Diffeomorphisms and Nonlinear Heat Flows

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Abstract

We show that the gradient flow $\mathbf{u}$ on L^2 generated by the energy functional $I[\mathbf{u}] := \int_U \Phi(\det D\mathbf{u})\,dx$ for vector-valued mappings is in some sense "integrable", meaning that (i) the inverse Jacobian $\beta := (\det D\mathbf{u})^{-1}$ satisfies a scalar nonlinear diffusion equation, and (ii) we can recover $\mathbf{u}$ by solving an ODE determined by β.

1 Introduction

1.1 Gradient flows for quasiconvex energies. This paper is a contribution to the mostly unsolved problem of understanding the gradient flow dynamics on L^2 generated by integral functionals having the form

$$I[\mathbf{v}] := \int_U F(D\mathbf{v})\,dx, \tag{1.1}$$

defined for functions $\mathbf{v} : U \to \mathbb{R}^m$, where U is an open subset of$\mathbb{R}^n$. The gradient $D\mathbf{v}$ belongs to $\mathbb{M}^{m\times n}$, the space of $m \times n$ matrices, and we are given the nonlinearity $F : \mathbb{M}^{m\times n} \to (-\infty, +\infty]$.

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Quasiconvexity. As is well known, the critical assumption for the existence of minimizers of $I[\cdot]$, subject to appropriate boundary conditions, is that F be *quasiconvex* in the sense of C. B. Morrey, Jr. This is the condition that

$$\int_U F(A)\,dx \le \int_U F(A + D\mathbf{v})\,dx \tag{1.2}$$

for all matrices $A \in \mathbb{M}^{m\times n}$ and all C^1 functions $\mathbf{v} : U \to \mathbb{R}^m$ vanishing on ∂U.

Dynamics. As the existence and (partial) regularity theories for minimizers are fairly well understood, it has long seemed natural to turn attention to related dynamical problems. The corresponding flow on L^2 generated by $I[\cdot]$ is the initial-value problem for the system of PDE

$$\begin{cases} \mathbf{u}_t = \operatorname{div}(DF(D\mathbf{u})) & (t > 0) \\ \mathbf{u} = \mathbf{u}^0 & (t = 0), \end{cases} \tag{1.3}$$

with appropriate boundary conditions.

Given the quasiconvexity hypothesis (1.2), the system (1.3) is parabolic, at least in some weak sense. However it is extremely nonlinear, so much so that it remains to date a challenging open problem to prove existence of even weak solutions, to understand uniqueness issues and/or to show partial regularity.

Time-step approximations. One obvious approach is to approximate by an implicit *time-step approximation*. For this, we fix a step size $h > 0$ and recursively find $\mathbf{u}_{k+1}$ to minimize

$$I_k[\mathbf{v}] := \frac{1}{2}\int_U |\mathbf{v} - \mathbf{u}_k|^2\,dx + h\int_U F(D\mathbf{v})\,dx, \tag{1.4}$$

with appropriate boundary conditions, given $\mathbf{u}_k$. The Euler-Lagrange equations read

$$\begin{cases} \frac{\mathbf{u}_{k+1}-\mathbf{u}_k}{h} = \operatorname{div}(DF(D\mathbf{u}_{k+1})) & (k = 0, 1, \dots) \\ \mathbf{u}_0 = \mathbf{u}^0. \end{cases} \tag{1.5}$$

This procedure generates a strong candidate for an approximation to the full dynamics (1.3). The fundamental point is that under our quasiconvexity assumption we can in fact iteratively find minimizers of (1.4).

The really hard task is passing to limits as $h \to 0$. Since our approximations $\mathbf{u}_k$ are minimizers, and not just critical points, of $I_k[\cdot]$, the expectation and hope is that we obtain in the limit some sort of reasonable weak solution of (1.3). It has however proved in practice impossible to carry out this program in general, owing to the usual problem in nonlinear PDE that we do not have very good uniform estimates on the approximate solutions $\mathbf{u}_k$.

(The paper [E] demonstrates a completely different minimization principle, but we have not been able to exploit this usefully.)

1.2 Nonlinearities depending only on the determinant. This paper documents some progress in this matter for the case $m = n$ and nonlinearities F with the special structure

$$F(P) = \Phi(\det P) \qquad (P \in \mathbb{M}^{n\times n}), \tag{1.6}$$

where Φ is a convex function and "det" means determinant. Such a nonlinearity is quasiconvex, and it has long been known that for the static calculus of variations the particular hypothesis (1.6) has strong implications: see for instance Dacorogna [D].

We begin by reviewing the issue of minimizing the functional

$$I[\mathbf{v}] := \int_U F(D\mathbf{v})\,dx = \int_U \Phi(\det D\mathbf{v})\,dx \tag{1.7}$$

among mappings $\mathbf{v} = (v^1, \dots, v^n)$ from a connected, open set $U \subset \mathbb{R}^n$ into $\mathbb{R}^n$. We write the gradient matrix of $\mathbf{v}$ as

$$D\mathbf{v} = \begin{pmatrix} v^1_{x_1} & \dots & v^1_{x_n} \\ \vdots & \ddots & \vdots \\ v^n_{x_1} & \dots & v^n_{x_n} \end{pmatrix}.$$

If $\mathbf{u} = (u^1, \dots, u^n)$ is a smooth minimizer of $I[\cdot]$, subject to boundary conditions which for the moment we do not specify, then $\mathbf{u}$ solves the Euler–Lagrange system of PDE

$$\operatorname{div}(DF(D\mathbf{u})) = \operatorname{div}(\Phi'(\det D\mathbf{u})(\operatorname{cof} D\mathbf{u})^T) = 0, \tag{1.8}$$

where $\operatorname{cof} D\mathbf{u}$ is the cofactor matrix formed from $D\mathbf{u}$. To derive (1.8) we employed the formula

$$\frac{\partial \det P}{\partial p^k_i} = (\operatorname{cof} P)^k_i \qquad (1 \le i, k \le n). \tag{1.9}$$

for the $n \times n$ matrix P, whose (i,k) entry is denoted p^k_i. Likewise, $(\operatorname{cof} P)^k_i$ means the (i,k) entry of $\operatorname{cof} P$. Formula (1.9) is a consequence of the matrix identity

$$(\operatorname{cof} P)^T P = I \det P, \tag{1.10}$$

But for any C^2 function $\mathbf{w} = (w^1, \dots, w^n)$ we have

$$\operatorname{div}((\operatorname{cof} D\mathbf{w})^T) \equiv 0; \tag{1.11}$$

that is,

$$(\operatorname{cof} D\mathbf{w})^k_{i,x_i} = 0 \qquad (k = 1, \dots, n).$$

Therefore (1.8) implies

$$0 = \Phi''(\det D\mathbf{u}) D(\det D\mathbf{u})(\operatorname{cof} D\mathbf{u})^T. \tag{1.12}$$

