\partial_t \rho_t + \operatorname{div}(\rho_t \mathbf{v}_t) = 0$ from ρ_0 to ρ_1 gives an admissible path in (2.9) with $r \equiv 0$ and cost exactly $\text{MK}_2^2(\rho_0, \rho_1)$. Likewise for arbitrary measures μ_0, μ_1 one can follow the Fisher-Rao geodesics $\partial_r \rho_t = \rho_t r_t$, which gives an admissible path with $\mathbf{v} \equiv 0$ and cost $\text{FR}^2(\mu_0, \mu_1)$. \square

Proposition 2.2. *The definition (2.9) of the KFR distance can be restricted to the subclass of admissible paths such that $\mathbf{v}_t = \nabla r_t$.*

Proof. By [13, thm. 2.1] there exists a minimizing curve $(\rho_t, \mathbf{v}_t, r_t)$ in (2.9), which by definition is a KFR-geodesic between ρ_0, ρ_1 (we also refer to [22, thm. 6] and [25] for the existence of geodesics). Here we stay at the formal and assume that ρ, \mathbf{v}, r are smooth with $\rho > 0$ everywhere.

Consider first an arbitrary smooth vector-field \mathbf{w} such that $\operatorname{div} \mathbf{w}_t = 0$ for all $t \in [0, 1]$, and let $\mathbf{v}^\varepsilon := \mathbf{v} + \varepsilon \frac{\mathbf{w}}{\rho}$. Then $\operatorname{div}(\rho \mathbf{v}^\varepsilon) = \operatorname{div}(\rho \mathbf{v}) + 0$ and the triplet

$(\rho_t, \mathbf{v}_t^\varepsilon, r_t)$ is an admissible competitor in (2.9). Writing the optimality condition we compute

$$\begin{aligned} 0 &= \frac{d}{d\varepsilon} \left(\frac{1}{2} \int_0^1 \int_\Omega (|\mathbf{v}_t^\varepsilon(x)|^2 + |r_t(x)|^2) d\rho_t(x) dt \right) \Big|_{\varepsilon=0} \\ &= \int_0^1 \int_\Omega \mathbf{v}_t(x) \cdot \frac{\mathbf{w}_t(x)}{\rho_t(x)} d\rho_t(x) dt = \int_0^1 \int_\Omega \mathbf{v}_t(x) \cdot \mathbf{w}_t(x) dx dt. \end{aligned}$$

This L^2 orthogonality with all divergence-free vector fields classically implies that \mathbf{v}_t is potential for all times, i.e. $\mathbf{v}_t = \nabla u_t$ for some u_t .

Fix now any smooth $\phi \in \mathcal{C}_c^\infty((0, 1) \times \Omega)$, and define $\tilde{\mathbf{v}}_t^\varepsilon := \mathbf{v}_t + \varepsilon \nabla \phi_t = \nabla(u_t + \varepsilon \phi_t)$. Defining s_t by $\rho_t s_t = \operatorname{div}(\rho_t \nabla \phi_t)$ and $\tilde{r}_t^\varepsilon := r_t + \varepsilon s_t$ it is easy to check that $(\rho_t, \tilde{\mathbf{v}}_t^\varepsilon, \tilde{r}_t^\varepsilon)$ solves the continuity equation, and this triplet is again an admissible competitor in (2.9). Writing the optimality condition we get now

$$\begin{aligned} 0 &= \frac{d}{d\varepsilon} \left(\frac{1}{2} \int_0^1 \int_\Omega (|\tilde{\mathbf{v}}_t^\varepsilon(x)|^2 + |\tilde{r}_t^\varepsilon(x)|^2) d\rho_t(x) dt \right) \Big|_{\varepsilon=0} \\ &= \int_0^1 \int_\Omega \left(\nabla u_t(x) \cdot \nabla \phi_t + r_t(x) s_t(x) \right) d\rho_t(x) dt \\ &= \int_0^1 \int_\Omega \nabla(u_t - r_t)(x) \cdot \nabla \phi_t d\rho_t(x) dt, \end{aligned}$$

where we used the identity $r_t s_t \rho_t = r_t \operatorname{div}(\rho_t \nabla \phi_t)$ to integrate by parts in the last equality. As ϕ was arbitrary this implies $\operatorname{div}(\rho_t \nabla u_t) = \operatorname{div}(\rho_t \nabla r_t)$ and $\|\mathbf{v}_t\|_{L^2(d\rho_t)}^2 = \|\nabla u_t\|_{L^2(d\rho_t)}^2 = \|\nabla r_t\|_{L^2(d\rho_t)}^2$. In particular the triplet $(\rho_t, \nabla r_t, r_t)$ is admissible and has the same cost as the optimal $(\rho_t, \mathbf{v}_t, r_t)$, which shows indeed that one can restrict to paths with $\mathbf{v} = \nabla r$ in the dynamical formulation (2.9). \square

As a consequence we have the alternative definition of the KFR distance as originally introduced in [22], which couples the reaction and velocity:

Theorem 3. *For all $\rho_0, \rho_1 \in \mathcal{M}^+(\Omega)$ there holds*

$$(2.10) \quad \text{KFR}^2(\rho_0, \rho_1) = \inf_{(\rho, u) \in \tilde{\mathcal{A}}_{\text{KFR}}[\rho_0, \rho_1]} \int_0^1 \int_\Omega (|\nabla u_t(x)|^2 + |u_t(x)|^2) d\rho_t(x) dt,$$

where $\tilde{\mathcal{A}}_{\text{KFR}}[\rho_0, \rho_1]$ is the set of weakly continuous curves $t \mapsto \rho_t \in \mathcal{C}_w([0, 1]; \mathcal{M}^+)$ with endpoints $\rho(0) = \rho_0$ and $\rho(1) = \rho_1$, with potentials $u \in L^2(0, 1; H^1(d\rho_t))$ such that

$$\partial_t \rho_t + \operatorname{div}(\rho_t \nabla u_t) = \rho_t u_t$$

in the sense of distributions.

This characterization of the KFR distance suggests that the metric space $(\mathcal{M}^+, \text{KFR})$ has in fact a Riemannian structure, inherited from the Lagrangian minimization. More precisely the tangent plane should be identified with

$$T_\rho \mathcal{M}_{\text{KFR}}^+ = \left\{ \partial_t \rho = -\operatorname{div}(\rho \nabla u) + \rho u \quad \text{evaluated at } t = 0 \right\}$$

endowed with the Riemannian metrics

$$\|\partial_t \rho\|_{T_\rho \mathcal{M}_{\text{KFR}}^+}^2 := \|u\|_{H^1(d\rho)}^2 \quad \text{with the identification } \partial_t \rho = -\operatorname{div}(\rho \nabla u) + \rho u,$$

where obviously $\|u\|_{H^1(d\rho)}^2 = \int_\Omega (|\nabla u|^2 + |u|^2) d\rho$.

Metric gradients $\text{grad}_{\text{KFR}} \mathcal{F}$ can be computed by the chain rule as earlier: if $\partial_t \rho_t + \text{div}(\rho_t \nabla u_t) = \rho_t u_t$ is a “ \mathcal{C}^1 ” curve passing through $\rho_t(0) = \rho$ with arbitrary initial velocity $\zeta = \partial_t \rho_t(0) = -\text{div}(\rho \nabla u) + \rho u$ then for functionals $\mathcal{F}(\rho) = \int_{\Omega} F(\rho(x), x) dx$ we have

$$\begin{aligned} \langle \text{grad}_{\text{KFR}} \mathcal{F}(\rho), \zeta \rangle_{T_{\rho} \mathcal{M}_{\text{KFR}}^+} &= \frac{d}{dt} \mathcal{F}(\rho_t) \Big|_{t=0} = \frac{d}{dt} \left(\int_{\Omega} F(\rho_t(x), x) dx \right) \Big|_{t=0} \\ &= \int_{\Omega} F'(\rho) \times \{-\text{div}(\rho \nabla u) + \rho u\} \\ &= \int_{\Omega} (\nabla F'(\rho) \cdot \nabla u + F'(\rho) u) d\rho = \langle F'(\rho), r \rangle_{H^1(d\rho)}, \end{aligned}$$

where $F'(\rho) = \frac{\delta F}{\delta \rho}$ as before. This shows that

$$(2.11) \quad \text{grad}_{\text{KFR}} \mathcal{F}(\rho) = -\text{div}(\rho \nabla F'(\rho)) + \rho F'(\rho)$$

through the canonical $H^1(d\rho)$ action. In particular gradient flows with respect to KFR read

$$(2.12) \quad \partial_t \rho = -\text{grad}_{\text{KFR}} \mathcal{F}(\rho) \quad \leftrightarrow \quad \partial_t \rho = \text{div}(\rho \nabla F'(\rho)) - \rho F'(\rho),$$

which should be compared with (2.5) and (2.8).

3. INFINITESIMAL UNCOUPLING OF THE INF-CONVOLUTION

Let us first summarize the previous informal discussion on each of the three metrics: the quadratic Monge-Kantorovich distance is modeled on the homogeneous $\dot{H}^1(d\rho)$ space, the Fisher-Rao distance is based on $L^2(d\rho)$, and the KFR metrics is constructed on the full $H^1(d\rho)$ structure. Each of these Riemannian structures are defined via identification of tangent vectors as

$$(3.1) \quad \begin{aligned} \text{MK}_2 : \quad & \|\partial_t \rho\|_{T_{\rho} \mathcal{M}_{\text{MK}}^+}^2 = \|\nabla p\|_{L^2(d\rho)}^2 = \int_{\Omega} |\nabla p|^2 d\rho, & \partial_t \rho + \text{div}(\rho \nabla p) &= 0, \\ \text{FR} : \quad & \|\partial_t \rho\|_{T_{\rho} \mathcal{M}_{\text{FR}}^+}^2 = \|r\|_{L^2(d\rho)}^2 = \int_{\Omega} |r|^2 d\rho, & \partial_t \rho &= \rho r, \\ \text{KFR} : \quad & \|\partial_t \rho\|_{T_{\rho} \mathcal{M}_{\text{KFR}}^+}^2 = \|u\|_{H^1(d\rho)}^2 = \int_{\Omega} (|\nabla u|^2 + u^2) d\rho, & \partial_t \rho + \text{div}(\rho \nabla u) &= \rho u. \end{aligned}$$

Note that in the uncoupled formulation (2.9) the velocity \mathbf{v} and the reaction r in the continuity equation $\partial_t \rho + \text{div}(\rho \mathbf{v}) = \rho r$ are completely independent. This suggests that, infinitesimally, we can decompose the tangent plane as an orthogonal sum

$$(3.2) \quad T_{\rho} \mathcal{M}_{\text{KFR}}^+ = T_{\rho} \mathcal{M}_{\text{MK}}^+ \oplus^{L^2(d\rho)} T_{\rho} \mathcal{M}_{\text{FR}}^+,$$

and thus $\text{KFR}^2 \approx \text{MK}_2^2 + \text{FR}^2$ in some vague sense. The same independence of (\mathbf{v}, r) also gives a natural strategy to send a measure ρ_0 to another ρ_1 : one can send first ρ_0 to the renormalized $\tilde{\rho}_0 := \frac{|\rho_0|}{|\rho_1|} \rho_1$ by pure Monge-Kantorovich transport (which is possible since $|\tilde{\rho}_0| = |\rho_0|$), and then send $\tilde{\rho}_0$ to ρ_1 by pure Fisher-Rao reaction. This amounts to following separately each of the “orthogonal” directions in the decomposition (3.2).

