



UNIVERSITÀ DEGLI STUDI DI PADOVA

Dipartimento di Fisica e Astronomia “Galileo  
Galilei”

Corso di Laurea in Fisica

Tesi di Laurea

Cosmological applications of Optimal Mass  
Transport

Applicazioni cosmologiche del Trasporto Ottimale  
di Massa

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Anno Accademico 2022/2023



## **Abstract**

La presente tesi si pone l'obiettivo di fornire una descrizione coesa, per quanto limitata a poche pagine e agli aspetti ritenuti essenziali dell'argomento, delle applicazioni della teoria del trasporto ottimale di massa, sviluppate negli scorsi decenni, al problema della ricostruzione della dinamica dell'Universo primordiale (EUR).

L'intuizione che fa da perno alla trattazione consiste nell'impiego dell'equazione di Monge-Ampère, la quale nella sua prima formulazione risale al 1781, per la costruzione di algoritmi efficaci per la computazione di soluzioni uniche del problema di Ricostruzione.

Oltre ad una breve contestualizzazione di carattere storico si è ritenuto opportuno richiamare alcuni risultati strettamente matematici per i quali si fa riferimento a [8]. Le sezioni centrali sono dedicate ad una breve discussione del modello di Monge-Ampère-Kantorovich (MAK) e del modello gravitazionale di Monge-Ampère (MAG). Quest'ultimo, proposto dal matematico Yann Brenier [9], sfrutta il principio di minima azione e la teoria del flusso di gradiente con potenziali convessi per realizzare un algoritmo uni-dimensionale e discreto, atto a ricostruire le soluzioni cercate.



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# 1 Introduction

Are we able to successfully rewind the dynamical history of the Universe we observe today and deterministically reconstruct the evolution, starting from its very early stages, of Universe's mass distribution at present time?

Cosmological reconstruction can be approached *directly* by assuming a certain model about primordial fluctuations, then compare the statistical properties expected for the present Universe with the observations.

On the other hand, reconstruction can be formulated as an *inverse problem*: reproduce and model as much as possible of the past dynamical history starting exactly where we are, from a sufficiently detailed map of the mass distribution we are able to observe today.

Over the past decades several great cosmologists and mathematicians have been addressing the issue in many different ways, in an effort to unravel this hidden mystery of our physical world.

It was first P.J.E. Peebles in July 1989 [1] to pave the way for this fascinating challenge of modern cosmology.

As he opens the introduction to his paper:

*"In the gravitational instability picture, the clumpy galaxy distribution grew by gravity out of smoother initial conditions. We can test this by comparing the motions needed to produce the clustering with observations of nearby galaxies, [...] I present a method of predicting velocities given present positions by adjusting trial orbits to minimize the action. As the action usually is applied the orbits have fixed initial and final positions, but the true orbits also minimize the action if the initial velocity vanishes."*

The major intuition in his words is that, assuming that galaxies trace the mass distribution, the latter depending on minor departures from primordial homogeneity, then galaxy orbits can be successfully estimated by adjusting them to make the action stationary.<sup>1</sup>

The action considered by Peebles is expressed for the  $i$ -th particle in co-moving coordinates  $\mathbf{x}_i(t)$  as

$$S = \int_0^{t_0} dt \left[ \sum \frac{m_i a^2}{2} \left( \frac{d\mathbf{x}_i}{dt} \right)^2 + \frac{G}{a} \sum_{i \neq j} \frac{m_i m_j}{|\mathbf{x}_i - \mathbf{x}_j|} + \frac{2}{3} \pi G \rho_b a^2 \sum m_i \mathbf{x}_i^2 \right]$$

---

<sup>1</sup>In the standard cosmological paradigm, the present distribution of galaxies and their peculiar motions result from gravitational amplification of small fluctuations in the initial density field.

The boundary conditions<sup>2</sup>

$$\delta \mathbf{x}_i = 0 \quad \text{at } t = t_0 \quad a^2 \frac{d\mathbf{x}_i}{dt} \rightarrow 0 \quad \text{at } a \rightarrow 0$$

are to satisfy by a least action solution in order to minimize  $S$ .

Feedbacks were sought experimentally in the studying of the peculiar velocities of the dwarf members of the Local Group. The group was assumed to be grown out of accretion of originally pressureless and smoothly distributed matter into seed masses at the Milky Way and Andromeda Nebula.

The following plot is displayed in Peebles' publication from 1990[2]:

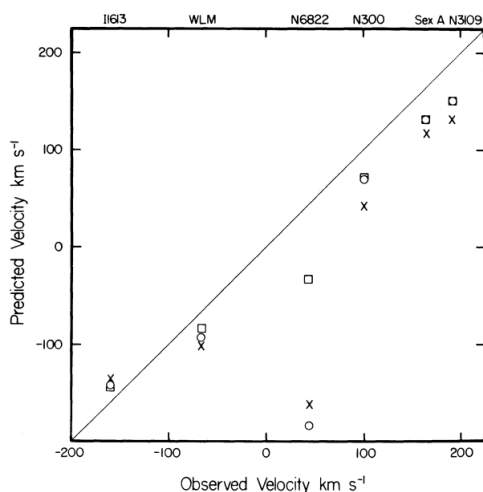


FIG. 5.—Predicted and observed velocities of outer members of the Local Group. (Open circles) the low-density solution that minimizes the action; (open squares) the standard solution with N6822 in a crossing orbit; (crosses) Einstein-de Sitter model.

Since Peebles' first papers many others have made the attempt to formulate effective methods for action minimization. As a matter of fact, most of the promising approaches to the problem are based on the least action principle.

In 1999 A. Nusser and E. Branchini [3] proposed a model named FAM, which stands for *Fast Action Minimization*, based on the use of the conjugate gradient method in order to locate the extremum of the action.