In view of (1.10), our multiplying (1.10) by $D\mathbf{u}$ gives

$$0 = \Phi''(\det D\mathbf{u}) D(\det D\mathbf{u})(\det D\mathbf{u}) = \frac{1}{2}\Phi''(\det D\mathbf{u}) D(\det D\mathbf{u})^2.$$

Assuming next the strict convexity condition that $\Phi'' > 0$, we deduce that that $(\det D\mathbf{u})^2$ is constant within U. Thus, if $\mathbf{u}$ is smooth, we conclude that

$$\det D\mathbf{u} \equiv C \quad \text{within} \quad U \tag{1.13}$$

for some constant C.

1.3 A gradient flow. We study in this paper the corresponding "heat flow" governed by the function $I[\cdot]$, that is, the system of PDE

$$\mathbf{u}_t = \operatorname{div}(DF(D\mathbf{u})) = \operatorname{div}(\Phi'(\det D\mathbf{u})(\operatorname{cof} D\mathbf{u})^T), \tag{1.14}$$

plus appropriate initial and boundary conditions, detailed later.

We are especially interested in the case that $\Phi(d) < \infty$ for $d > 0$, $\Phi(d) = \infty$ for $d < 0$, and $\lim_{d \to 0^+} \Phi(d) = +\infty$. Then (1.14) enforces the constraint

$$\det D\mathbf{u} > 0.$$

We can hope therefore that for each time t the mapping $x \mapsto y = \mathbf{u}(x,t)$ is a diffeomorphism, with inverse $y \mapsto x = \mathbf{v}(y,t)$. And since the static problem, recalled in §1.1, is so simple, we hope as well that the analysis of the system (1.14) may not be so complicated.

This is in fact so, for as we will see in Section 2, the quantity

$$\beta := (\det D\mathbf{u})^{-1} > 0, \tag{1.15}$$

regarded as a function of y and t, solves the nonlinear parabolic PDE

$$\beta_t = \operatorname{div}\left(\Phi''\left(\frac{1}{\beta}\right)\frac{D\beta}{\beta^2}\right) = \operatorname{div}\left(\beta\Psi'(\beta)D\beta\right) \tag{1.16}$$

with Neumann boundary conditions, where

$$\Psi(d) := d\Phi\left(\frac{1}{d}\right) \quad \text{for } d > 0.$$

Now (1.16) is singular in regimes where $\beta \to 0$ or ∞, but the maximum principle implies that if the initial data β^0 is bounded away from 0 and ∞, then so is the solution.

We will show furthermore that given β, the solution of (1.16) with appropriate initial conditions, we can then recover the mappings $\mathbf{u}$ by solving a system of ODE governed by β and proving then that the PDE (1.14) holds. In this sense, we can regard the parabolic system PDE (1.14) as being somehow "integrable".

1.4 Outline. Our paper introduces in Section 2 the formal computations showing how (1.16) results from (1.14). Section 3 then reverses this process, to provide careful proofs: we start with the solution β of the nonlinear diffusion equation and build from it the mappings $\mathbf{u}(\cdot, t)$ for $t > 0$.

Section 4 introduces some interesting variants of our construction, the first for more general integrands than in (1.7). We discuss also a situation when the range of the initial mapping $\mathbf{u}^0$ is a proper subset W_0 of the target V. In this case we can design Φ so that the flow "fills up" V in finite time. Interesting complications occur if U and V are not in fact diffeomorphic.

The concluding Section 5 introduces and analyzes a related "time stepping" dynamic variational principle. This discussion will make much clearer the connections between our PDE (1.16) and (1.14).

2 Calculations for smooth solutions

Suppose now U is a smooth, open, bounded, connected subset of $\mathbb{R}^n$, and

$$\mathbf{u} : \bar{U} \times [0, \infty) \to \mathbb{R}^n$$

is smooth, $\mathbf{u} = (u^1, \dots, u^n)$. In this section we suppose as well that $\mathbf{u}$ solves the system (1.14). Let $\mathbf{u}^0 = \mathbf{u}(\cdot, 0)$ denote the initial mapping.

2.1 Changing variables. Suppose that for each time $t \geq 0$, the mapping

$$\mathbf{u}(\cdot, t) : \bar{U} \to \bar{V}$$

is a diffeomorphism, where $V \subset \mathbb{R}^n$ is a fixed open subset of $\mathbb{R}^n$ We can then invert the relationship

$$y = \mathbf{u}(x, t) \qquad (x \in \bar{U}, y \in \bar{V}) \tag{2.1}$$

to give

$$x = \mathbf{v}(y,t) \qquad \text{for } \mathbf{v} := \mathbf{u}^{-1}. \tag{2.2}$$

Set

$$\beta(y,t) := \det D\mathbf{v}(y,t) = (\det D\mathbf{u}(x,t))^{-1}. \tag{2.3}$$

2.2 A partial differential equation for $\boldsymbol{\beta}$. Our main observation is that β solves a scalar, nonlinear diffusion equation:

Theorem 2.1 *We have*

$$\begin{cases} \beta_t = \operatorname{div}\left(\Phi''\left(\frac{1}{\beta}\right)\frac{1}{\beta^2}D\beta\right) & \text{in } V \times (0,\infty) \\ \frac{\partial \beta}{\partial \nu} = 0 & \text{on } \partial V \times (0,\infty), \end{cases} \tag{2.4}$$

ν denoting the unit outward pointing normal vectorfield to ∂V.