An immediate consequence of this observation is

Proposition 3.1. *For arbitrary measures $\rho_0, \rho_1 \in \mathcal{M}^+$ let $\tilde{\rho}_0 := \frac{|\rho_0|}{|\rho_1|} \rho_1$. Then*

$$(3.3) \quad \text{KFR}^2(\rho_0, \rho_1) \leq 2(\text{MK}_2^2(\rho_0, \tilde{\rho}_0) + \text{FR}^2(\tilde{\rho}_0, \rho_1)).$$

Proof. It is enough to follow first a pure Monge-Kantorovich geodesics ($r \equiv 0$) from ρ_0 to $\tilde{\rho}_0$ in time $t \in [0, 1/2]$ and then a pure Fisher-Rao geodesic ($\mathbf{v} \equiv 0$) from $\tilde{\rho}_0$ to ρ_1 in time $t \in [1/2, 1]$. Because of the rescaling in time each of these half-paths has an extra factor 2, amounting to a total cost of $2\text{MK}_2^2(\rho_0, \tilde{\rho}_0) + 2\text{FR}^2(\tilde{\rho}_0, \rho_1)$. The result then follows from the definition (2.9) of KFR^2 as an infimum over all paths. \square

Note that estimate (3.3) holds for any arbitrary measure $\rho_0, \rho_1 \in \mathcal{M}^+$, but has a multiplicative factor 2 which is certainly not optimal and came from the rescaling in time. Consider now two very close measures $\text{KFR}(\rho_0, \rho_1) \ll 1$. Then the above transformation from ρ_0 to ρ_1 can essentially be considered as occurring infinitesimally in the tangent plane $T_{\rho_0}\mathcal{M}_{\text{KFR}}^+$, which can be decomposed as $T_{\rho_0}\mathcal{M}_{\text{MK}}^+ \oplus T_{\rho_0}\mathcal{M}_{\text{FR}}^+$ with “ $L^2(\text{d}\rho_0)$ orthogonality”. Roughly speaking, this means that the two advection and reaction processes from ρ_0 to $\tilde{\rho}_0$ and from $\tilde{\rho}_0$ to ρ_1 in the previous proof can be considered as occurring *simultaneously and independently* at the infinitesimal level. Thus we do not need to follow *first* a Monge-Kantorovich path from ρ_0 to $\tilde{\rho}_0$ and *then* a Fisher-Rao path from $\tilde{\rho}_0$ to ρ_1 , the factor 2 in the previous proposition is unnecessary, and therefore one should expect in fact

$$(3.4) \quad \text{KFR}^2(\rho_0, \rho_1) \approx \text{MK}_2^2(\rho_0, \tilde{\rho}_1) + \text{FR}^2(\tilde{\rho}_0, \rho_1)$$

for very close measures $\text{KFR}(\rho_0, \rho_1) \ll 1$. This can be made more rigorous at least for one-point mass particles

$$\rho_0 = k_0 \delta_{x_0}, \quad \rho_1 = k_1 \delta_{x_1}$$

at close distance, i-e $|x_1 - x_0| \ll 1$ and $k_1 \approx k_0$. Intuitively the geodesics ρ_t from ρ_0 to ρ_1 should be a moving one-point mass of the form $\rho_t = k_t \delta_{x_t}$ for some curve $t \mapsto (x_t, k_t) \in \Omega \times \mathbb{R}^+$ to be determined. This has been shown heuristically in [22, Section 3.3] and proved rigorously [13, thm. 4.1] and [25, thm. 3.1].

Remark 3.1. *The one-point ansatz $\rho_t = k_t \delta_{x_t}$ is in fact correct not only for short distances $|x_1 - x_0| \ll 1$, but also as long as $|x_1 - x_0| < \pi$. Past this threshold $|x_1 - x_0| = \pi$ it is more efficient to virtually displace mass from x_0 to x_1 by pure reaction, i-e by killing mass at x_0 while simultaneously creating some at x_1 .*

In the continuity equation $\partial_t \rho_t + \text{div}(\rho_t \mathbf{v}_t) = \rho_t r_t$ the advection moves particles around according to $\frac{d}{dt}x_t = \mathbf{v}_t$ and the reaction reads $\frac{d}{dt}k_t = k_t r_t$, each with infinitesimal cost $k_t |\mathbf{v}_t|^2$ and $k_t |r_t|^2$. The optimal (\mathbf{v}_t, r_t) for the one-point ansatz $\rho_t = k_t \delta_{x_t}$ can be obtained explicitly by looking at the coupled formulation (2.10) with $\mathbf{v}_t = \nabla u_t, r_t = u_t$, and optimizing the cost with respect to admissible potentials u_t . Omitting the details (see again [22, 24]), the optimal cost can be computed explicitly as

$$(3.5) \quad \text{KFR}^2(\rho_0, \rho_1) = 4 \left(k_0 + k_1 - 2\sqrt{k_0 k_1} \cos \left(\frac{|x_1 - x_0|}{2} \right) \right) \quad \text{for } |x_1 - x_0| < \pi.$$

Remark 3.2. *It was shown in [24, 25] that the KFR distance can be constructed by suitably lifting measures in Ω to probability measures on a cone space $C_\Omega = \{[x, r] \in \Omega \times \mathbb{R}^+\} / \sim$ over Ω , where \sim is the identification of all the tips $[x, 0]$ into a single point $\diamond \in C_\Omega$, and then projecting back onto $(\mathcal{P}_2(C_\Omega), \text{MK}_2) \rightarrow (\mathcal{M}^+(\Omega), \text{KFR})$. In order to retrieve exactly the KFR distance one should endow the Polish space C_Ω with the cone distance $d_C^2([x_0, r_0], [x_1, r_1]) = r_0^2 + r_1^2 - 2r_0 r_1 \cos_\pi(|x_1 - x_0|/2)$ and $\cos_\pi(z) = \cos(\pi \wedge |z|)$, see [24] for details. In formula (3.5) one sees in fact, up to the normalizing factor 4, the natural Monge-Kantorovich distance $\text{MK}_2^2(\delta_{[x_0, \sqrt{k_0}]}, \delta_{[x_1, \sqrt{k_1}]}) = d_C^2([x_0, \sqrt{k_0}], [x_1, \sqrt{k_1}])$ between unit Dirac masses in the overlying space $\mathcal{P}_2(C_\Omega)$.*

In this setting and with the previous notation $\tilde{\rho}_0 = \frac{|\rho_0|}{|\rho_1|}\rho_1 = k_0\delta_{x_1}$ we have of course

$$\text{MK}_2^2(\rho_0, \tilde{\rho}_0) = \text{MK}_2^2(k_0\delta_{x_0}, k_0\delta_{x_1}) = k_0|x_1 - x_0|^2,$$

and by (2.6)

$$\text{FR}^2(\tilde{\rho}_0, \rho_1) = 4 \int_{\Omega} \left| \sqrt{\frac{d(k_1\delta_{x_1})}{d\delta_{x_1}}} - \sqrt{\frac{d(k_0\delta_{x_1})}{d\delta_{x_1}}} \right|^2 d\delta_{x_1} = 4 \left| \sqrt{k_1} - \sqrt{k_0} \right|^2.$$

Taylor-expanding (3.5) at order two in $|x_1 - x_0|$, $|\sqrt{k_1} - \sqrt{k_0}| \ll 1$ gives

$$\begin{aligned} (3.6) \quad \text{KFR}^2(\rho_0, \rho_1) &= k_0|x_1 - x_0|^2 + 4|\sqrt{k_1} - \sqrt{k_0}|^2 + \mathcal{O}(|x_1 - x_0|^2|\sqrt{k_1} - \sqrt{k_0}|) \\ &= \text{MK}_2^2(\rho_0, \tilde{\rho}_0) + \text{FR}^2(\tilde{\rho}_0, \rho_1) + \text{lower order}, \end{aligned}$$

which shows that our claim (3.4) holds true at least for one-point particles and at order one in the squared distances.

Remark 3.3. Due to $4|\sqrt{k_1} - \sqrt{k_0}|^2 = \text{FR}^2(\tilde{\rho}_0, \rho_1) \ll 1$ we have $k_1 = k_0 + \mathcal{O}(|\sqrt{k_1} - \sqrt{k_0}|)$. The previous expression can therefore be rewritten as

$$\text{KFR}^2(\rho_0, \rho_1) = \frac{k_0 + k_1}{2}|x_1 - x_0|^2 + 4|\sqrt{k_1} - \sqrt{k_0}|^2 + \text{lower order}$$

and the apparent loss of symmetry in k_0, k_1 in (3.6) is thus purely artificial.

Remark 3.4. An interesting question would be to determine how much information on the transport/reaction coupling is encoded in the remainder.

Justifying and/or quantifying the above discussion and (3.4) for general measures with $d(\rho_0, \rho_1) \ll 1$ is an interesting question left for future work. One can think that the superposition principle should apply: viewing any measure as a continuum of one-point Lagrangian particles and taking for granted that the infinitesimal uncoupling holds for single particles, it seems natural that the result should also hold for all measures.

4. MINIMIZING SCHEME

We turn now our attention to gradient-flows

$$(4.1) \quad \partial_t \rho = -\text{grad}_{\text{KFR}} \mathcal{F}(\rho)$$

of functionals

$$\mathcal{F}(\rho) = \begin{cases} \int_{\Omega} \{U(\rho) + \Psi(x)\rho + \frac{1}{2}\rho K \star \rho\} dx & \text{if } d\rho \ll dx \\ \infty & \text{otherwise} \end{cases}$$

with respect to the KFR distance. Without further mention we implicitly restrict to absolutely continuous measures (with respect to Lebesgue), and still denote their Radon-Nikodym derivatives $\rho = \frac{d\rho}{dx}$ with a slight abuse of notations. According to (2.12) this corresponds in terms of PDEs to equations of the form

$$(4.2) \quad \partial_t \rho = \text{div}(\rho \nabla (U'(\rho) + \Psi + K \star \rho)) - \rho(U'(\rho) + \Psi + K \star \rho),$$

which appear for example in the tumor growth model studied in [31].

The natural minimizing movement for (4.1) should be

$$(4.3) \quad \rho^{n+1} \in \underset{\rho \in \mathcal{M}^+}{\text{Argmin}} \left\{ \frac{1}{2\tau} \text{KFR}^2(\rho, \rho^n) + \mathcal{F}(\rho) \right\}$$

for some small time step $\tau > 0$. In order to obtain an Euler-Lagrange equation, a classical and natural strategy would be to consider perturbations $\varepsilon \mapsto \rho_\varepsilon$ of the minimizer $\rho_\varepsilon(0) = \rho^{n+1}$ starting with velocity $\partial_\varepsilon \rho_\varepsilon(0) = -\operatorname{div}(\rho^{n+1} \nabla \phi) + \rho^{n+1} \phi$ for some arbitrary smooth ϕ , corresponding to choosing arbitrary directions of perturbation in the tangent plane $T_{\rho^{n+1}} \mathcal{M}_{\text{KFR}}^+$. Writing down the optimality criterion $\frac{d}{d\varepsilon} \left(\frac{1}{2\tau} \text{KFR}^2(\rho_\varepsilon, \rho^n) + \mathcal{F}(\rho_\varepsilon) \right) \Big|_{\varepsilon=0} = 0$ should then give the sought Euler-Lagrange equation. In order to exploit this, one should in particular know how to differentiate the squared distance $\rho \mapsto \text{KFR}^2(\rho, \mu)$ with respect to such perturbations ρ_ε of the minimizer. At this stage the theory does not provide yet the necessary tools, even though what the formula should be is quite clear: For any reasonable smooth Riemannian manifold and curve $x(t)$ with $x(0) = x$ we have

$$\frac{d}{dt} \left(\frac{1}{2} d^2(x(t), y) \right) \Big|_{t=0} = \langle x'(0), \zeta \rangle_{T_x \mathcal{M}},$$

where ζ is the terminal velocity $y'(1) \in T_x \mathcal{M}$ of the geodesics from y to x . Here the KFR-geodesics $(\mu_s)_{s \in [0,1]}$ from μ to ρ should solve $\partial_s \mu_s + \operatorname{div}(\mu_s \nabla u_s) = \mu_s u_s$ and the terminal velocity $\zeta = \partial_s \mu(1)$ should be identified with some potential $u_s(1) = u \in H^1(d\rho)$, see section 2.3. We should therefore expect

$$\frac{d}{d\varepsilon} \left(\frac{1}{2} \text{KFR}^2(\rho_\varepsilon, \mu) \right) \Big|_{\varepsilon=0} = \langle \partial_\varepsilon \rho(0), \partial_s \mu(1) \rangle_{T_\rho \mathcal{M}_{\text{KFR}}^+} = \int_\Omega (\nabla \phi \cdot \nabla u + \phi u) d\rho.$$

However, this can give rise to difficult issues at the cut-locus, where geodesics cease to be minimizing and prevent any differentiability of the squared distance. Indeed, it was shown in [25, section 5.2], [13, thm. 4.1], and [22, section 3.5] that such cut-locuses do exist for $\Omega = \mathbb{R}^d$, and even that the set of non-unique geodesics generically spans an infinite-dimensional convex set. This is related to the threshold $|x_1 - x_0| = \pi$ for one-point measures, see Remark 3.1. In other words the squared distance may very well not be differentiable, even in the case of the simplest geometry $\Omega = \mathbb{R}^d$ of the underlying space. This is in sharp contrast with classical mass conservative optimal transportation, where the cut-locus in $\mathcal{P}(X)$ is intimately related to the geometry of the underlying Riemannian manifold X [38].

