

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

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

defined for functions $\mathbf{v} : U \rightarrow \mathbb{R}^m$, 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 $F : \mathbb{M}^{m \times n} \rightarrow (-\infty, +\infty]$.

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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. [M]. This is the condition that

$$(1.2) \quad \int_U F(A) dx \leq \int_U F(A + D\mathbf{v}) dx$$

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

Dynamics. As 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

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

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

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

given \mathbf{u}_k . The Euler-Lagrange equations read

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

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 $h \rightarrow 0$. 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 . We

will discuss these matters more in §5. (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

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

where Φ is a convex function and “det” means determinant. Such a nonlinearity is quasi-convex, 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].

Let us start by reviewing the problem of minimizing the functional

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

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

$$D\mathbf{v} = \begin{pmatrix} v_{x_1}^1 & \cdots & v_{x_n}^1 \\ \vdots & \ddots & \vdots \\ v_{x_1}^n & \cdots & v_{x_n}^n \end{pmatrix}.$$

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

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

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

$$(1.9) \quad \frac{\partial \det P}{\partial p_i^k} = (\operatorname{cof} P)_i^k \quad (1 \leq i, k \leq n).$$

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

$$(1.10) \quad (\operatorname{cof} P)^T P = I \det P.$$

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

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

that is,

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

Therefore (1.8) implies

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

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 the Euler-Lagrange system (1.8) greatly simplifies, to become

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

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

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

plus appropriate initial and boundary conditions, detailed later. We hope that just as (1.8) lead to (1.13) for the static problem, so also (1.14) somehow simplifies.

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

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

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 §1.2, 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

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

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

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

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 $\beta \rightarrow 0$ 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 mapping \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 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.

The concluding Section 5 explains more about the time stepping variational principle (1.4) and (1.5). 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

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

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

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

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

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

to give

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

Set

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

2.2 A partial differential equation for β . Our main observation is that β solves a scalar, nonlinear diffusion equation:

Theorem 2.1 *We have*

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

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

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

$$(2.5) \quad \zeta(\cdot, 0) \equiv \zeta(\cdot, T) \equiv 0.$$

Then employing (2.1), we compute

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

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

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

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

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

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

$$\frac{\partial}{\partial \nu} \left(\Phi' \left(\frac{1}{\beta} \right) \right) = -\Phi'' \left(\frac{1}{\beta} \right) \frac{1}{\beta^2} \frac{\partial \beta}{\partial \nu} \equiv 0 \quad \text{on} \quad \partial V \times (0, T).$$

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

2.3 Recovering the mapping \mathbf{u} from β . 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

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

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

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

Then

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

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

Next, perform these calculations:

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

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

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

where $\dot{\cdot} = \frac{d}{dt}$. 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

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

of our system

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

under some additional assumptions.

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

$$(4.2) \quad \beta^0 := \det D\mathbf{v}^0$$

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

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

We ask also that this *compatibility condition* hold:

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

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

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

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

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

has a unique, smooth solution β , with

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

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

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

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 $\mathbf{y} : [0, \infty) \rightarrow \bar{V}$, 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*

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

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

$$(3.6) \quad \beta \equiv \det D\mathbf{v}.$$

(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

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

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

$$(3.8) \quad \alpha_t = -\alpha \Delta_y \Psi'(\beta).$$

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

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

Finally let us calculate:

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

□

4 Some variants

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

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

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

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

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

which simplifies to read

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

As in Section 1.1 this implies that

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

for some constant C .

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

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

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*

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

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

Then

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

But according to (4.3), we have

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

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

4.2 “Filling up” the target domain. We mention next an interesting variant of our construction. Select $\mathbf{u}^0 : \bar{U} \rightarrow \bar{W}_0$ be a diffeomorphism, where the smooth open set $W_0 \subset\subset V$ is given

Our goal is to find Φ and \mathbf{u} so that the sets

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

expand, “filling 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 (1.16) becomes the porous medium equation

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

So we turn attention to the initial/boundary–value problem:

$$(4.8) \quad \begin{cases} \beta_t = \Delta(\beta^{m+1}) & \text{in } V \times (0, \infty) \\ \frac{\partial \beta}{\partial \nu} = 0 & \text{on } \partial V \times (0, \infty) \\ \beta = \beta^0 & \text{on } V \times \{t = 0\}. \end{cases}$$

The support of the initial data β^0 is the set \bar{W}_0 .

We write $W(t)$ to denote the interior of the support of $\beta(\cdot, t)$ for times $t \geq 0$. According to standard theory for the porous medium equation, the sets $\{W(t)\}_{t \geq 0}$ are increasing and $W(t) \equiv V$ for $t \geq T$, for a first time T when the sets “fill up” the target V . The solution β is smooth in the interior of its support, and is continuous on $V \times [0, \infty)$.