Proof. 1. Fix any time $T > 0$ and select a smooth function $\zeta : \bar{V} \times [0,T] \to \mathbb{R}$ such that

$$\zeta(\cdot,0) \equiv \zeta(\cdot,T) \equiv 0. \tag{2.5}$$

Then employing (2.1), we compute

$$\begin{aligned} &\int_0^T \int_V \beta\zeta_t + D_y\left(\Phi'\left(\frac{1}{\beta}\right)\right)\cdot D_y\zeta \, dydt \\ = &\int_0^T \int_U \left[\beta(\mathbf{u},t)\zeta_t(\mathbf{u},t) + D_x\left(\Phi'\left(\frac{1}{\beta}\right)\right)(D\mathbf{u})^{-1}\cdot D_y\zeta\right]\frac{dx}{\beta(\mathbf{u},t)}\, dt \\ = &\int_0^T \int_U \frac{\partial}{\partial t}(\zeta(\mathbf{u},t)) - D_y\zeta\cdot\mathbf{u}_t + D_x\left(\Phi'\left(\frac{1}{\beta}\right)\right)\frac{(D\mathbf{u})^{-1}}{\beta}\cdot D_y\zeta\, dxdt \\ = &-\int_0^T \int_U D_y\zeta\cdot\left[\mathbf{u}_t - D_x\left(\Phi'\left(\frac{1}{\beta}\right)\right)\frac{(D\mathbf{u})^{-1}}{\beta}\right] dxdt. \end{aligned} \tag{2.6}$$

Now our PDE (1.14) reads

$$\mathbf{u}_t = \operatorname{div}_x(\Phi'(\det D\mathbf{u})\det D\mathbf{u}(D\mathbf{u})^{-1}) = D_x\left(\Phi'\left(\frac{1}{\beta}\right)\right)\frac{(D\mathbf{u})^{-1}}{\beta},$$

since $\operatorname{div}((\det D\mathbf{u})(D\mathbf{u})^{-1}) = \operatorname{div}(\operatorname{cof} D\mathbf{u}^T) \equiv 0$. Consequently the expression within the square brackets in the last term of (2.6) vanishes. So

$$\int_0^T \int_V \beta\zeta_t + D_y\left(\Phi'\left(\frac{1}{\beta}\right)\right)\cdot D_y\zeta\, dydt = 0$$

for all test functions ζ as above.

2. If also $\zeta \equiv 0$ on $\partial V \times [0,T]$, we may integrate by parts to deduce

$$\beta_t + \operatorname{div}_y \left(D_y \Phi' \left(\frac{1}{\beta} \right) \right) \equiv 0 \tag{2.7}$$

and this is the PDE in (2.4). Now drop the assumption that $\zeta = 0$ on the boundary and again integrate by parts:

$$\int_0^T \int_{\partial V} \frac{\partial}{\partial \nu} \left(\Phi' \left(\frac{1}{\beta} \right) \right) \zeta \, d\mathcal{H}^{n-1} \, dt = 0.$$

It follows that

$$\frac{\partial}{\partial \nu} \left(\Phi' \left(\frac{1}{\beta} \right) \right) = -\Phi'' \left(\frac{1}{\beta} \right) \frac{\partial \beta}{\partial \nu} \equiv 0 \quad \text{on} \quad \partial V \times (0,T).$$

Since $\Phi'' > 0$, the proof is done. □

2.3 Recovering the mapping u from $\boldsymbol{\beta}$. We next address the question of how to recover the mapping $\mathbf{u}$ from knowledge of β. One possibility is for each time t to try to find $x \mapsto \mathbf{u}(x,t)$ solving

$$\begin{cases} \beta(\mathbf{u}(x,t),t) \det D\mathbf{u}(x,t) \equiv 1 & \text{in } \bar{U}, \\ \mathbf{u}(\cdot,t) \in \operatorname{Diff}(\bar{U},\bar{V}), \end{cases} \tag{2.8}$$

where $\operatorname{Diff}(\bar{U},\bar{V})$ denotes the set of all diffeomorphisms of $\bar{U}$ onto $\bar{V}$. As we will discuss later in Section 5, this approach works, provided U and V are convex sets.

However there is a simpler construction available. First, define the new nonlinearity

$$\Psi(d) := d\Phi \left(\frac{1}{d} \right) \qquad (d > 0). \tag{2.9}$$

Then

$$\Psi'(d) = \Phi \left(\frac{1}{d} \right) - \frac{1}{d} \Phi' \left(\frac{1}{d} \right), \quad \Psi''(d) = \frac{1}{d^3} \Phi'' \left(\frac{1}{d} \right); \tag{2.10}$$

and so $\Psi : (0,\infty) \to \mathbb{R}$ is convex.

Next, perform these calculations:

$$
\begin{aligned}
\mathbf{u}_t &= \operatorname{div}_x(\Phi'(\det D\mathbf{u}) \det D\mathbf{u}(D\mathbf{u})^{-1}) \\
&= D_x(\Phi'(\det D\mathbf{u})) \cdot (\det D\mathbf{u}(D\mathbf{u})^{-1}) \\
&= \Phi''(\det D\mathbf{u}) D_x(\det D\mathbf{u}) \cdot (\det D\mathbf{u}(D\mathbf{u})^{-1}) \\
&= \Phi''\left(\frac{1}{\beta}\right) \frac{1}{\beta} D_x \left(\frac{1}{\beta}\right) (D\mathbf{u})^{-1} \\
&= -\Phi''\left(\frac{1}{\beta}\right) \frac{1}{\beta^3} D_x \beta (D\mathbf{u})^{-1} \\
&= -\Psi''(\beta) D_y \beta = -D_y \Psi'(\beta).
\end{aligned} \tag{2.11}
$$

This computation suggests that we fix a point $x \in \bar{U}$ and then solve the ODE

$$
\begin{cases} \dot{\mathbf{y}}(t) = -\Psi''(\beta(\mathbf{y}(t), t)) D\beta(\mathbf{y}(t), t) & \text{for } t > 0 \\ \mathbf{y}(0) = y = \mathbf{u}^0(x) \end{cases} \tag{2.12}
$$

where $\dot{} = \frac{d}{dt}$. Then by uniqueness of solutions we have $\mathbf{u}(x, t) = \mathbf{y}(t)$ for $t \geq 0$.