In the context of minimizing movements one should expect two successive steps to be extremely close, typically $\text{KFR}(\rho^{n+1}, \rho^n) = \mathcal{O}(\sqrt{\tau})$ as $\tau \rightarrow 0$. It seems reasonable to hope that geodesics then become unique at short distance, and one might therefore think that the previous cut-locus issue actually does not arise here. However, even assuming that we could somehow compute a unique minimizing geodesics ρ_s from ρ^n to ρ^{n+1} and safely evaluate the terminal velocity $\partial_s \rho(1) = -\operatorname{div}(\rho^{n+1} \nabla u^{n+1}) + \rho^{n+1} u^{n+1}$ at $s = 1$ in order to differentiate the squared distance, it would remain to derive a (possibly approximated) relation between the Riemannian point of view and the more classical PDE framework, e.g. by proving an estimate like

$$\int_\Omega (\nabla u^{n+1} \cdot \nabla \phi + u^{n+1} \phi) d\rho^{n+1} \approx \int_\Omega \frac{\rho^{n+1} - \rho^n}{\tau} \phi + \text{remainder}.$$

In this last display we see the interplay between the forward tangent vector $u^{n+1} \in H^1(d\rho^{n+1}) \longleftrightarrow T_{\rho^{n+1}} \mathcal{M}_{\text{KFR}}^+$, encoding the Riemannian variation from ρ^n to ρ^{n+1} , and the standard difference quotient $\frac{\rho^{n+1} - \rho^n}{\tau}$. One should then typically prove that the remainder is quadratic $\mathcal{O}(\text{KFR}^2(\rho^{n+1}, \rho^n))$. Within the framework of classical optimal transport this is usually done exploiting the explicit representation of the MK_2 metrics in terms of optimal transport maps (or transference plans, or Kantorovich potentials), which are in turn related to some static formulations of the problem.

See later on section 4.1 and in particular the Taylor expansion (4.11) for details, and also remark 4.1. However, and even though static formulations of the KFR distance have been derived in [24], the current theory does not provide yet such an asymptotic expansion.

In order to tackle these technical issues, let us recall from the discussion in section 3 that the inf-convolution formally uncouples at short distance. This strongly suggests replacing KFR^2 by the approximation $\text{MK}_2^2 + \text{FR}^2 \approx \text{KFR}^2$, and as a consequence we naturally substitute the direct one-step minimizing scheme (4.3) by a sequence of two elementary substeps

$$\rho^n \xrightarrow{\text{MK}_2^2} \rho^{n+\frac{1}{2}} \xrightarrow{\text{FR}^2} \rho^{n+1}.$$

Each of these substeps are pure Monge-Kantorovich/transport and Fisher-Rao/reaction variational steps, respectively and successively

$$(4.4) \quad \rho^{n+\frac{1}{2}} \in \underset{\rho \in \mathcal{M}_2^+, |\rho| = |\rho^n|}{\text{Argmin}} \left\{ \frac{1}{2\tau} \text{MK}_2^2(\rho, \rho^n) + \mathcal{F}(\rho) \right\}$$

and

$$(4.5) \quad \rho^{n+1} \in \underset{\rho \in \mathcal{M}^+}{\text{Argmin}} \left\{ \frac{1}{2\tau} \text{FR}_2^2(\rho, \rho^{n+\frac{1}{2}}) + \mathcal{F}(\rho) \right\}.$$

Note that the first Monge-Kantorovich step is mass preserving by construction, while the second will account for mass variations.

The underlying idea is that the scheme follows alternatively the two privileged directions in $T_\rho \mathcal{M}_{\text{KFR}}^+ = T_\rho \mathcal{M}_{\text{MK}}^+ \oplus T_\rho \mathcal{M}_{\text{FR}}^+$, corresponding to pure Monge-Kantorovich transport and pure Fisher-Rao reaction respectively. Another possible interpretation is that of an operator-splitting method: from (2.5)(2.7)(2.12) we get

$$\begin{aligned} -\text{grad}_{\text{KFR}} \mathcal{F}(\rho) &= \text{div}(\rho \nabla(U'(\rho) + \Psi + K \star \rho)) - \rho(U'(\rho) + \Psi + K \star \rho) \\ &= -\text{grad}_{\text{MK}} \mathcal{F}(\rho) - \text{grad}_{\text{FR}} \mathcal{F}(\rho). \end{aligned}$$

Viewing the same functional $\mathcal{F}(\rho)$ through distinct “differential” lenses (i-e using respectively the MK_2 and FR differential structures) gives the two transport and reaction terms in the PDE (4.2). Thus it is very natural to split the PDE into two separate transport/reaction operators and treat separately each of them in their own and intrinsic differential framework. This idea of hybrid variational structures has been successfully applied e.g. in [20, 6, 7] for systems of equations where each component is viewed from separate differential perspectives, but not to the splitting of one single equation as it is the case here. A related splitting scheme was employed in [9] to construct weak solutions of fractional Fokker-Planck equations $\partial_t \rho = \Delta^{2s} \rho + \text{div}(\rho \nabla \Psi)$, using a Monge-Kantorovich variational scheme in order to handle the transport term. However the discretization of the fractional Laplacian was treated in a non metric setting, the PDE cannot be viewed as the sum of gradient-flows of the same functional for two different “orthogonal” metrics, and the approach is thus more a technical tool than an intrinsic variational feature.

Another natural consequence of this formal point of view is the following: From the “ $L^2(d\rho)$ orthogonality” in $T_\rho \mathcal{M}_{\text{KFR}}^+ = T_\rho \mathcal{M}_{\text{MK}}^+ \oplus T_\rho \mathcal{M}_{\text{FR}}^+$ we can compute using Pythagora’s theorem

$$\mathcal{D}(t) := -\frac{d}{dt} \mathcal{F}(\rho(t)) = -\|\text{grad}_d \mathcal{F}\|_{T_\rho \mathcal{M}_{\text{KFR}}^+}^2 = -\|\text{grad}_{\text{MK}} \mathcal{F}\|_{T_\rho \mathcal{M}_{\text{MK}}^+}^2 - \|\text{grad}_{\text{FR}} \mathcal{F}\|_{T_\rho \mathcal{M}_{\text{FR}}^+}^2,$$

which really means that the total dissipation for the coupled KFR metrics is just the sum of the two MK_2, FR dissipations. One can of course check this formula by

differentiating $\frac{d}{dt}F(\rho_t)$ along solutions of the PDE. This may be useful at the discrete level, since regularity is essentially related to dissipation. For example λ -convexity ensures that the energy is dissipated at a minimum rate, which in turn can be viewed as a quantifiable regularization in the spirit of Brézis-Pazy. This is illustrated in Proposition 5.4, where we show that one indeed recovers an Energy Dissipation Inequality with respect to KFR from the two elementary MK, FR geodesic convexity and dissipation.

Before detailing each of the substeps we collect some general properties of our two-steps MK₂/FR splitting scheme, which shares common features with the intrinsic one-step scheme (4.3). Testing $\rho = \rho^n$ in (4.4) and $\rho = \rho^{n+\frac{1}{2}}$ in (4.5) we get as usual

$$\begin{aligned} \frac{1}{2\tau} \text{MK}_2^2(\rho^{n+\frac{1}{2}}, \rho^n) + \mathcal{F}(\rho^{n+\frac{1}{2}}) &\leq \mathcal{F}(\rho^n), \\ \frac{1}{2\tau} \text{FR}^2(\rho^{n+1}, \rho^{n+\frac{1}{2}}) + \mathcal{F}(\rho^{n+1}) &\leq \mathcal{F}(\rho^{n+\frac{1}{2}}). \end{aligned}$$

Summing over $n \geq 0$ we end-up with the mixed total-square distance estimate

$$(4.6) \quad \frac{1}{\tau} \sum_{n \geq 0} \left\{ \text{FR}^2(\rho^{n+1}, \rho^{n+\frac{1}{2}}) + \text{MK}_2^2(\rho^{n+\frac{1}{2}}, \rho^n) \right\} \leq 2 \left(\mathcal{F}(\rho^0) - \inf_{\mathcal{M}^+} \mathcal{F} \right),$$

which is finite if $\mathcal{F}(\rho^0) < \infty$ and \mathcal{F} is bounded from below (this is a reasonable assumption, which is true e.g. if $U(\rho) = \rho^m$ for some $m > 1$ and the external potential $\Psi(x) \geq 0$ outside of a finite measure set). By triangular inequality and Proposition 2.1 it is easy to check that

$$(4.7) \quad \text{KFR}^2(\rho^{n+1}, \rho^n) \leq 2 \left(\text{FR}^2(\rho^{n+1}, \rho^{n+\frac{1}{2}}) + \text{MK}_2^2(\rho^{n+\frac{1}{2}}, \rho^n) \right),$$

and from (4.6)(4.7) we obtain the more intrinsic

$$(4.8) \quad \frac{1}{\tau} \sum_{n \geq 0} \text{KFR}^2(\rho^{n+1}, \rho^n) \leq 4 \left(\mathcal{F}(\rho^0) - \inf_{\mathcal{M}^+} \mathcal{F} \right).$$

As already discussed the factor 2 in (4.7) is not optimal, and from the infinitesimal decoupling we should expect $\text{KFR}^2(\rho^{n+1}, \rho^n) \approx \text{FR}^2(\rho^{n+1}, \rho^{n+\frac{1}{2}}) + \text{MK}_2^2(\rho^{n+\frac{1}{2}}, \rho^n)$. Thus the previous (4.8) should have a factor 2 instead of 4 in the right-hand side, which is exactly what one would get when applying a direct one-step minimizing scheme with distance KFR as in (4.3).

We detail now each substep and retrieve the two corresponding Euler-Lagrange equations. In order to keep our notations light we write μ for the previous step and ρ^* for the minimizer. Thus $\mu = \rho^n$ and $\rho^* = \rho^{n+\frac{1}{2}}$ in the first MK₂ step $\rho^n \rightarrow \rho^{n+\frac{1}{2}}$, while $\mu = \rho^{n+\frac{1}{2}}$ and $\rho^* = \rho^{n+1}$ in the next FR step $\rho^{n+\frac{1}{2}} \rightarrow \rho^{n+1}$.

4.1. The Monge-Kantorovich substep. For some fixed absolutely continuous measure $\mu \in \mathcal{M}_2^+$ (finite second moment) and mass $|\mu| = m$, let us consider here an elementary minimization step

$$(4.9) \quad \rho^* \in \underset{\rho \in \mathcal{M}_2^+, |\rho|=m}{\text{Argmin}} \left\{ \frac{1}{2\tau} \text{MK}_2^2(\rho, \mu) + \mathcal{F}(\rho) \right\}.$$

Note that, if Ω is bounded, the restriction on finite second moments can be relaxed. Further assuming that \mathcal{F} is lower semi-continuous with respect to the weak L^1 convergence (which is typically satisfied for the classical models), it is easy to obtain a minimizer $\rho^* \in \mathcal{M}_2^+$ with mass $|\rho^*| = m = |\mu|$. Additional assumptions (e.g. strict convexity) sometimes guarantee uniqueness. Here we do not take interest in optimal

conditions guaranteeing existence and/or uniqueness of minimizers, and this should be checked on a case-to-case basis depending on the structure of U, Ψ, K .