By solving as before the ODE (3.4), we should in principle be able to construct a family of diffeomorphisms $\mathbf{u}(\cdot, t) : \bar{U} \rightarrow \bar{W}(t)$ for times $t \geq 0$, the images of which fill up V at $t = T$. Since however β is not smooth across $\partial W(t)$ for times $0 \leq t < T$, we are not able to make these interpretations precise.

Numerical simulations would be interesting here, especially for the case that U and V are not diffeomorphic.

5 Time step minimization, optimal mass transfer

As noted in §1, the time step minimization process (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 both the connections with Monge–Kantorovich mass transfer theory and the difficulties of proving convergence. These comments are meant also to underscore the advantages of our differential equations methods in §2–4.

We are primarily motivated by Otto [O] and Jordan–Kinderlehrer–Otto [J-K-O]. The novelty of Otto’s paper [O] was to interpret (1.16) 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 for β . Assume for this section that that U and V are two bounded, open, *convex* sets with smooth boundaries. Fix a time step size $h > 0$. We recall from §1 the implicit scheme of recursively finding \mathbf{u}_{k+1} to solve

$$(5.1) \quad \begin{cases} \frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} = \operatorname{div}(DF(D\mathbf{u}_{k+1})) \\ \mathbf{u}_{k+1} \in \operatorname{Diff}(\bar{U}, \bar{V}), \end{cases}$$

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

$$(5.2) \quad I_k[\mathbf{v}] := \frac{1}{2} \int_U |\mathbf{v} - \mathbf{u}_k|^2 dx + h \int_U F(D\mathbf{v}) dx.$$

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

$$(5.3) \quad \min_{\mathbf{v}} \{I_k[\mathbf{v}] \mid \mathbf{v} \in \operatorname{Diff}(\bar{U}, \bar{V})\}.$$

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 variables $y = \mathbf{v}(x)$ and set $\beta := \det(D\mathbf{v}^{-1})$, $\beta_k := \det(D\mathbf{u}_k^{-1})$, 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

$$\begin{aligned} & \min_{\mathbf{v} \in \text{Diff}(\bar{U}, \bar{V})} I_k[\mathbf{v}] \\ (5.4) \quad &= \inf_{\beta} \left\{ h \int_V \Psi(\beta) dy + \inf_{\mathbf{v}} \left\{ \frac{1}{2} \int_V |y - \mathbf{u}_k(\mathbf{v}^{-1}(y))|^2 dy \mid \beta = \det(D\mathbf{v}^{-1}) \right\} \right\} \\ &= \inf_{\beta} \left\{ h \int_V \Psi(\beta) dy + \inf_{\mathbf{w}} \left\{ \frac{1}{2} \int_V |y - \mathbf{w}(y)|^2 dy \mid \beta_k = \beta(\mathbf{w}) \det D\mathbf{w} \right\} \right\} \\ &= \inf_{\beta} \left\{ h \int_V \Psi(\beta) dy + W_2^2(\beta_k, \beta) \right\}, \end{aligned}$$

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 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 (5.4) to minimization problems over $\mathcal{P}_a(V)$, the set of probability densities supported in V .

Define the new functional

$$(5.5) \quad J_k(\beta) := W_2^2(\beta_k, \beta) + h \int_V \Psi(\beta) dy.$$

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

$$(5.6) \quad \inf_{\beta \in \mathcal{P}_a(V)} J_k(\beta)$$

has a unique solution β_{k+1} .

5.2 Time-step approximations for \mathbf{u} . Next we discuss how to build \mathbf{u}_{k+1} , given β_{k+1} . We study the minimization problem

$$(5.7) \quad \inf_{\mathbf{v}} \left\{ \int_V |y - \mathbf{v}(y)|^2 dy \mid \beta_k = \beta_{k+1}(\mathbf{v}) \det D\mathbf{v} \right\}$$

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 $\psi_{k+1} : \bar{V} \rightarrow \mathbb{R}$, satisfying the Monge-Ampere problem

$$(5.8) \quad \beta_k = \beta_{k+1}(D\psi_{k+1}) \det D^2\psi_{k+1}, \quad D\psi_{k+1}(\bar{V}) = \bar{V},$$

in the sense that

$$(5.9) \quad D\psi_{k+1} : \bar{V} \rightarrow \bar{V} \text{ a.e.} \quad \text{and} \quad \int_V f(D\psi_{k+1})\beta_k dx = \int_V f\beta_{k+1} dy$$

for all $f \in C(\mathbb{R}^n)$.

Agueh [A] and Otto [O] have shown that

$$(5.10) \quad C_1 \leq \beta_{k+1} \leq C_2,$$

provided

$$(5.11) \quad C_1 \leq \beta_k \leq C_2$$

for constants $0 < C_1 \leq C_2$

Let ϕ_{k+1} denote the Legendre transform of ψ_{k+1} . The Euler Lagrange equations of (5.6) turn out to read

$$(5.12) \quad D\phi_{k+1}(y) = y + hD[\Psi'(\beta_{k+1}(y))],$$

and we conclude from (5.12) that

$$(5.13) \quad \beta_{k+1}(y) = (\Psi^*)' \left((\phi_{k+1}(y) - \frac{|y|^2}{2})/h \right),$$

where Ψ^* is the Legendre transform of Ψ .