3 Building diffeomorphisms

The formal calculations from the previous section done with, we turn now to building rigorously a smooth solution

$$
\mathbf{u} : \bar{U} \times [0, \infty) \to \bar{V}
$$

of our system

$$
\begin{cases} \mathbf{u}_t = \operatorname{div}(\Phi'(\det D\mathbf{u})(\operatorname{cof} D\mathbf{u})^T) & \text{in } \bar{U} \times (0, \infty) \\ \mathbf{u} = \mathbf{u}^0 & \text{on } \bar{U} \times \{t = 0\} \\ \mathbf{u}(\cdot, t) \in \operatorname{Diff}(\bar{U}, \bar{V}) \end{cases} \tag{3.1}
$$

under some additional assumptions.

3.1 Hypotheses. We require that the initial mapping $\mathbf{u}^0 : \bar{U} \to \bar{V}$ be a diffeomorphism, mapping ∂U onto ∂V. We write

$$
\beta^0 := \det D\mathbf{v}^0 \tag{4.2}
$$

for $\mathbf{v}^0 := (\mathbf{u}^0)^{-1}$ and assume that there exist positive constants $0 < C_1 \leq C_2$ such that

$$
C_1 \leq \beta^0 \leq C_2 \quad \text{on } \bar{V}. \tag{$H1$}
$$

We ask also that this *compatibility condition* hold:

$$\frac{\partial \beta^0}{\partial \nu} = 0 \quad \text{on} \quad \partial V. \tag{$H2$}$$

Finally we require that Φ be smooth and convex on $(0, \infty)$, with the lower bound

$$\Phi''\left(\frac{1}{\beta}\right) > 0 \quad \text{for } C_1 \leq \beta \leq C_2. \tag{$H3$}$$

3.2 Solving PDE and ODE. In view of $(H1)$, $(H2)$, the initial/ boundary value problem

$$\begin{cases} \beta_t = \operatorname{div}\left(\Phi''\left(\frac{1}{\beta}\right)\frac{D\beta}{\beta^2}\right) & \text{in } V \times (0, \infty) \\ \frac{\partial \beta}{\partial \nu} = 0 & \text{on } \partial V \times [0, \infty) \\ \beta = \beta^0 & \text{on } \bar{V} \times \{t = 0\} \end{cases} \tag{3.2}$$

has a unique, smooth solution β, with

$$0 < C_1 \leq \beta \leq C_2 \qquad \text{in } \bar{V} \times [0, \infty). \tag{3.3}$$

Next, for each $y \in \bar{V}$, solve the ODE (2.12):

$$\begin{cases} \dot{\mathbf{y}}(t) = -\Psi''(\beta(\mathbf{y}(t), t))D\beta(\mathbf{y}(t), t) & \text{for } t > 0 \\ \mathbf{y}(0) = y. \end{cases} \tag{3.4}$$

We write $\mathbf{y}(t) = \mathbf{y}(t, y)$ to display dependence on the initial point y.

Theorem 3.1 (i) *For each given $x \in \bar{U}$, the* ODE (3.4) *has a unique solution $\mathbf{y} : [0, \infty) \to \bar{V}$, existing for all times $t \geq 0$.*
(ii) *If $y \in \partial V$, then $\mathbf{y}(t) \in \partial V$ for all times $t \geq 0$.*
(iii) *For each $t \geq 0$, the mapping*

$$\mathbf{u}(x, t) := \mathbf{y}(t, \mathbf{u}^0(x)) \qquad (x \in \bar{U},\ t \geq 0) \tag{3.5}$$

is a smooth diffeomorphism from $\bar{U}$ to $\bar{V}$, mapping ∂U onto ∂V.

Proof. Since $\frac{\partial \beta}{\partial \nu} = 0$ on ∂V, $D\beta$ is tangent to ∂V and consequently the flow does not leave $\bar{V}$. In particular, if $\mathbf{u}^0(x) \in \partial V$, then $\mathbf{x}(t) \in \partial V$ for times $t \geq 0$.
Assertion (iii) is standard. □

Define $\mathbf{u} : \bar{U} \times [0, \infty) \to \bar{V}$ by (3.5) and set $\mathbf{v}(\cdot, t) := \mathbf{u}^{-1}(\cdot, t)$ for each time $t \geq 0$.

Theorem 3.2 (i) *We have*

$$\beta \equiv \det D\mathbf{v}. \tag{3.6}$$

(ii) *Furthermore,* $\mathbf{u}$ *solves the system of* PDE (2.1)*, and the mapping*

$$t \mapsto \int_U \Phi(\det D\mathbf{u})(x,t)\,dx$$

is nonincreasing.

Proof. 1. As before, set $\alpha = \det D\mathbf{u}$, $\alpha = \alpha(x,t)$. Then

$$\alpha_t = \alpha D_x \mathbf{u}_t (D\mathbf{u})^{-1}. \tag{3.7}$$

Now

$$\mathbf{u}_t = -D_y \Psi'(\beta)$$

and so

$$D_x \mathbf{u}_t = -D_y^2 \Psi'(\beta)(D_x \mathbf{u}).$$

Hence

$$\alpha_t = -\alpha \Delta_y \Psi'(\beta). \tag{3.8}$$

Next, regarding $\beta = \beta(\mathbf{u}, t)$ as a function of (x,t), we have

$$\begin{aligned} (\alpha\beta)_t &= \alpha_t \beta + \alpha \beta_t + \alpha D_y \beta \cdot \mathbf{u}_t \\ &= -\alpha\beta\Delta_y \Psi'(\beta) + \alpha \operatorname{div}(\Psi''(\beta)\beta D_y \beta) - \alpha D_y \beta \cdot (\Psi''(\beta) D_y \beta) \\ &= 0. \end{aligned}$$