From the classical theory of optimal transportation we know that there exists an optimal map \mathbf{t} from ρ^* to μ , such that

$$\mathbf{MK}_2^2(\rho^*, \mu) = \int_{\Omega} |x - \mathbf{t}(x)|^2 d\rho^*(x).$$

A by-now standard computation [34, 37] shows that the Euler-Lagrange equation associated with (4.9) can be written in the form

$$(4.10) \quad \forall \zeta \in \mathcal{C}_c^\infty(\Omega; \mathbb{R}^d) : \quad \int_{\Omega} \frac{\text{id} - \mathbf{t}}{\tau} \cdot \zeta d\rho^* + \int_{\Omega} \nabla(U'(\rho^*) + \Psi + K \star \rho^*) \cdot \zeta d\rho^* = 0.$$

Using the definition of the pushforward $\mu = \mathbf{t}\#\rho^*$ we recall the classical Taylor expansion

$$(4.11) \quad \begin{aligned} \int_{\Omega} (\rho^* - \mu)\phi &= \int_{\Omega} (\rho^* - \mathbf{t}\#\rho^*)\phi = \int_{\Omega} (\phi(x) - \phi(\mathbf{t}(x)))\rho^*(x) \\ &= \int_{\Omega} \left(x - \mathbf{t}(x) \right) \cdot \nabla \phi(x) + \mathcal{O}(\|D^2\phi\|_{\infty}|x - \mathbf{t}(x)|^2) d\rho^*(x) \\ &= \int_{\Omega} (\text{id} - \mathbf{t}) \cdot \nabla \phi d\rho^* + \mathcal{O}(\|D^2\phi\|_{\infty}\mathbf{MK}_2^2(\rho^*, \mu)) \end{aligned}$$

for all $\phi \in \mathcal{C}_c^\infty(\Omega)$. Taking $\zeta = \nabla \phi$ in (4.10) and substituting yields

$$(4.12) \quad \int_{\Omega} (\rho^* - \mu)\phi = -\tau \int_{\Omega} \nabla(U'(\rho^*) + \Psi + K \star \rho^*) \cdot \nabla \phi d\rho^* + \mathcal{O}(\|D^2\phi\|_{\infty}\mathbf{MK}_2^2(\rho^*, \mu))$$

for all smooth test functions ϕ . This is of course an approximation of the implicit implicit Euler scheme

$$\frac{\rho^* - \mu}{\tau} = \text{div}(\rho^* \nabla(U'(\rho^*) + \Psi + K \star \rho^*)),$$

the approximate error being controlled quadratically in the \mathbf{MK}_2 distance. Note that this corresponds to the pure transport part $\partial_t \rho = \text{div}(\rho \nabla(U'(\rho) + \Psi + K \star \rho)) + (\dots)$ in the PDE (4.2).

4.2. The Fisher-Rao substep. Let us fix as before an arbitrary measure $\mu \in \mathcal{M}^+$ (no restriction on the second moment), and assume that there exists somehow an absolutely continuous minimizer

$$(4.13) \quad \rho^* \in \underset{\rho \in \mathcal{M}^+}{\text{Argmin}} \left\{ \frac{1}{2\tau} \mathbf{FR}^2(\rho, \mu) + \mathcal{F}(\rho) \right\}.$$

Again, the existence and uniqueness of minimizers can be obtained under suitable superlinearity, lower semi-continuity, and convexity assumptions on U, Ψ, K , and we do not worry about this issue.

Let us start by differentiating the squared distance for suitable perturbations ρ_ε of the minimizer ρ^* . According to section 2.2 an arbitrary $\psi \in \mathcal{C}_c^\infty(\Omega)$ can be considered as a tangent vector in $T_{\rho^*} \mathcal{M}_{\text{FR}}^+$ through

$$\begin{cases} \partial_\varepsilon \rho_\varepsilon = \rho_\varepsilon \psi \\ \rho_\varepsilon(0) = \rho^* \end{cases} \quad \Leftrightarrow \quad \rho_\varepsilon = \rho^* e^{\varepsilon \psi}.$$

Denoting by $\mu_s = [(1-s)\sqrt{\mu} + s\sqrt{\rho^*}]^2$ the Fisher-Rao geodesics from μ to ρ^* , the terminal velocity $\partial_s \mu(1) = 2\sqrt{\rho^*}(\sqrt{\rho^*} - \sqrt{\mu})$ can be represented by the $L^2(d\rho^*)$ action of $r = 2\frac{\sqrt{\rho^*} - \sqrt{\mu}}{\sqrt{\rho^*}}$. Using the first variation formula $\frac{d}{dt} \left(\frac{1}{2} d^2(x(t), y) \right) \Big|_{t=0} =$

$\langle x'(0), y'(1) \rangle_{x(0)}$ and our $L^2(d\rho)$ identification of the tangent spaces in section 2.3 we can guess that

$$\begin{aligned} \left. \frac{d}{d\varepsilon} \left(\frac{1}{2} \text{FR}^2(\rho_\varepsilon, \mu) \right) \right|_{\varepsilon=0} &= \langle \partial_\varepsilon \rho(0), \partial_s \mu(1) \rangle_{T_{\rho^*} \mathcal{M}_{\text{FR}}^+} \\ &= (\psi, r)_{L^2(d\rho^*)} = 2 \int_{\Omega} (\sqrt{\rho^*} - \sqrt{\mu}) \sqrt{\rho^*} \psi, \end{aligned}$$

which can be checked by differentiating w.r.t. ε in the explicit representation (2.6). Using the same Riemannian formalism we anticipate that

$$\begin{aligned} \left. \frac{d}{d\varepsilon} \mathcal{F}(\rho_\varepsilon) \right|_{\varepsilon=0} &= \langle \text{grad}_{\text{FR}} \mathcal{F}, \partial_\varepsilon \rho(0) \rangle_{T_{\rho^*} \mathcal{M}_{\text{FR}}^+} \\ &= \langle F'(\rho^*), \psi \rangle_{L^2(d\rho^*)} = \int_{\Omega} \rho^* (U'(\rho^*) + \Psi + K \star \rho^*) \psi, \end{aligned}$$

and this can be checked again by differentiating $\mathcal{F}(\rho_\varepsilon) = \int_{\Omega} (\dots)$ under the integral sign. Writing the optimality condition $\left. \frac{d}{d\varepsilon} \left(\frac{1}{2\tau} \text{FR}^2(\rho_\varepsilon, \mu) + \mathcal{F}(\rho_\varepsilon) \right) \right|_{\varepsilon=0} = 0$ thus gives the Euler-Lagrange equation

$$(4.14) \quad \forall \psi \in \mathcal{C}_c^\infty(\Omega) : \quad \int_{\Omega} (\sqrt{\rho^*} - \sqrt{\mu}) \sqrt{\rho^*} \psi = -\frac{\tau}{2} \int_{\Omega} \{U'(\rho^*) + \Psi + K \star \rho^*\} \rho^* \psi.$$

In order to relate this with the more standard Euclidean difference quotient, we first assume that $U'(\rho^*) + \Psi + K \star \rho^* \in L^2(d\rho^*)$, or in other words that $\text{grad}_{\text{FR}} \mathcal{F}(\rho^*)$ can indeed be considered as a tangent vector of $T_{\rho^*} \mathcal{M}_{\text{FR}}^+$. This should be natural, but may require a case-to-case analysis depending on the structure of U, Ψ, K . Ignoring this technical issue and thus assuming the $L^2(d\rho^*)$ regularity, an easy density argument shows that the previous equality holds for all $\psi \in L^2(d\rho^*)$. Taking in particular $\psi = \frac{\sqrt{\rho^*} + \sqrt{\mu}}{\sqrt{\rho^*}} \phi \in L^2(d\rho^*)$ for arbitrary $\phi \in \mathcal{C}_c^\infty(\Omega)$, we obtain a slight variant of the previous Euler-Lagrange equation (4.14) in the form

$$(4.15) \quad \forall \phi \in \mathcal{C}_c^\infty(\Omega) : \quad \int_{\Omega} (\rho^* - \mu) \phi = -\tau \int_{\Omega} \frac{\sqrt{\rho^*}(\sqrt{\rho^*} + \sqrt{\mu})}{2} \{U'(\rho^*) + \Psi + K \star \rho^*\} \phi.$$

Recalling that in the minimizing scheme we only deal with measures at short $\mathcal{O}(\sqrt{\tau})$ distance, one should essentially think of this as if $\rho^* \approx \mu$ in the right-hand side, and (4.15) is thus an approximation to the implicit Euler scheme

$$\frac{\rho^* - \mu}{\tau} = -\rho^* (U'(\rho^*) + \Psi + K \star \rho^*).$$

Note that this is the reaction part $\partial_t \rho = (\dots) - \rho(U'(\rho) + \Psi + K \star \rho^*)$ in the PDE (4.2).

Remark 4.1. *Contrarily to the corresponding approximate Euler-Lagrange equation (4.12) for one elementary Monge-Kantorovich substep, (4.15) does not involve any quadratic remainder $\mathcal{O}(\text{FR}^2(\rho^*, \mu))$. The price to pay for this is that the right-hand side appears now as a slight “twist” of the more natural and purely Riemannian object $-\rho^*(U'(\rho^*) + \Psi) = -\text{grad}_{\text{FR}} \mathcal{F}(\rho^*)$ in (4.15), the twist occurring through the approximation $\frac{\sqrt{\rho^*}(\sqrt{\rho^*} + \sqrt{\mu})}{2} \approx \rho^*$.*

Remark 4.2. *A technical issue might appear here for unbounded domains Ω . Indeed since we construct recursively $\rho^n \xrightarrow{\text{MK}_2^2} \rho^{n+\frac{1}{2}} \xrightarrow{\text{FR}^2} \rho^{n+1}$ one should make sure that, in the second reaction substep, the minimizer ρ^{n+1} keeps finite second moment so that*

the scheme can be safely iterated afterward. This should be generally guaranteed if the external potential Ψ is quadratically confining, but may require once again a delicate analysis depending on the structure of U, Ψ, K (see section 5 for a simple example $\Psi, K \equiv 0$).

4.3. Convergence to a weak solution. Assuming that we can solve recursively (4.4)-(4.5) for some given initial datum

$$\rho_0 \in \mathcal{M}^+, \quad \mathcal{F}(\rho^0) < \infty,$$

we construct two piecewise-constant interpolating curves

$$(4.16) \quad t \in ((n-1)\tau, n\tau], n \geq 0 : \quad \begin{cases} \tilde{\rho}^\tau(t) = \rho^{n+\frac{1}{2}}, \\ \rho^\tau(t) = \rho^{n+1}. \end{cases}$$

By construction we have the energy monotonicity

$$(4.17) \quad \forall 0 \leq t_1 \leq t_2 : \quad \mathcal{F}(\rho^\tau(t_2)) \leq \mathcal{F}(\tilde{\rho}^\tau(t_2)) \leq \mathcal{F}(\rho^\tau(t_1)) \leq \mathcal{F}(\tilde{\rho}^\tau(t_1)) \leq \mathcal{F}(\rho^0),$$

and an easy application of the Cauchy-Schwarz inequality with the total square-distance estimate (4.8) gives moreover the classical $\frac{1}{2}$ -Hölder estimate

$$(4.18) \quad \forall 0 \leq t_1 \leq t_2 : \quad \begin{cases} \text{KFR}(\rho^\tau(t_2), \rho^\tau(t_1)) \leq C|t_2 - t_1 + \tau|^{\frac{1}{2}} \\ \text{KFR}(\tilde{\rho}^\tau(t_2), \tilde{\rho}^\tau(t_1)) \leq C|t_2 - t_1 + \tau|^{\frac{1}{2}} \end{cases}.$$

Moreover for all $t > 0$ we have $\tilde{\rho}^\tau(t) = \rho^{n+\frac{1}{2}}$ and $\rho^\tau(t) = \rho^{n+1}$ for some $n \geq 0$. From the total square estimate (4.6) we have therefore $\text{FR}^2(\tilde{\rho}^\tau(t), \rho^\tau(t)) \leq C\tau$, and by Proposition 2.1 we conclude that the two curves $\rho^\tau, \tilde{\rho}^\tau$ stay close

$$(4.19) \quad \forall t \geq 0 : \quad \text{KFR}(\tilde{\rho}^\tau(t), \rho^\tau(t)) \leq \text{FR}(\tilde{\rho}^\tau(t), \rho^\tau(t)) \leq C\sqrt{\tau}$$

uniformly in τ .

We begin with a fairly general result, giving pointwise convergence in time when $\tau \rightarrow 0$ for a weak topology:

Proposition 4.1. *Assume that $\mathcal{F}(\rho^0) < \infty$ and \mathcal{F} is bounded from below on \mathcal{M}^+ . Then there exists a KFR-continuous curve $\rho \in \mathcal{C}^{\frac{1}{2}}([0, \infty); \mathcal{M}_{\text{KFR}}^+)$ and a discrete subsequence $\tau \rightarrow 0$ (not relabeled here) such that*

$$(4.20) \quad \forall t \geq 0 : \quad \rho^\tau(t), \tilde{\rho}^\tau(t) \rightarrow \rho(t) \quad \text{weakly-}^* \text{ when } \tau \rightarrow 0.$$

We recall that the weak-* convergence of measures is defined in duality with $\mathcal{C}_c(\Omega)$ test-functions. Observe that the two interpolated curves converge to the *same* limit, and note that because $\rho \in \mathcal{C}([0, \infty); \mathcal{M}_{\text{KFR}}^+)$ the initial datum $\rho(0) = \rho^0$ is taken continuously in the KFR metric sense. In particular since KFR metrizes the narrow convergence of measures [22, thm. 3] the initial datum $\rho(0) = \rho^0$ will be taken at least in the narrow sense, which is stronger than weak-* or distributional convergence.