Assume that $\beta_k \in C^{l,\alpha}(\bar{V})$ for some $0 < \alpha < 1$ and some integer $l \geq 0$. Then (5.8) and the deep regularity theory of Caffarelli and Urbas for the Monge-Ampere equations (see, for instance, [C1], [C2],[C3],[C4]) imply that $\psi_{k+1}, \phi_{k+1} \in C^{l+2,\alpha}(\bar{V})$. This and (5.13) demonstrate that $\beta_{k+1} \in C^{l,\alpha}(\bar{V})$. Also

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

The map

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

is then the unique solution to (5.1), and $\mathbf{u}_{k+1} \in C^{l+1,\alpha}(\bar{U}, \bar{V})$ if $\mathbf{u}_0 \in C^{l+1,\alpha}(\bar{U}, \bar{V})$.

5.3 Estimates, convergence? Finally, we consider the convergence problem as $h \rightarrow 0$. We record first some uniform estimates:

Lemma 5.1 *Fix $h > 0$ and inductively define \mathbf{u}_{k+1} to be the unique minimizer of $I_k[\cdot]$ over $\text{Diff}(\bar{U}, \bar{V})$. Define*

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

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

(i) *There are constants $C_1, C_2 > 0$, depending only on \mathbf{u}_0 , such that*

$$C_1 \leq \det D(\mathbf{u}^h(\cdot, t))^{-1} \leq C_2.$$

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

$$(5.14) \quad \sum_{k=0}^{M-1} \int_U |\mathbf{u}_{k+1} - \mathbf{u}_k|^2 dx \leq Ch.$$

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

$$(5.15) \quad \left| \int_0^T \int_U \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v} dx dt + \int_U \mathbf{u}_0 \cdot \mathbf{v}(\cdot, 0) dx \right| = O(h) \quad \text{as } h \rightarrow 0.$$

Proof. 1. Assertion (i) follows from the remarks above. The inequality $I_k(\mathbf{u}_{k+1}) \leq I_k(\mathbf{u}_k)$ implies that

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

Therefore

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

2. 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

$$\int_0^T \int_U \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v} dx dt = \sum_{k=0}^{M-1} \int_{U_k} \mathbf{u}_{k+1} \cdot \mathbf{v}_t dx - DF(D\mathbf{u}_{k+1}) : D\mathbf{v} dx.$$

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

$$\begin{aligned}
\int_0^T \int_U \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v} \, dx dt &= \sum_{k=0}^{M-1} \int_{U_k} \mathbf{u}_{k+1} \cdot \mathbf{v}_t + \left(\frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} \right) \cdot \mathbf{v} \, dx dt \\
&= \sum_{k=0}^{M-1} \int_U \mathbf{u}_{k+1} \cdot (\mathbf{v}_{k+1} - \mathbf{v}_k) \, dx \\
&\quad + \int_U (\mathbf{u}_{k+1} - \mathbf{u}_k) \cdot \mathbf{v}_k \, dx \\
&\quad + \sum_{k=0}^{M-1} \int_U \left(\frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} \right) \cdot \left(\int_{t_k}^{t_{k+1}} \mathbf{v} - \mathbf{v}_k \, dt \right) \, dx \\
&= \int_U \mathbf{u}_M \cdot \mathbf{v}_M - \mathbf{u}_0 \cdot \mathbf{v}_0 \, dx \\
&\quad + \sum_{k=0}^{M-1} \int_U \left(\frac{\mathbf{u}_{k+1} - \mathbf{u}_k}{h} \right) \cdot \left(\int_{t_k}^{t_{k+1}} \mathbf{v} - \mathbf{v}_k \, dt \right) \, dx.
\end{aligned}$$

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

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

we conclude that

$$\begin{aligned}
&\left| \int_0^T \int_U \mathbf{u}^h \cdot \mathbf{v}_t - DF(D\mathbf{u}^h) : D\mathbf{v} \, dx dt + \int_U \mathbf{u}_0 \cdot \mathbf{v}(\cdot, 0) \, dx \right| \\
&\leq Ch \sum_{k=0}^{M-1} \int_U |\mathbf{u}_{k+1} - \mathbf{u}_k| \, dx \\
&\leq Ch \left(\sum_{k=0}^{M-1} \int_U |\mathbf{u}_{k+1} - \mathbf{u}_k|^2 \, dx \right)^{\frac{1}{2}} M^{\frac{1}{2}}.
\end{aligned}$$

We combine (5.14) and (5.16) to finish up the proof of (iii). \square

5.4 Evaluation. This lemma provides some uniform estimates, but it remains an unsolved problem to exploit (5.15) to show that as $h \rightarrow 0$, 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 (5.1), (5.2) and (5.3) 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 §2–4 provide a way around this difficulty for the special case of the nonlinearity (1.6).

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