Since $\alpha\beta \equiv 1$ at $t = 0$, we deduce that

$$\beta = \alpha^{-1} = \det D\mathbf{v}.$$

2. We have shown that $\beta \equiv \det D\mathbf{v}$, where $\mathbf{v} = \mathbf{u}^{-1}$ and $\mathbf{u}$ is defined by (3.5). We then return to the computation (2.11) to deduce that

$$\mathbf{u}_t = \dot{\mathbf{x}} = -\Psi''(\beta) D\beta = \operatorname{div}(\Phi'(\det D\mathbf{u})(\operatorname{cof} D\mathbf{u})^T). \tag{3.9}$$

Finally let us calculate:

$$\begin{aligned}\frac{d}{dt}\int_U \Phi(\det D\mathbf{u})\,dx &= \frac{d}{dt}\int_V \Phi\left(\frac{1}{\beta}\right)\beta\,dy\\ &= \int_V \left(\Phi\left(\frac{1}{\beta}\right) - \frac{1}{\beta}\Phi'\left(\frac{1}{\beta}\right)\right)\beta_t\,dy\\ &= \int_V \Psi'(\beta)\,\mathrm{div}(\beta\Psi''(\beta)D\beta)\,dy\\ &= -\int_V \Psi''(\beta)^2\beta|D\beta|^2\,dy \leq 0.\end{aligned}$$

□

4 Some variants

4.1 More general nonlinearities. Our methods extend with little difficulty to the functional

$$I[\mathbf{v}] := \int_U \Phi(f(\mathbf{v})\det D\mathbf{v})\,dx, \tag{4.1}$$

for Φ as before and $f : \bar{V} \to (0, \infty)$.

Euler-Lagrange equation. The corresponding Euler-Lagrange equation is

$$-\,\mathrm{div}(\Phi'(f\det D\mathbf{u})f(\mathrm{cof}\,D\mathbf{u})^T) + \Phi'(f\det D\mathbf{u})(\det D\mathbf{u})Df = 0,$$

which simplifies to read

$$\Phi''(f\det D\mathbf{u})D(f\det D\mathbf{u})f(\mathrm{cof}\,D\mathbf{u})^T = 0. \tag{4.2}$$

As in Section 1.1 this implies that

$$f(\mathbf{u})\det D\mathbf{u} \equiv C \quad \text{within} \quad U$$

for some constant C.

A gradient flow. The evolution associated with (4.1) is

$$\mathbf{u}_t - \mathrm{div}(\Phi'(f\det D\mathbf{u})f(\mathrm{cof}\,D\mathbf{u})^T) + \Phi'(f\det D\mathbf{u})(\det D\mathbf{u})Df = 0, \tag{4.3}$$

plus initial and boundary conditions.

As before assume $\mathbf{v} := \mathbf{u}^{-1}$ exists and write

$$\beta := \det D\mathbf{v}.$$

Theorem 4.1 *We have*

$$\begin{cases} \beta_t = -\operatorname{div}\left(\Phi''\left(\frac{f}{\beta}\right) f D\left(\frac{f}{\beta}\right)\right) & \text{in } V \times (0,\infty) \\ \frac{\partial}{\partial \nu}\left(\frac{f}{\beta}\right) = 0 & \text{on } \partial V \times (0,\infty). \end{cases} \tag{4.4}$$

Proof. 1. Fix any time $T > 0$ and select a smooth function $\zeta : \bar{V} \times [0,T] \to \mathbb{R}$ satisfying (2.5)

Then

$$\begin{aligned} &\int_0^T \int_V \beta\zeta_t + D_y\left(\Phi'\left(\frac{f}{\beta}\right)\right) \cdot D_y\zeta f \; dydt \\ =& \int_0^T \int_U \left[\beta(\mathbf{u},t)\zeta_t(\mathbf{u},t) + D_x\left(\Phi'\left(\frac{f}{\beta}\right)\right)(D\mathbf{u})^{-1} \cdot D_y\zeta f\right] \frac{dx}{\beta(\mathbf{u},t)} \; dt \\ =& \int_0^T \int_U \frac{\partial}{\partial t}(\zeta(\mathbf{u},t)) - D_y\zeta \cdot \mathbf{u}_t + D_x\left(\Phi'\left(\frac{f}{\beta}\right)\right)\frac{(D\mathbf{u})^{-1}}{\beta} \cdot D_y\zeta f \; dxdt \\ =& -\int_0^T \int_U D_y\zeta \cdot \left[\mathbf{u}_t - D_x\left(\Phi'\left(\frac{f}{\beta}\right)\right)\frac{(D\mathbf{u})^{-1}}{\beta} f\right] \; dxdt. \end{aligned} \tag{4.5}$$

But according to (4.3), we have

$$\begin{aligned} \mathbf{u}_t &= D(\Phi'(f \det D\mathbf{u})) f(\det D\mathbf{u})(D\mathbf{u})^{-1} \\ &= D\left(\Phi'\left(\frac{f}{\beta}\right)\right)\frac{f}{\beta}(D\mathbf{u})^{-1} \end{aligned} \tag{4.6}$$

Consequently the expression within the square brackets in the last term above vanishes.

□

4.2 "Filling up" the target domain. An interesting variant of our construction is as follows. Select $\mathbf{u}^0 : \bar{U} \to \bar{W}_0$ be a diffeomorphism, where $W_0 \subset\subset V$ is given We will choose Φ and $\mathbf{u}$ so that

$$\begin{cases} W(t) := \mathbf{u}(U,t) & (t \geq 0) \\ W(0) = W_0 \end{cases} \tag{4.7}$$

expands, to "fill up" the target V in finite time.

For this, let us take $m > 0$ and

$$\Phi(d) := \begin{cases} \frac{1}{m} d^{-m} & (d > 0) \\ +\infty & (d \leq 0). \end{cases}$$

Therefore

$$\Psi(d) = d\Phi\left(\frac{1}{d}\right) = \frac{1}{m}d^{m+1}$$

for $d > 0$. Then β solves porous medium equation

$$\beta_t = \operatorname{div}(\Psi''(\beta)\beta D\beta) = \Delta(\beta^{m+1}).$$

5 Connections with optimal mass transfer problems

As noted in the Introduction, the time step minimization method (1.4) and (1.5) provides an extremely natural approximation method, but one which we have not been able to prove converges. This section recalls more about this procedure, to highlight the connections with Monge-Kantorovich mass transfer theory.