Proof. From the proof of [22, lem. 2.2] it is easy to see that we have mass control

$$\forall \mu, \nu \in \mathcal{M}^+ : \quad |\nu| \leq |\mu| + \text{KFR}^2(\nu, \mu).$$

Applying this with $\nu = \rho^\tau(t), \tilde{\rho}^\tau(t)$ and $\mu = \rho^0$, and noting that the square-distance estimate (4.8) controls $\text{KFR}^2(\rho^\tau(t), \rho^0), \text{KFR}^2(\tilde{\rho}^\tau(t), \rho^0) \leq C(t + \tau)$, we see that the masses are controlled as $|\rho^\tau(t)| + |\tilde{\rho}^\tau(t)| \leq C_T$ uniformly in τ in any finite time interval $t \in [0, T]$. By the Banach-Alaoglu in $\mathcal{M} = \mathcal{C}_c^*$ we see that $\rho^\tau(t), \tilde{\rho}^\tau(t)$ lie in the fixed weakly-* relatively compact set $\mathcal{K}_T = \{|\rho| \leq C_T\}$ for all $t \in [0, T]$. By [22, thm. 5] we know that the KFR distance is lower semi-continuous with respect to the weak-* convergence of measures, and the metric space $(\mathcal{M}^+, \text{KFR})$ is complete [22,

thm. 3]. Exploiting the time equicontinuity (4.18), the lower semi-continuity, and the completeness, we can apply a refined version of the Arzelà-Ascoli theorem [2, prop. 3.3.1] to conclude that, up to extraction of a discrete subsequence if needed, $\rho^\tau(t) \rightarrow \rho(t)$ and $\tilde{\rho}^\tau(t) \rightarrow \tilde{\rho}(t)$ pointwise in $t \in [0, T]$ for the weak-* convergence and for some limit curves $\rho, \tilde{\rho} \in \mathcal{C}^{\frac{1}{2}}([0, T]; \mathcal{M}_{\text{KFR}}^+)$. Moreover $\rho(t), \tilde{\rho}(t) \in \mathcal{K}_T$ for all $t \in [0, T]$, and by diagonal extraction we can assume that this holds for all $T > 0$. Finally as we already know that $\rho^\tau(t)$ and $\tilde{\rho}^\tau(t)$ converge weakly-* to $\rho(t)$ and $\tilde{\rho}(t)$ respectively, we conclude by (4.19) and the same lower semi-continuity that $\text{KFR}(\rho(t), \tilde{\rho}(t)) \leq \liminf_{\tau \rightarrow 0} \text{KFR}(\rho^\tau(t), \tilde{\rho}^\tau(t)) = 0$ for any arbitrary $t \geq 0$. Thus $\rho = \tilde{\rho}$ as desired and the proof is complete. \square

Our next statement is more vague and requires some compactness conditions to be checked in each particular case, but guarantees that the previous limit should generically be a weak solution of the original PDE:

Theorem 4. *Assume that one could strengthen the convergence $\rho^\tau, \tilde{\rho}^\tau \rightarrow \rho$ from Proposition 4.1 into any strong convergence (e.g. pointwise a.e. $t, x \in (0, \infty) \times \Omega$), guaranteeing that*

$$(4.21) \quad \begin{cases} \tilde{\rho}^\tau \nabla (U'(\tilde{\rho}^\tau) + \Psi + K \star \tilde{\rho}^\tau) & \rightharpoonup \rho \nabla (U'(\rho) + \Psi + K \star \rho) \\ \sqrt{\rho^\tau} \frac{\sqrt{\rho^\tau} + \sqrt{\tilde{\rho}^\tau}}{2} (U'(\rho^\tau) + \Psi + K \star \rho^\tau) & \rightharpoonup \rho (U'(\rho) + \Psi + K \star \rho) \end{cases}$$

at least in $\mathcal{D}'((0, \infty) \times \Omega)$ as $\tau \rightarrow 0$ with limits in $L_{\text{loc}}^1((0, \infty) \times \Omega)$. Then ρ is a nonnegative weak solution of

$$(4.22) \quad \begin{cases} \partial_t = \text{div}(\rho \nabla (U'(\rho) + \Psi + K \star \rho)) - \rho (F'(\rho) + \Psi + K \star \rho) & \text{in } (0, \infty) \times \Omega \\ \rho|_{t=0} = \rho^0 & \text{in } \mathcal{M}^+(\Omega) \end{cases}$$

For the sake of generality we simply assumed here that the nonlinear terms pass to the limit as in (4.21). This is of course a strong hypothesis, and we shall discuss in section 5 some strategies to retrieve such compactness.

Proof. As already discussed just after Proposition 4.1, the initial datum $\rho(0) = \rho^0$ is taken continuously at least in the metric sense $(\mathcal{M}^+, \text{KFR})$, and any limit $\rho = \lim_{\tau \rightarrow 0} \rho^\tau$ in any weak sense will automatically be nonnegative.

Fix now any $0 < t_1 < t_2$ and $\phi \in \mathcal{C}_c^\infty(\Omega)$. For fixed τ we have $\rho^\tau(t_i) = \rho^{N_i}$ for $N_i = \lceil t_i/\tau \rceil$, and $T_i = N_i \tau \rightarrow t_i$ as $\tau \rightarrow 0$. Moreover for fixed $n \geq 0$ we have by construction the two Euler-Lagrange equations (4.12)(4.15), one for each Monge-Kantorovich and Fisher-Rao substep as in section 4.1 and section 4.2 respectively. More explicitly, there holds

$$\begin{aligned} \int_{\Omega} (\rho^{n+\frac{1}{2}} - \rho^n) \phi &= -\tau \int_{\Omega} \rho^{n+\frac{1}{2}} \nabla (U'(\rho^{n+\frac{1}{2}}) + \Psi + K \star \rho^{n+\frac{1}{2}}) \cdot \nabla \phi \\ &\quad + \mathcal{O} \left(\|D^2 \phi\|_{\infty} \text{MK}_2^2(\rho^{n+\frac{1}{2}}, \rho^n) \right) \end{aligned}$$

and

$$\int_{\Omega} (\rho^{n+1} - \rho^{n+\frac{1}{2}}) \phi = -\tau \int_{\Omega} \frac{\sqrt{\rho^{n+1}}(\sqrt{\rho^{n+1}} + \sqrt{\rho^{n+\frac{1}{2}}})}{2} \{U'(\rho^{n+1}) + \Psi + K \star \rho^{n+1}\} \phi.$$

Summing from $n = N_1$ to $n = N_2 - 1$, using the square-distance estimate (4.6) to control the remainder term in the first Euler-Lagrange equation above, and recalling

that the interpolated curves are piecewise constant, we immediately get

$$\begin{aligned} \int_{\Omega} (\rho^{\tau}(t_2) - \rho^{\tau}(t_1)) \phi &= \sum_{n=N_1}^{N_2-1} \int_{\Omega} (\rho^{n+1} - \rho^n) \phi = \sum_{n=N_1}^{N_2-1} \tau \int_{\Omega} (\dots) \\ &= - \int_{T_1}^{T_2} \int_{\Omega} \frac{\sqrt{\rho^{\tau}}(\sqrt{\rho^{\tau}} + \sqrt{\tilde{\rho}^{\tau}})}{2} \{U'(\rho^{\tau}) + \Psi + K \star \rho^{\tau}\} \phi \\ &\quad - \int_{T_1}^{T_2} \int_{\Omega} \tilde{\rho}^{\tau} \nabla(U'(\tilde{\rho}^{\tau}) + \Psi + K \star \tilde{\rho}^{\tau}) \cdot \nabla \phi + \mathcal{O}(\|D^2 \phi\|_{\infty} \tau). \end{aligned}$$

From the previous Proposition we know that $\rho^{\tau}(t)$ converge weakly-* to $\rho(t)$ pointwise in time, so the left-hand side immediately passes to the limit when $\tau \rightarrow 0$. Due to our strong assumption (4.21) and because $T_i \rightarrow t_i$ the right-hand side also passes to the limit. As a consequence we get

(4.23)

$$\int_{\Omega} (\rho(t_2) - \rho(t_1)) \phi = - \int_{t_1}^{t_2} \int_{\Omega} \rho \left(\nabla(U'(\rho) + \Psi + K \star \rho) \cdot \nabla \phi + (U'(\rho) + \Psi + K \star \rho) \phi \right)$$

for all $0 < t_1 < t_2$ and $\phi \in \mathcal{C}_c^{\infty}(\Omega)$, which is clearly an admissible weak formulation of $\partial_t \rho = \operatorname{div}(\rho \nabla(U'(\rho) + \Psi + K \star \rho)) - \rho(U'(\rho) + \Psi + K \star \rho)$. \square

If Ω has a nontrivial boundary, some further work may be needed to retrieve the homogeneous Neumann condition $\rho \nabla(U'(\rho) + \Psi + K \star \rho) \cdot \nu = 0$ on $\partial\Omega$. This amounts to extending the class of $\mathcal{C}_c^{\infty}(\Omega)$ test functions to $\mathcal{C}_{loc}^1(\overline{\Omega})$ and should generically hold with just enough regularity on the solution, but we will not consider this technical issue for the sake of simplicity.

5. COMPACTNESS ISSUES: AN ILLUSTRATIVE EXAMPLE

In Theorem 4 we assumed that the nonlinear terms pass to the limit, mainly in the distributional sense. In order to prove this, the usual strategy is to obtain first some energy/dissipation-type estimates to show that the nonlinear terms have a weak limit, and then prove pointwise convergence $\rho^{\tau}(t, x) \rightarrow \rho(t, x)$ a.e. $(t, x) \in \mathbb{R}^+ \times \Omega$ to identify the weak limit (typically as weak-strong products of limits). Thus the problem should amount to retrieving enough compactness on the interpolating curves $\rho^{\tau}, \tilde{\rho}^{\tau}$. With the help of any Aubin-Lions-Simon type results this essentially requires compactness in time and space, which can be handled separately for different topologies in a flexible way. Compactness in space usually follows from the aforementioned energy estimates, and the energy monotonicity should of course help: if e.g. the total energy $\mathcal{F}(\rho) = \int_{\Omega} U(\rho) + (\dots)$ controls any $L^q(\Omega)$ norm then $\mathcal{F}(\rho^{\tau}(t)) \leq \mathcal{F}(\rho^0)$ immediately controls $\|\rho^{\tau}\|_{L^{\infty}(0, \infty; L^q)}$ uniformly in τ . A rule of thumbs for parabolic equations is usually that space regularity can be transferred to time regularity. Thus the parabolic nature of the scheme should allow here to transfer space estimates, if any, to time estimates. Note also that some sort of compactness (approximate equicontinuity in time) is already guaranteed by (4.18), but in a very weak metric sense for which the standard Aubin-Lions-Simon theory does not apply directly.

A slight modification of the usual arguments should however be required here, because the scheme is decomposed in two separate substeps. The first Monge-Kantorovich substep (4.9) encodes the higher order part of the PDE, which is parabolic and should therefore be smoothing. This regularization can often be quantified using by-now classical methods in (Monge-Kantorovich) optimal transport theory, such as BV estimates [15], the *flow-interchange* technique from [26], regularizing

λ -displacement convexity in the spirit of [27, 2], or any other strategy. On the other hand the second Fisher-Rao substep (4.13) encodes the reaction part of the PDE, hence we cannot expect any smoothing at this stage. One should therefore make sure that, in the step $\rho^{n+\frac{1}{2}} \xrightarrow{\text{FR}} \rho^{n+1}$, the regularity of $\rho^{n+\frac{1}{2}}$ inherited from the previous step $\rho^n \xrightarrow{\text{MK}_2} \rho^{n+\frac{1}{2}}$ propagates to ρ^{n+1} at least to some extent.

At this stage we would like to point out one other possible advantage of our splitting scheme: it is well known [2] that λ -geodesic convexity is a central tool in the setting of gradient flows in abstract metric spaces, and leads to quantified regularization properties at the discrete level. Second order differential calculus *à la Otto* [30] with respect to the KFR Riemannian structure was discussed in [22, 25] (also earlier suggested in [23]) and allows to determine at least formally if a given functional \mathcal{F} is λ -geodesically convex for the distance KFR. However, in our scheme each step only sees either one of the differential MK₂/FR structures and therefore only separate geodesic convexity comes into play. Consider for example the case of internal energies $\mathcal{F}(\rho) = \int_{\Omega} U(\rho)$. Then the celebrated condition for McCann's displacement convexity [27] with respect to MK₂ reads $\rho P'(\rho) - (1 - \frac{1}{d}) P(\rho) \geq 0$ in space dimension d , where the pressure $P(\rho) = \rho U'(\rho) - U(\rho)$. On the other hand using the Riemannian formalism in section 2.2 it is easy to see that, at least formally, this same functional is λ -geodesically convex with respect to FR if and only if $\rho U''(\rho) + \frac{U'(\rho)}{2} \geq \lambda$. This condition can be interpreted as $s \mapsto U(s^2)$ being $\lambda/4$ -convex in $s = \sqrt{\rho}$, the latter change of variables naturally arising through (2.6) and $\text{FR}^2(\rho_0, \rho_1) = 4\|\sqrt{\rho_1} - \sqrt{\rho_0}\|_{L^2}^2$. Those two conditions are very easy to check separately and, in the light of the infinitesimal uncoupling, it seems likely that simultaneous convexity with respect to each of the MK, FR metrics is equivalent to convexity with respect to the coupled KFR structure. See [22, section 3] and [25, section 5.1] for related discussions.

The rest of this section is devoted to the illustration of this compactness strategy in the simple case

$$(H) \quad \begin{cases} \Psi, K \equiv 0, \\ U \in \mathcal{C}^1([0, \infty)) \cap \mathcal{C}^2(0, \infty) \quad \text{with } U(0) = 0, \\ U', U'' \geq 0, \\ \rho U''(\rho) \quad \text{is bounded for small } \rho \in (0, \rho_0], \end{cases}$$

which from now is assumed without further mention. We would like to stress here that (H) holds for any Porous-Medium-type nonlinearity $U(\rho) = \rho^m$, $m > 1$, but *not* for the Boltzmann entropy $U(\rho) = \rho \log \rho - \rho$. Even though the latter is well behaved (displacement convex) with respect to the Monge-Kantorovich structure [18, 37], it is *not* with respect to the Fisher-Rao one. Indeed it is easy to check that $\rho \log \rho - \rho$ is not convex in $\sqrt{\rho}$, so that the Boltzmann entropy is not λ -displacement convex with respect to FR for any $\lambda \in \mathbb{R}$. This would require $\rho U''(\rho) + \frac{U'(\rho)}{2} = 1 + \frac{\log \rho}{2} \geq \lambda$ for some constant λ , which obviously fails for small ρ (this can be related to $\rho = 0$ being an extremal point in \mathcal{M}^+ , where all the Riemannian formalism from section 2.3 degenerates).

5.1. Propagation of regularity at the discrete level. Whenever $U', U'' \geq 0$, the PDE $\partial_t \rho = \text{div}(\rho \nabla U'(\rho)) - \rho U'(\rho) = \text{div}(\rho U''(\rho) \nabla \rho) - \rho U'(\rho)$ should be parabolic, satisfy the maximum principle in the form $\|\rho(t)\|_{\infty} \leq \|\rho^0\|_{\infty}$, and initial regularity should propagate. We prove below that this holds at the discrete level:

Proposition 5.1 (BV and L^∞ estimates). *Assume that the initial datum $\rho^0 \in BV \cap L^\infty(\Omega)$. Then for any $\tau < 2/U'(\|\rho^0\|_\infty)$ there holds*

$$\forall t \geq 0 : \quad \|\rho^\tau(t)\|_{BV(\Omega)} \leq \|\tilde{\rho}^\tau(t)\|_{BV(\Omega)} \leq \|\rho^0\|_{BV(\Omega)}$$

and

$$\forall t \geq 0 : \quad \|\rho^\tau(t)\|_{L^\infty(\Omega)} \leq \|\tilde{\rho}^\tau(t)\|_{L^\infty(\Omega)} \leq \|\rho^0\|_{L^\infty(\Omega)}.$$

Proof. We argue at the discrete level by showing that the estimates propagate in each substep. We shall actually prove a more precise result, namely

$$(5.1) \quad \|\rho^{n+\frac{1}{2}}\|_{BV} \leq \|\rho^n\|_{BV}, \quad \|\rho^{n+\frac{1}{2}}\|_{L^\infty} \leq \|\rho^n\|_{L^\infty}$$

and

$$(5.2) \quad \|\rho^{n+1}\|_{BV} \leq \|\rho^{n+\frac{1}{2}}\|_{BV}, \quad \rho^{n+1}(x) \leq \rho^{n+\frac{1}{2}}(x) \text{ a.e.}$$

The propagation (5.1) in the first MK₂ only requires convexity $U'' \geq 0$ and no smallness condition on the time step τ . This should be expected since the MK₂ step is an implicit discretization of $\partial_t \rho = \operatorname{div}(\rho \nabla U'(\rho)) = \operatorname{div}(\rho U''(\rho) \nabla \rho)$, which is formally parabolic as soon as $U'' \geq 0$. We recall first that by construction the step is mass preserving, $\|\rho^{n+\frac{1}{2}}\|_{L^1} = \|\rho^n\|_{L^1}$. With our assumption $U'' \geq 0$ we can directly apply [15, thm. 1.1] to obtain $\|\rho^{n+\frac{1}{2}}\|_{TV} \leq \|\rho^n\|_{TV}$, which immediately entails the BV estimate. An early proof of $\|\rho^{n+\frac{1}{2}}\|_{L^\infty} \leq \|\rho^n\|_{L^\infty}$ can be found in [29] for the particular case $U(\rho) = \rho^2$, and the case of general convex U is covered by [34, prop. 7.32] (see also [11, 35]).

For the propagation (5.2) in the FR step we show below that the minimizer ρ^{n+1} can be written as

$$\rho^{n+1}(x) = R(\rho^{n+\frac{1}{2}}(x)) \quad \text{a.e. } x \in \Omega$$

for some 1-Lipschitz function $R : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ with $R(0) = 0$. This will ensure that $0 \leq \rho^{n+1}(x) \leq \rho^{n+\frac{1}{2}}(x)$ and entail the L^∞ and L^1 bounds as well as the total variation estimate (see [1] for the composition of $\operatorname{Lip} \circ BV$ maps). Note that $\rho^{n+1}(x) \leq \rho^{n+\frac{1}{2}}(x)$ shows in particular that the second moments propagate to the next step, which might be difficult to check in general and should require further assumptions on U, Ψ . In the rest of the proof we write $\rho^* = \rho^{n+1}$ and $\mu = \rho^{n+\frac{1}{2}}$ for simplicity, in agreement with the notations in section 4.2.

By (4.14) with $\Psi, K \equiv 0$ we see that

$$(5.3) \quad (\sqrt{\rho^*} - \sqrt{\mu})\sqrt{\rho^*} = -\frac{\tau}{2}\rho^*U'(\rho^*)$$

at least in $L^1_{\text{loc}}(\Omega)$, hence a.e. $x \in \Omega$. From $U' \geq 0$ we immediately get that either $\rho^* = 0$ or $\sqrt{\rho^*} \leq \sqrt{\mu}$, which gives in any case $\rho^*(x) \leq \mu(x)$ a.e.

We show now that if the CFL condition $\tau \leq U'(\|\rho^0\|_\infty)/2$ holds then ρ^* and μ share the same support, i.e. $\rho^*(x) > 0 \Leftrightarrow \mu(x) > 0$. From the previous inequality $\rho^* \leq \mu$ we only have to show that $\rho^*(x) > 0$ as soon as $\mu(x) > 0$. Assume by contradiction that there is some subset $E \subset \Omega$ with positive Lebesgue measure such that $\rho^*(x) = 0$ but $\mu(x) > 0$ in E . We claim that

$$\bar{\rho} := \rho^*\chi_{E^c} + \mu\chi_E$$

is then a strictly better competitor than the minimizer ρ^* . In order to check this we first compute the square distance

$$\begin{aligned} \frac{1}{4} (\text{FR}^2(\bar{\rho}, \mu) - \text{FR}^2(\rho^*, \mu)) &= \int_{\Omega} |\sqrt{\bar{\rho}} - \sqrt{\mu}|^2 - \int_{\Omega} |\sqrt{\rho^*} - \sqrt{\mu}|^2 \\ &= \left(\int_{E^c} |\sqrt{\rho^*} - \sqrt{\mu}|^2 + \int_E |\sqrt{\mu} - \sqrt{\mu}|^2 \right) \\ &\quad - \left(\int_{E^c} |\sqrt{\rho^*} - \sqrt{\mu}|^2 + \int_E |0 - \sqrt{\mu}|^2 \right) = - \int_E \mu < 0. \end{aligned}$$

For the energy contribution we have by convexity

$$\begin{aligned} \mathcal{F}(\bar{\rho}) - \mathcal{F}(\rho^*) &= \int_{\Omega} U(\bar{\rho}) - U(\rho^*) \leq \int_{\Omega} U'(\bar{\rho})(\bar{\rho} - \rho^*) \\ &= \int_E U'(\bar{\rho})(\mu - 0) \leq U'(\|\rho^0\|_{\infty}) \int_E \mu. \end{aligned}$$

Note that $0 \leq \rho^*, \bar{\rho}, \mu \leq \|\rho^0\|_{\infty}$ almost everywhere, so that all these integrals are well-defined. Gathering these two inequalities we obtain

$$\frac{1}{2\tau} (\text{FR}^2(\bar{\rho}, \mu) - \text{FR}^2(\rho^*, \mu)) + (\mathcal{F}(\bar{\rho}) - \mathcal{F}(\rho^*)) \leq \left(-\frac{2}{\tau} + U'(\|\rho^0\|_{\infty}) \right) \int_E \mu < 0$$

because $\int_E \mu > 0$ and $\tau < 2/U'(\|\rho^0\|_{\infty})$. This shows that $\bar{\rho}$ is a strictly better competitor and yields the desired contradiction, thus $\rho^* > 0 \Leftrightarrow \mu > 0$.

Now inside the common support of ρ^*, μ we can divide (5.3) by $\sqrt{\rho^*} > 0$, and $\rho^*(x)$ is a solution of the implicit equation

$$f(\rho, \mu) = 0 \quad \text{with} \quad f(\rho, \mu) := \sqrt{\rho} \left(1 + \frac{\tau}{2} U'(\rho) \right) - \sqrt{\mu}.$$

An easy application of the implicit functions theorem shows that, for any $\mu > 0$, this has a unique solution $\rho = R(\mu)$ for a $\mathcal{C}^1(0, \infty)$ function R satisfying $0 < R(\mu) \leq \mu$. Moreover one can compute explicitly for all $\mu > 0$

$$\begin{aligned} 0 < \frac{dR}{d\mu}(\mu) &= - \frac{\partial_{\mu} f}{\partial_{\rho} f} \Big|_{\rho=R(\mu)} = \frac{\frac{1}{2\sqrt{\mu}}}{\frac{1}{2\sqrt{\rho}} \left(1 + \frac{\tau}{2} U'(\rho) \right) + \frac{\tau}{2} \sqrt{\rho} U''(\rho)} \\ &\leq \frac{\frac{1}{2\sqrt{\mu}}}{\frac{1}{2\sqrt{\rho}} \left(1 + \frac{\tau}{2} U'(\rho) \right)} = \frac{1}{\frac{\sqrt{\mu}}{\sqrt{\rho}} \left(1 + \frac{\tau}{2} U'(\rho) \right)} = \frac{\rho}{\mu} \leq 1, \end{aligned}$$

where we used successively $U'' \geq 0$, $f(\rho, \mu) = 0 \Leftrightarrow 1 + \frac{\tau}{2} U'(\rho) = \frac{\sqrt{\mu}}{\sqrt{\rho}}$, and $\rho = R(\mu) \leq \mu$. Extending by continuity $R(0) = 0$, we have shown that $\rho^*(x) = R(\mu(x))$ for some 1-Lipschitz function $R: \mathbb{R}^+ \rightarrow \mathbb{R}^+$ with $R(0) = 0$, and the proof is complete. \square

Remark 5.1. A closer analysis of the implicit functions theorem above reveals that the argument only requires $U' \geq 0$ and $\rho U''(\rho) + U'(\rho)/2 \geq 0$, which is less stringent than our assumption $U', U'' \geq 0$ as in (H). As already suggested this former condition corresponds to convexity of $U(\rho)$ in the square root variable $s = \sqrt{\rho}$, or more intrinsically to geodesic convexity of $\mathcal{F}(\rho) = \int_{\Omega} U(\rho)$ with respect to the distance FR. We also point out that the same approach should work with external potentials $\Psi \not\equiv 0$ under suitable structural assumptions: one should show first that strict positivity is preserved in the sense that $\text{supp } \rho^{n+1} = \text{supp } \rho^{n+\frac{1}{2}}$, which is to be expected since the ODE $\partial_t \rho = -\rho(U'(\rho) + \Psi(x))$ formally preserves positivity. Exploiting the Euler-Lagrange equations (4.14)(4.15), an implicit functions theorem

$f(\rho, \mu, \Psi) = 0 \Leftrightarrow \rho = R(\mu, \Psi)$ should then apply inside the common support to propagate the regularity. This should still control $\nabla \rho = \partial_\mu R \nabla \mu + \partial_\Psi R \nabla \Psi$ provided that Ψ is smooth enough. Nonlocal interaction terms $\int \rho K * \rho$ are more involved.