We are primarily motivated by Otto [O] and Jordan–Kinderlehrer–Otto [J-K-O]. The novelty of Otto's paper [O] was to interprete (5.8) as a gradient flux of the "entropy" $S(\beta) := \int_V \Psi(\beta)dy$ with respect to the Wasserstein distance.

5.1 Time step approximations. Assume for this section that that U and V are two bounded, open, *convex* sets with smooth boundaries.

We discuss a time–discrete algorithm for the flow

$$\text{(5.1)} \qquad \begin{cases} \mathbf{u}_t = \operatorname{div}(DF(D\mathbf{u})) \\ \mathbf{u}(\cdot, 0) = \mathbf{u}_0, \\ \mathbf{u}(\cdot, t) \in \operatorname{Diff}(\bar{U}, \bar{V}), \end{cases}$$

where, as before,

$$F(P) = \begin{cases} \Phi(\det P) & \det P > 0 \\ +\infty & \det P \leq 0. \end{cases}$$

The system (5.1) is a gradient flux of the functional $I[\cdot]$ with respect to the L^2–metric. In Section 2 we have shown that (5.1) is related to (1.16), which, as we will recall below, is the gradient flow governed by of $\int_V \Psi(\beta)\, dy$ with respect to the Wasserstein distance. The algorithm which we discuss is another way to view that relation.

A discrete time approximation. First, let us fix a time step size $h > 0$. We introduce the implicit scheme of recursively finding $\mathbf{u}_{k+1}$ to solve

$$\text{(5.2)} \qquad \begin{cases} \frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} = \operatorname{div}(DF(D\mathbf{u}_{k+1})) \\ \mathbf{u}_{k+1} \in \operatorname{Diff}(\bar{U}, \bar{V}), \end{cases}$$

given $\mathbf{u}_k$. More precisely, set

$$I_k[\mathbf{v}] := \frac{1}{2}\int_U |\mathbf{v}-\mathbf{u}_k|^2\,dx + h\int_U F(D\mathbf{v})\,dx. \tag{5.3}$$

We intend to find $\mathbf{u}_{k+1}$ to be the unique minimizer of

$$\min_{\mathbf{v}}\{I_k[\mathbf{v}] \mid \mathbf{v}\in \mathrm{Diff}(\bar{U},\bar{V})\}. \tag{5.4}$$

Changing variables. Since our nonlinearity F is neither coercive nor convex, standard calculus of variations methods do not apply. However recent papers by Gangbo–Van der Putten [G-VP] and Maroofi [Ma] demonstrate how to exploit the special structure of $F(P) = \Phi(\det P)$ to find minimizers.

Indeed, if we change of variables $y = \mathbf{u}(x)$ and set $\beta := \det(D\mathbf{u}^{-1})$, $\beta_k := \det(D\mathbf{u}_k^{-1})$, we discover that

$$I_k[\mathbf{v}] = \frac{1}{2}\int_V |y-\mathbf{u}_k(\mathbf{v}^{-1}(y))|^2 dy + h\int_V \Psi(\beta)\,dy.$$

Consequently

$$\begin{aligned}
&\min_{\mathbf{v}\in\mathrm{Diff}(\bar{U},\bar{V})} I_k[\mathbf{v}]\\
&= \inf_\beta\Big\{h\int_V \Psi(\beta)\,dy + \inf_{\mathbf{v}}\{\frac{1}{2}\int_V |y-\mathbf{u}_k(\mathbf{v}^{-1}(y))|^2 dy \mid \beta = \det(D\mathbf{v}^{-1})\}\Big\}\\
&= \inf_\beta\Big\{h\int_V \Psi(\beta)\,dy + \inf_{\mathbf{w}}\{\frac{1}{2}\int_V |y-\mathbf{w}(y)|^2 dy \mid \beta_k = \beta(\mathbf{w})\det D\mathbf{w}\}\Big\}\\
&= \inf_\beta\Big\{h\int_V \Psi(\beta)\,dy + W_2^2(\beta_k,\beta)\Big\},
\end{aligned} \tag{5.5}$$

where W_2, the *Wasserstein distance* between two Borel measures μ and ν, is defined as

$$W_2^2(\mu,\nu) := 1/2 \inf_{\gamma\in\Gamma(\mu,\nu)} \iint |x-y|^2 d\gamma(x,y).$$

Here $\Gamma(\mu,\nu)$ is the set of Borel measures γ on $\mathbb{R}^{2n}$ that have μ and ν as their marginals. The notation $W_2^2(\beta_k,\beta)$ means that we have identified β with the measure whose density is β.

We assume that for $k = 0$ that

$$\int_V \beta_0\,dy = 1,$$

where $\beta_0 = \det D\mathbf{u}_0^{-1}$. This reduces the last three problems in (5.5) to minimization problems over $\mathcal{P}_a(V)$, the set of probability densities supported in V.

Define the new functional

$$J_k(\beta) := W_2^2(\beta, \beta_k) + h \int_V \Psi(\beta)\, dy. \tag{5.6}$$

Now $W_2^2(\beta_k, \cdot)$ is convex and is weakly-$*$ lower semicontinuous. Since Ψ is strictly convex, we see also that $\beta \to \int_V \Psi(\beta)\, dy$ is a strictly convex functional of β and is weakly-$*$ lower semicontinuous on subsets of L^1 that are weakly-$*$ compact. Consequently, the minimization problem

$$\inf_{\beta \in \mathcal{P}_a(V)} J_k(\beta) \tag{5.7}$$

has a unique solution β_{k+1}.

5.2 Time-step approximations for β. This subsection quickly reviews a time–discrete algorithm based on the Wasserstein distance, for solving

$$\begin{cases} \beta_t = \operatorname{div}\Big(\beta D[\Psi'(\beta)]\Big) \\ \beta(\cdot, 0) = \beta_0. \end{cases} \tag{5.8}$$

Let us now deal with the following nonlinear problem appearing in (5.5), where we replace β by β_{k+1}. We study the minimization problem

$$\inf_{\mathbf{v}} \{ \int_V |y - \mathbf{v}(y)|^2 dy \mid \beta_k = \beta_{k+1}(\mathbf{v}) \det D\mathbf{v} \} \tag{5.9}$$

which, thanks to the Monge-Kantorovich theory, is known to admit a unique minimizer $\mathbf{v}_{k+1}$ (see Brenier [B]). Furthermore, $\mathbf{v}_{k+1}$ is the gradient of a convex function $\psi_{k+1} : \bar{V} \to \mathbb{R}$, satisfying the Monge-Ampere problem

$$\beta_k = \beta_{k+1}(D\psi_{k+1}) \det D^2\psi_{k+1}, \quad D\psi_{k+1}(\bar{V}) = \bar{V}, \tag{5.10}$$

in the sense that

$$D\psi_{k+1} : \bar{V} \to \bar{V} \ a.e. \quad \text{and} \quad \int_V f(D\psi_{k+1})\beta_k\, dx = \int_V f\beta_{k+1}\, dy \tag{5.11}$$

for all $f \in C(\mathbb{R}^n)$. Equivalently, if ϕ_{k+1} is the Legendre transform of ψ_{k+1}, then

$$D\phi_{k+1} : \bar{V} \to \bar{V} \ a.e. \qquad \text{and} \quad \int_V g(D\phi_{k+1})\beta_{k+1}\, dy = \int_V g\beta_k\, dx, \tag{5.12}$$

for all $g \in C(\mathbb{R}^n)$. We write that

$$(D\psi_{k+1})_\# \beta_k = \beta_{k+1}, \quad (D\phi_{k+1})_\# \beta_{k+1} = \beta_k,$$

the symbol # denoting push-forward. Agueh [A] has shown that

$$C_1 \leq \beta_{k+1} \leq C_2, \tag{5.13}$$

provided

$$C_1 \leq \beta_k \leq C_2 \tag{5.14}$$

for constants $0 < C_1 \leq C_2$

The Euler Lagrange equations of (5.7) read

$$D\phi_{k+1}(y) = y + hD[\Psi'(\beta_{k+1}(y))], \tag{5.15}$$

and we conclude from (5.15) that

$$\beta_{k+1}(y) = (\Psi^*)'\Big((\phi_{k+1}(y) - \frac{|y|^2}{2})/h\Big) \tag{5.16}$$

where Ψ^* is the Legendre transform of Ψ.

Assume that $\beta_k \in C^{l,\alpha}(\bar{V})$ for some $\alpha > 0$ and some integer $l \geq 0$. By (5.16), $\beta_{k+1} \in W^{1,\infty}(V) \subset C^{0,\alpha}(\bar{V})$. Regularity theory for the Monge-Ampere equations ([C1], [C2],[C3],[C4]) and (5.10) imply that $\psi_{k+1}, \phi_{k+1} \in C^{2,\alpha}(\bar{V})$. This and (5.16) demonstrate that $\beta_{k+1} \in C^{2,\alpha}(\bar{V})$. Thus

$$\gamma_{k+1} := D\phi_{k+1} \circ D\phi_k \circ \cdots \circ D\phi_1 \in C^{l+1,\alpha}(\bar{V}, \bar{V}).$$

The map

$$\mathbf{u}_{k+1} = \gamma_{k+1} \circ \mathbf{u}_0$$

is then the unique solution to (5.2), and $\mathbf{u}_{k+1} \in C^{l+1,\alpha}(\bar{U}, \bar{V})$ if $\mathbf{u}_0 \in C^{l+1,\alpha}(\bar{U}, \bar{V})$.

We record next that the time step approximations converge as $h \to 0$:

Theorem 5.1 *For $h > 0$, inductively define β_{k+1} to be the unique minimizer of $J_k[\cdot]$ over $\mathcal{P}_a(V)$. Set*

$$\beta^h(y,t) = \begin{cases} \beta_0(y) & \text{if} \quad t = 0, \\ \beta_k(y) & \text{if} \quad t \in ((k-1)h, kh]. \end{cases}$$

Fix $T > 0$ and assume that $T = Mh$ for an integer $M > 0$.

Then

(i) *for each test function $\eta \in C_c^2$, we have*

$$\Big|\int_{V_T} \partial_t^h \eta (\beta^h - \beta_0)\, dxdt + \int_{V_T} \operatorname{div}\Big(\beta^h D[\Psi'(\beta^h)]\Big)\, dxdt\Big| \leq C_\eta h,$$

where $\partial_t^h \eta(x,t) = (\eta(x,t+h) - \eta(x,t))/h$ and $V_T = V \times (0,T)$.

(ii) *There exists a subsequence $\{h_m\}_{m=1}^\infty$ converging to 0 and $\beta \in L^1(V_T)$ such that $\{\beta^{h_m}\}_{m=1}^\infty$ converges to β. Furthermore, β satisfies the parabolic equation (5.8).*

5.3 Time-step approximations for u. Finally, we return to the approximation scheme (5.2), and consider the convergence problem as $h \to 0$.

We first record some uniform estimates:

Theorem 5.2 *Fix $h > 0$ and inductively define $\mathbf{u}_{k+1}$ to be the unique minimizer of $I_k[\cdot]$ over* $\mathrm{Diff}(\bar{U}, \bar{V})$. *Define*

$$\mathbf{u}^h(\cdot, t) = \begin{cases} \mathbf{u}_0(\cdot) & \text{if} \quad t = 0, \\ \mathbf{u}_k(\cdot) & \text{if} \quad t \in ((k-1)h, kh]. \end{cases}$$

Fix $T > 0$ and assume that $T = Mh$ for an integer $M > 0$. Set $U_T = U \times (0, T)$.