5.2. Compactness and Energy Dissipation Inequality. Here we intend to show how the strong compactness in space from Proposition 5.1 can be transferred to full compactness, thus allowing to check our strong assumption (4.21) in Theorem 4 and passing to the limit in the nonlinear terms.

Proposition 5.2. *Assume (H). Then*

$$\rho^\tau, \tilde{\rho}^\tau \rightarrow \rho \quad \text{in } L^1_{\text{loc}}([0, \infty); L^1)$$

for some (discrete) subsequence $\tau \rightarrow 0$.

We give two proofs: the first one is elementary and fully exploits the uniform-in-time compactness estimates from Proposition 5.1. The second is less straightforward but enlightens the transfer of space to time regularity.

First proof of Proposition 5.2. Let us recall from Proposition 4.1 that $\rho^\tau(t), \tilde{\rho}^\tau(t)$ both converge weakly-* to the same limit $\rho(t)$ pointwise in time. We claim that this weak-* convergence can be strengthened into strong $L^1(\Omega)$ convergence. Indeed for any fixed $t \geq 0$ we have $\|\rho^\tau(t)\|_{\text{BV}}, \|\tilde{\rho}^\tau(t)\|_{\text{BV}} \leq \|\rho^0\|_{\text{BV}}$ so by compactness $\text{BV}(\Omega) \subset\subset L^1(\Omega)$ we see that $\{\rho^\tau(t)\}, \{\tilde{\rho}^\tau(t)\}$ are L^1 relatively compact. Because strong L^1 convergence implies in particular weak-* convergence of measures, and because we already know that these sequences are weakly-* relatively compact, the uniqueness of the limit shows in fact that the whole sequences are strongly converging in L^1 to the same limit

$$\forall t \geq 0 : \quad \lim_{L^1} \rho^\tau(t) = \lim_{w-*} \rho^\tau(t) = \rho(t) = \lim_{w-*} \tilde{\rho}^\tau(t) = \lim_{L^1} \tilde{\rho}^\tau(t).$$

From this strong pointwise-in time L^1 convergence and the uniform $L^\infty(0, \infty; L^1)$ bounds from Proposition 5.1, an easy application of Lebesgue's dominated convergence theorem in any finite time interval $[0, T]$ finally gives $\|\rho^\tau - \rho\|_{L^1((0, T); L^1)} \rightarrow 0$ and $\|\tilde{\rho}^\tau - \rho\|_{L^1((0, T); L^1)} \rightarrow 0$ for all $T > 0$. \square

Before giving the second proof we need a well known technical result:

Lemma 5.1. *Let μ_0, μ_1 be any absolutely continuous measures with finite second moments, same mass $|\mu_0| = |\mu_1|$, and bounded in $L^p(\Omega)$ for some $1 \leq p \leq \infty$ by the same constant C_p . Then*

$$\forall \phi \in W^{1, 2p'}(\Omega) : \quad \left| \int_{\Omega} (\mu_1 - \mu_0) \phi \right| \leq \sqrt{C_p} \text{MK}_2(\mu_0, \mu_1) \|\nabla \phi\|_{L^{2p'}},$$

with the convention $1' = \infty$ and $\infty' = 1$.

Proof. Let $(\mu_t, \mathbf{v}_t)_{t \in [0, 1]}$ be the unique Monge-Kantorovich geodesics from μ_0 to μ_1 , satisfying $\partial_t \mu_t + \text{div}(\mu_t \mathbf{v}_t) = 0$ with constant metric speed $\|\mathbf{v}_t\|_{L^2(\text{d}\mu_t)} = cst = \text{MK}(\mu_0, \mu_1)$. We first claim that $\|\mu_t\|_{L^p} \leq C_p$ as well along this geodesics. Indeed if $p = 1$ this is simply the mass conservation, and the proof for $p = \infty$ can be found in [29]. For $1 < p < \infty$ this is a simple consequence of the well-known displacement convexity of $\mathcal{E}_p[\mu] = \int_{\Omega} \frac{\mu^p}{p-1}$, [37, thm. 5.15]. Using the weak formulation of the

continuity equation, we compute by Hölder's inequality

$$\begin{aligned} \left| \int_{\Omega} (\mu_1 - \mu_0) \phi \right| &= \left| \int_0^1 \int_{\Omega} \mathbf{v}_t \cdot \nabla \phi \, d\mu_t \, dt \right| \leq \int_0^1 \left(\int_{\Omega} |\mathbf{v}_t|^2 \, d\mu_t \right)^{\frac{1}{2}} \left(\int_{\Omega} |\nabla \phi|^2 \, d\mu_t \right)^{\frac{1}{2}} \, dt \\ &\leq \mathbf{MK}_2(\mu_0, \mu_1) \int_0^1 (\|\mu_t\|_{L^p} \|\nabla \phi\|_{L^{p'}}^2)^{\frac{1}{2}} \, dt \leq \sqrt{C_p} \mathbf{MK}_2(\mu_0, \mu_1) \|\nabla \phi\|_{L^{2p'}} \end{aligned}$$

and the proof is complete. \square

Second proof of Proposition 5.2. We assume here that Ω is bounded for simplicity, but the same argument would actually work for unbounded domains simply replacing all the functional spaces by their local counterparts (\mathbf{BV}_{loc} , H_{loc}^1 , $L_{\text{loc}}^p \dots$).

We first control the difference quotient $\|\rho^{n+1} - \rho^n\|_Y$ in the dual space $Y := H^1(\Omega)^*$. For the Monge-Kantorovich step we can apply the previous Lemma 5.1 with $p = \infty$, $2p' = 2$, $\|\rho^{n+\frac{1}{2}}\|_{L^\infty} \leq \|\rho^n\|_{L^\infty} \leq \|\rho^0\|_{L^\infty}$ and obtain by duality

$$\|\rho^{n+\frac{1}{2}} - \rho^n\|_Y \leq C \mathbf{MK}_2(\rho^{n+\frac{1}{2}}, \rho^n).$$

For the reaction step we recall the Euler-Lagrange equation (4.15), which reads for $\Psi, K \equiv 0$

$$\forall \phi \in \mathcal{C}_c^\infty(\Omega) : \quad \int_{\Omega} (\rho^{n+1} - \rho^{n+\frac{1}{2}}) \phi = -\tau \int_{\Omega} \frac{\sqrt{\rho^{n+1}}(\sqrt{\rho^{n+1}} + \sqrt{\rho^{n+\frac{1}{2}}})}{2} U'(\rho^{n+1}) \phi.$$

Because in the right-hand side $\rho^{n+\frac{1}{2}}, \rho^{n+1}$ are bounded in $L^1 \cap L^\infty(\Omega)$ uniformly in n this gives

$$\|\rho^{n+1} - \rho^{n+\frac{1}{2}}\|_Y \leq \|\rho^{n+\frac{1}{2}} - \rho^{n+1}\|_{L^2} \leq C\tau.$$

By triangular inequality we deduce from the previous two estimates that

$$\|\rho^{n+1} - \rho^n\|_Y \leq C(\tau + \mathbf{MK}_2(\rho^{n+1}, \rho^n)),$$

and using the square distance estimate (4.6) and Cauchy-schwarz inequality we obtain the approximate equicontinuity

$$\forall 0 \leq t_1 \leq t_2 : \quad \|\rho^\tau(t_2) - \rho^\tau(t_1)\|_Y \leq C(|t_2 - t_1 + \tau| + |t_2 - t_1 + \tau|^{\frac{1}{2}}).$$

Because the embedding $H^1 \subset\subset L^2$ is compact we have $L^2 \subset\subset Y$ as well. Thanks to the $L^1 \cap L^\infty(\Omega)$ bounds from Proposition 5.1 we have τ -uniform bounds $\|\rho^\tau(t)\|_{L^2} \leq C$, and we see that there is a Y -relatively compact set $\mathcal{K}_Y = \{\|\rho\|_{L^2} \leq C\}$ such that $\rho^\tau(t) \in \mathcal{K}_Y$ for all $t \geq 0$. Exploiting the above equicontinuity we can apply again the same variant of the Arzelà-Ascoli theorem [2, prop. 3.3.1] in any bounded time interval to deduce that there exists a subsequence (not relabeled) and $\rho \in \mathcal{C}([0, T]; Y)$ such that $\rho^\tau(t) \rightarrow \rho(t)$ in Y for all $t \in [0, T]$. A further application of Lebesgue's dominated convergence theorem with $\|\rho^\tau(t)\|_Y \leq C$ shows that $\rho^\tau \rightarrow \rho$ in $L^p([0, T]; Y)$ for all $p \geq 1$ and fixed $T > 0$, and by Cantor's procedure

$$\rho^\tau \rightarrow \rho \quad \text{in } L_{\text{loc}}^p([0, \infty); Y).$$

Let now $X := \mathbf{BV} \cap L^\infty(\Omega) \subset\subset L^2(\Omega) =: B$. We just proved that

$$X \subset\subset B \subset Y \quad \text{and} \quad \begin{cases} \rho^\tau \text{ is bounded in } L^\infty(0, \infty; X), \\ \rho^\tau \text{ is relatively compact in } L_{\text{loc}}^p([0, \infty); Y) \end{cases}$$

for all $p \geq 1$. By standard Aubin-Lions-Simon theory [36, lem. 9] we get that ρ^τ is relatively compact in $L_{\text{loc}}^p([0, \infty); B)$ for all $p \geq 1$. In particular we get pointwise a.e. convergence $\rho^\tau(t, x) \rightarrow \rho(t, x)$ (up to extraction of a further subsequence), and a last

application of Lebesgue's dominated convergence allows to conclude. The argument is identical for $\tilde{\rho}^\tau$. \square

In order to show that the nonlinear terms pass to the limit as in (4.21) we shall need the following variant of the Banach-Alaoglu theorem with varying measures:

Lemma 5.2 (compactness for vector-fields). *Let $\mathcal{O} \subset \mathbb{R}^m$ be an open set (not necessarily bounded), $\{\sigma_n\}_{n \geq 0} \subset \mathcal{M}^+(\mathcal{O})$ a sequence of finite nonnegative Radon measures narrowly converging to $\sigma \in \mathcal{M}^+(\mathcal{O})$, and \mathbf{v}_n a sequence of vector fields on \mathcal{O} . If*

$$\|\mathbf{v}_n\|_{L^2(\mathcal{O}, d\sigma_n; \mathbb{R}^m)} \leq C$$

then there exists $\mathbf{v} \in L^2(\mathcal{O}, d\sigma; \mathbb{R}^m)$ such that, up to extraction of some subsequence,

$$\forall \zeta \in \mathcal{C}_c^\infty(\mathcal{O}; \mathbb{R}^m) : \quad \lim_{n \rightarrow \infty} \int_{\mathcal{O}} \mathbf{v}_n \cdot \zeta d\sigma_n = \int_{\mathcal{O}} \mathbf{v} \cdot \zeta d\sigma$$

and

$$\|\mathbf{v}\|_{L^2(\mathcal{O}, d\sigma; \mathbb{R}^m)} \leq \liminf_{n \rightarrow \infty} \|\mathbf{v}_n\|_{L^2(\mathcal{O}, d\sigma_n; \mathbb{R}^m)}.$$

The proof can be found in [2, thm. 5.4.4] for probability measures, see also [22, prop. 5.3] for an abstract version. As anticipated, we have now

Proposition 5.3. *Assume (H). Then $\rho^\tau, \tilde{\rho}^\tau$ satisfy the compactness assumption (4.21) in Theorem 4.*

Proof. From the strong $L_{\text{loc}}^1([0, \infty); L^1)$ convergence in Proposition 5.2 and the uniform $L^1 \cap L^\infty(\Omega)$ bounds in Proposition 5.1, a straightforward application of Lebesgue's dominated convergence theorem yields strong convergence $\sqrt{\rho^\tau} \frac{\sqrt{\tilde{\rho}^\tau} + \sqrt{\rho^\tau}}{2} U'(\rho^\tau) \rightarrow \rho U'(\rho)$ at least in $L_{\text{loc}}^1((0, \infty) \times \Omega)$. Therefore the reaction terms pass to the limit as in (4.21), and we only have to check that the diffusion part does too.