Then

(i) *For each $t \in [0, T]$ we have that $\mathbf{u}^h(\cdot, t) \in \mathrm{Diff}(\bar{U}, \bar{V}) \cap C^{l+1,\alpha}(\bar{U}, \mathbb{R}^n)$ and there are constants $C_1, C_2 > 0$ depending only on $\mathbf{u}_0$ such that*

$$C_1 \le \det D(\mathbf{u}^h)^{-1} \le C_2.$$

(ii) *There exists a constant $C > 0$, depending only on $\mathbf{u}_0$, such that*

$$\sum_{k=0}^{M-1} \int_U |\mathbf{u}_{k+1} - \mathbf{u}_k|^2 \, dx \le Ch.$$

(iii) *For each test function $\mathbf{v} \in C^2$, we have*

$$(5.17) \qquad |\int_{U_T} \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v} \, dxdt + \int_U \mathbf{u}_0 \cdot \mathbf{v}(\cdot, 0) \, dx| \le \frac{h}{2} C \sqrt{T} ||\mathbf{v}_t||_{L^\infty(U_T)}.$$

Proof. 1. Set $\beta_0 = \det D\mathbf{u}_0^{-1}$. Since $\mathbf{u}_0 \in \mathrm{Diff}(\bar{U}, \bar{V})$ we have that

$$0 < C_1 := \min_{\bar{V}} \beta_0, C_2 := \max_{\bar{V}} \beta_0 < +\infty.$$

According to the discussion above, we can choose inductively $\mathbf{u}_{k+1}$ to be the unique minimizer of I_k over $\mathrm{Diff}(\bar{U}, \bar{V})$.

2. The inequality $I_k(\mathbf{u}_{k+1}) \le I_k(\mathbf{u}_k)$ implies that

$$\sum_{k=0}^{M-1} I_k(\mathbf{u}_{k+1}) \le \sum_{k=0}^{M-1} I_k(\mathbf{u}_k).$$

Therefore

$$(5.18) \qquad \frac{1}{2} \sum_{k=0}^{M-1} \int_V |\mathbf{u}_{k+1} - \mathbf{u}_k|^2 dx \le h \int_U \Phi(\det D\mathbf{u}_0) - \Phi(\det D\mathbf{u}_M) dx \le 2h|U| \max_{[\frac{1}{C_2}, \frac{1}{C_1}]} |\Phi|.$$

This proves (ii).

3. Suppose now that $\mathbf{v} \in C^2$, and set $t_k = kh$, $\mathbf{v}_k = \mathbf{v}(\cdot, kh)$, and $U_k = U \times (t_k, t_{k+1})$. Then

$$\int_{U_T} \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v}\, dxdt = \sum_{k=0}^{M-1} \int_{U_k} \mathbf{u}_{k+1} \cdot \mathbf{v}_t \, dxdt - DF(D\mathbf{u}_{k+1}) : D\mathbf{v}\, dxdt.$$

We recall that $(\mathbf{u}_{k+1} - \mathbf{u}_k)/h = \operatorname{div}(DF(D\mathbf{u}_{k+1}))$, and continue to calculate that

$$\begin{aligned}
\int_{U_T} \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v}\, dxdt &= \sum_{k=0}^{M-1} \int_{U_k} \mathbf{u}_{k+1} \cdot \mathbf{v}_t + \left(\frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} \right) \cdot \mathbf{v}\, dxdt \\
&= \sum_{k=0}^{M-1} \int_U \mathbf{u}_{k+1} \cdot (\mathbf{v}_{k+1} - \mathbf{v}_k)\, dx \\
&\quad + \int_U (\mathbf{u}_{k+1} - \mathbf{u}_k) \cdot \mathbf{v}_k \, dx \\
&\quad + \sum_{k=0}^{M-1} \int_U \left(\frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} \right) \cdot \left(\int_{t_k}^{t_{k+1}} \mathbf{v} - \mathbf{v}_k \, dt \right) dx \\
&= \int_U \mathbf{u}_M \cdot \mathbf{v}_M - \mathbf{u}_0 \cdot \mathbf{v}_0 \, dx \\
&\quad + \sum_{k=0}^{M-1} \int_U \left(\frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} \right) \cdot \left(\int_{t_k}^{t_{k+1}} \mathbf{v} - \mathbf{v}_k \, dt \right) dx.
\end{aligned}$$

Taking into account $\mathbf{v}_M = \mathbf{v}(T) = 0$ and

$$\left| \int_{t_k}^{t_{k+1}} \mathbf{v} - \mathbf{v}_k \, dt \right| \le \frac{h^2}{2} \max_{U_T} |\mathbf{v}_t|,$$

we conclude that

$$\begin{aligned}
&\left| \int_{U_T} \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v}\, dxdt + \int_U \mathbf{u}_0 \cdot \mathbf{v}(\cdot, 0)\, dx \right| \\
&\quad \le \frac{h}{2} ||\mathbf{v}_t||_{L^\infty} \sum_{k=0}^{M-1} \int_U |\mathbf{u}_{k+1} - \mathbf{u}_k| \, dx \\
&\quad \le \frac{h}{2} ||\mathbf{v}_t||_{L^\infty(U_T)} \left(\sum_{k=0}^{M-1} \int_U |\mathbf{u}_{k+1} - \mathbf{u}_k|^2 \, dx \right)^{\frac{1}{2}} M^{\frac{1}{2}}. \qquad (5.19)
\end{aligned}$$

We combine (5.18) and (5.19) to finish up the proof of (iii). □

This theorem provides some uniform estimates, but it remains an unsolved problem to show that as $h \to 0$, the approximation $\mathbf{u}^h$ converges somehow to a solution $\mathbf{u}$ of (1.3). One particular issue is that we do not know if the gradients $D\mathbf{u}^h$ converge strongly in L^2.

Our belief is that although the scheme (5.2), (5.3) and (5.4) is obviously extremely natural, we do not currently know how fully to exploit the minimization structure. We have here a problem in the "time-dependent calculus of variations"; but we do not have enough experience to understand, for instance, the proper choices of comparison functions to employ in our variational principles. The direct PDE and ODE methods in Sections 2 and 3 provide a way around this difficulty for the special case of the nonlinearity (1.6).

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