Let $\mathbf{t}^{n+\frac{1}{2}}$ be the (backwards) optimal map from $\rho^{n+\frac{1}{2}}$ to ρ^n , and recall that the Euler-Lagrange equation (4.10) holds with $\mu = \rho^n$ and minimizer $\rho^* = \rho^{n+\frac{1}{2}}$. An easy density argument shows that (4.10) can in fact be written as $\frac{\text{id} - \mathbf{t}^{n+\frac{1}{2}}}{\tau} = -\nabla U'(\rho^{n+\frac{1}{2}})$ in $L^2(d\rho^{n+\frac{1}{2}})$, which should be interpreted as an equality in the tangent plane $T_{\rho^{n+\frac{1}{2}}} \mathcal{M}_{\text{MK}}^+$. Taking thus the $L^2(d\rho^{n+\frac{1}{2}})$ norm we obtain

$$\tau \|\nabla U'(\rho^{n+\frac{1}{2}})\|_{L^2(d\rho^{n+\frac{1}{2}})}^2 = \frac{1}{\tau} \|\text{id} - \mathbf{t}^{n+\frac{1}{2}}\|_{L^2(d\rho^{n+\frac{1}{2}})}^2 = \frac{1}{\tau} \text{MK}_2^2(\rho^{n+\frac{1}{2}}, \rho^n).$$

Recalling that the interpolated curve $\tilde{\rho}^\tau(t)$ is piecewise constant and summing from $n = 0$ to $n = \lceil T/\tau \rceil + 1$ for fixed any $T > 0$, we obtain from the total square-distance estimate (4.6)

$$(5.4) \quad \int_0^T \int_{\Omega} |\nabla U'(\tilde{\rho}^\tau(t))|^2 d\tilde{\rho}^\tau(t) dt \leq C \quad \Leftrightarrow \quad \int_{\mathcal{O}} |\nabla U'(\tilde{\rho}^\tau)|^2 d\sigma^\tau \leq C$$

with $\mathcal{O} = (0, T) \times \Omega \subset \mathbb{R}^{1+d}$ and $d\sigma^\tau(t, x) = d\tilde{\rho}_t^\tau(x) \otimes dt$. Recall that $\|\tilde{\rho}^\tau(t)\|_{L^1(\Omega)} \leq \|\rho^0\|_{\Omega}$, so that σ^τ is really a *finite* measure on \mathcal{O} for finite $T > 0$. From the strong $L_{\text{loc}}^1([0, \infty); L^1)$ convergence $\tilde{\rho}^\tau \rightarrow \rho$ (Proposition 5.2) it is easy to check that σ^τ converges narrowly to $d\sigma(t, x) = d\rho_t(x) \otimes dt = \rho(t, x) dx dt$. Applying Lemma 5.2 we see that there is a vector-field $\mathbf{v} \in L^2(\mathcal{O}, d\sigma) = L^2(0, T; L^2(d\rho_t))$ such that, up to extraction of a subsequence,

$$(5.5) \quad \int_0^T \int_{\Omega} \tilde{\rho}^\tau \nabla U'(\tilde{\rho}^\tau) \cdot \zeta \rightarrow \int_0^T \int_{\Omega} \rho(t, x) \mathbf{v}(t, x) \cdot \zeta(t, x) dx dt$$

for all $\zeta \in \mathcal{C}_c^\infty((0, T) \times \Omega; \mathbb{R}^n)$. In order to identify the weak limit \mathbf{v} , recall that the thermodynamic pressure $P(\rho) := \rho U'(\rho) - U(\rho)$. Since $P'(\rho) = \rho U''(\rho)$ our assumptions on U show that P is Lipschitz in any bounded interval $\rho \in [0, M]$. With the strong convergence $\rho^\tau \rightarrow \rho$ and the uniform $L^1 \cap L^\infty(\Omega)$ bounds one immediately gets $P(\tilde{\rho}^\tau) \rightarrow P(\rho)$ in $L^1_{\text{loc}}((0, \infty) \times \Omega)$, and as a consequence $\nabla P(\tilde{\rho}^\tau) \rightharpoonup \nabla P(\rho)$ in the sense of distributions $\mathcal{D}'((0, T) \times \Omega)$. Note that the measure $d\sigma(t, x) = d\rho_t(x) \otimes dt$ is finite on any subdomain $(0, T) \times \Omega$, hence $\mathbf{v} \in L^2(\mathcal{O}, d\sigma) \subset L^1(\mathcal{O}, d\sigma)$ and $\rho \mathbf{v} \in L^1((0, T) \times \Omega)$. Using the chain rule $\nabla P(\rho) = P'(\rho) \nabla \rho = \rho U''(\rho) \nabla \rho = \rho \nabla U'(\rho)$ we conclude that $\rho \mathbf{v} = \nabla P(\rho) = \rho \nabla U'(\rho)$, thus $\mathbf{v} = \nabla U'(\rho)$ at least in $L^2(d\rho)$. A further diagonal extraction shows that the limit \mathbf{v} can be chosen independent of T , and the proof is complete. \square

At this stage we can safely apply Theorem 4 to conclude that $\rho = \lim \rho^\tau = \lim \tilde{\rho}^\tau$ is a weak solution of the PDE. Our next and final result illustrates perhaps even better the deep interplay between our two-steps variational discretization and the three metrics:

Proposition 5.4. *In addition to (H), assume that $\mathcal{F}(\rho)$ is geodesically convex with respect to the MK_2 structure, i.e. $\rho P'(\rho) \geq (1 - \frac{1}{d}) P(\rho)$ with $P(\rho) = \rho U'(\rho) - U(\rho)$ [37]. Then we have*

$$(5.6) \quad \mathcal{F}(\rho(t_2)) + \int_{t_1}^{t_2} \int_{\Omega} (|\nabla U'(\rho)|^2 + |U'(\rho)|^2) d\rho dt \leq \mathcal{F}(\rho(t_1))$$

for all $0 \leq t_1 \leq t_2$.

From the discussion in section 2.3 we know that $\|U'(\rho)\|_{H^1(d\rho)}^2$ can be interpreted either as the metric slope $|\partial \mathcal{F}(\rho)|^2 = \|\text{grad}_{\text{KFR}} \mathcal{F}(\rho)\|^2$ or, through the continuity equation $\partial_t \rho = \text{div}(\rho \nabla U'(\rho)) - \rho U'(\rho)$, as the metric speed $|\rho'(t)|^2$ with respect to our distance KFR . Therefore (5.6) can be rephrased as the classical Energy Dissipation Inequality

$$\mathcal{F}(\rho(t_2)) + \int_{t_1}^{t_2} \left\{ \frac{1}{2} |\rho'(t)|^2 + \frac{1}{2} |\partial \mathcal{F}(\rho(t))|^2 \right\} dt \leq \mathcal{F}(\rho(t_1)),$$

which is one of the possible formulations of gradient flows in abstract metric spaces as in [2]. Note also that (H) already implies $\rho U''(\rho) + U'(\rho)/2 \geq 0$, which is equivalent to geodesic convexity with respect to FR . Thus we essentially assumed here that \mathcal{F} is geodesically convex with respect to each of the MK_2, FR structures, and it is not surprising that we recover in the end a dissipation inequality for the full KFR metrics.

Proof. Let $\mathbf{t}^{n+\frac{1}{2}}$ be the optimal map from $\rho^{n+\frac{1}{2}}$ to ρ^n . By the above-tangent characterization of the displacement convexity with respect to MK_2 [37, prop. 5.29] we have

$$\begin{aligned} \mathcal{F}(\rho^n) &\geq \mathcal{F}(\rho^{n+\frac{1}{2}}) + \int_{\Omega} (\mathbf{t}^{n+\frac{1}{2}} - \text{id}) \cdot \nabla U'(\rho^{n+\frac{1}{2}}) d\rho^{n+\frac{1}{2}} \\ &= \mathcal{F}(\rho^{n+\frac{1}{2}}) + \tau \int_{\Omega} |\nabla U'(\rho^{n+\frac{1}{2}})|^2 d\rho^{n+\frac{1}{2}}, \end{aligned}$$

where the last equality follows by noticing that the Euler-Lagrange (4.10) really means $\mathbf{t}^{n+\frac{1}{2}} - \text{id} = \tau \nabla U'(\rho^{n+\frac{1}{2}})$ in $L^2(d\rho^{n+\frac{1}{2}})$.

For the reaction part let us recall that $\rho U''(\rho) + \frac{U'(\rho)}{2} \geq 0$ can be reinterpreted as the convexity of $s \mapsto U(s^2)$ in $s = \sqrt{\rho}$. Using this convexity we obtain

$$\begin{aligned} \mathcal{F}(\rho^{n+\frac{1}{2}}) &\geq \mathcal{F}(\rho^{n+1}) + \int_{\Omega} 2\sqrt{\rho^{n+1}} U'(\rho^{n+1}) \left(\sqrt{\rho^{n+\frac{1}{2}}} - \sqrt{\rho^{n+1}} \right) \\ &= \mathcal{F}(\rho^{n+1}) + \tau \int_{\Omega} |U'(\rho^{n+1})|^2 d\rho^{n+1}, \end{aligned}$$

where the second line follows now by reinterpreting the Euler-Lagrange equation (4.14) as $2\frac{\sqrt{\rho^{n+1}} - \sqrt{\rho^{n+\frac{1}{2}}}}{\sqrt{\rho^{n+1}}} = -\tau U'(\rho^{n+1})$ in $L^2(d\rho^{n+1})$. We get altogether

$$\mathcal{F}(\rho^{n+1}) + \tau \left(\int_{\Omega} |\nabla U'(\rho^{n+\frac{1}{2}})|^2 d\rho^{n+\frac{1}{2}} + \int_{\Omega} |U'(\rho^{n+1})|^2 d\rho^{n+1} \right) \leq \mathcal{F}(\rho^n).$$

For any $0 \leq t_1 \leq t_2$ let now $N_1, N_2 \in \mathbb{N}$ such that $\rho^\tau(t_i) = \rho^{N_i}$, and $T_i = N_i \tau$. Summing the previous inequality from $n = N_1$ to $n = N_2 - 1$ gives

$$(5.7) \quad \mathcal{F}(\rho^\tau(t_2)) + \int_{T_1}^{T_2} \int_{\Omega} |\nabla U'(\tilde{\rho}^\tau)|^2 d\tilde{\rho}^\tau dt + \int_{T_1}^{T_2} \int_{\Omega} |U'(\rho^\tau)|^2 d\rho^\tau dt \leq \mathcal{F}(\rho^\tau(t_1)).$$

We proved in Proposition 5.3 that $\tilde{\rho}^\tau \nabla U'(\tilde{\rho}^\tau) \rightharpoonup \rho \nabla U'(\rho)$, and observe that $T_i \rightarrow t_i$ as $\tau \rightarrow 0$. From the energy estimate (5.4) and the lower semi-continuity in Lemma 5.2 we deduce that

$$\int_{t_1}^{t_2} \int_{\Omega} |\nabla U'(\rho)|^2 d\rho dt \leq \liminf_{\tau \rightarrow 0} \int_{T_1}^{T_2} \int_{\Omega} |\nabla U'(\tilde{\rho}^\tau)|^2 d\tilde{\rho}^\tau dt,$$

and from the strong convergence in Proposition 5.2 with the uniform $L^1 \cap L^\infty(\Omega)$ bounds (Proposition 5.1) it is easy to see that

$$\int_{t_1}^{t_2} \int_{\Omega} |U'(\rho)|^2 d\rho dt = \lim_{\tau \rightarrow 0} \int_{T_1}^{T_2} \int_{\Omega} |U'(\rho^\tau)|^2 d\rho^\tau dt.$$

Similarly one can verify that

$$\forall t \geq 0 : \quad \mathcal{F}(\rho^\tau(t)) = \int_{\Omega} U(\rho^\tau(t)) \rightarrow \int_{\Omega} U(\rho(t)) = \mathcal{F}(\rho(t)).$$

Indeed with our assumptions U is Lipschitz in any bounded interval $\rho \in [0, M]$, $\|\rho^\tau(t)\|_{L^\infty} \leq M = \|\rho^0\|_{L^\infty}$ uniformly in τ , and in the first proof of Proposition 5.2 we obtained strong $L^1(\Omega)$ convergence $\rho^\tau(t) \rightarrow \rho(t)$ pointwise in time. As a consequence we can pass to the \liminf in (5.7) to retrieve (5.6) and the proof is complete. \square

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