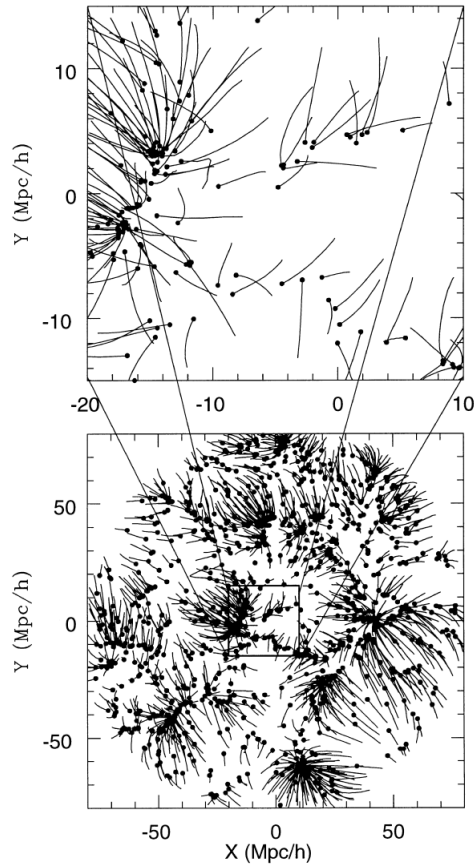
FAM is able to reconstruct the flow field down to cluster scales<sup>3</sup> and thus recover both the present peculiar velocities of mass particles and the initial fluctuations field.

<sup>2</sup>  $a(t)$  is the expansion parameter and its present value is  $a_0 = a(t_0) = 1$ .

<sup>3</sup> At those scales deviations from the Zel'dovich solution become significant.



The  $N$ -body simulation using FAM successfully retraces the orbits of a limited distribution of particles in real space, lessening the effects of the so-called *multivalued zones*, redshift distortions coming from galaxy surveys.



**Figure 1.** Recovered orbits from the FAM. Filled dots show present time positions for a random selection of  $N$ -body particles contained within a slice of thickness  $10 h^{-1}$  Mpc. The solid lines represent their projected orbits. The upper plot is an enlargement of the central region in the lower plot.

In the early 2000' a *Monge-Ampère-Kantorovich*<sup>4</sup> (MAK) kind of reconstruction was introduced [6], taking a new direction: the model re-established the problem as an assignment problem in optimization theory.

<sup>4</sup>The reason behind the name will be more clear in the next sections.

MAK is built starting from mass conservation, under the following assumptions:

- (i) the final positions of the particles are known;
- (ii) the initial distribution is homogeneous;
- (iii) the Lagrangian map ( $\mathbf{q} \rightarrow \mathbf{x}$ ) is the gradient of a convex potential<sup>5</sup>.

These assumptions imply that the inverse map also has a convex potential representation, related to the previous one by the corresponding Legendre-Fenchel transform.

By combining the expression for the inverse map with mass conservation one would obtain the Monge-Ampère equation (see section 2.4).

The solution to this well-known equation provides a unique solution to an optimization problem: while previous approaches rendered non-unique solutions MAK shows that the initial positions of dark matter fluid elements, under the hypothesis that their displacement is the gradient of a convex potential, can be reconstructed *uniquely*.

In the following work an attempt will be made to provide an insight into the problem of the Reconstruction of the early Universe dynamics (EUR).

Section 2 will be spent to deliver some of the main mathematical results that contribute to the abstract framework describing the EUR problem in a rather rigorous way.

Section 3 will be an overview of the Monge-Ampère gravitational model, mainly developed by the french mathematician Yann Brenier, aiming, once again, to answer to the great question this introduction was opened with.

## 2 the Reconstruction problem

The evolution of the present non-uniform distribution of mass in the Universe can be traced back to minor primordial fluctuations<sup>6</sup> and successfully modelled as the motion of a self-gravitating continuum of cold dark matter described by the Euler-Poisson system.

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<sup>5</sup>The convexity condition guarantees that there is no multistreaming and will be further discussed in the next sections.

<sup>6</sup>It is widely accepted that the primeval perturbations originated at the inflationary stage.

In its non relativistic form:

$$\begin{aligned}
\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) &= 0 \\
\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) &= -\rho \nabla \phi_g \\
\nabla_{\mathbf{x}}^2 \phi_g &= \rho
\end{aligned} \tag{1}$$

where  $\mathbf{v} = v(t, \mathbf{x}) \in \mathbb{R}^3$  indicates the velocity vector-field,  $\rho$  indicates the density field and  $\phi_g = \phi_g(t, \mathbf{x})$  is the gravitational scalar-potential.

The product  $\rho \mathbf{v}$  will be later defined as the flux of matter.

Performing the correct adjustments in order to take into account the expanding motion for the Einstein-De Sitter Universe, system (1) can be expressed in the appropriate co-moving coordinates, as it follows:

$$\begin{aligned}
\partial_\tau \rho + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) &= 0 \\
\partial_\tau \mathbf{v} + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{v} &= -\left(\frac{3}{2\tau}\right)(\mathbf{v} + \nabla_{\mathbf{x}} \phi_g) \\
\nabla_{\mathbf{x}}^2 \phi_g &= \frac{\rho - 1}{\tau}
\end{aligned} \tag{2}$$

The Poisson equation is formulated in accordance with the condition of normalization given by

$$\int_{\mathbb{T}^d} \rho(\cdot, x) dx = 1$$

calculated for simplicity over the flat torus  $\mathbb{T}^d = \mathbb{R}^d / \mathbb{Z}^d$ .

The assumption of a particular constraint, named *slaving*, seems to be not only necessary in an effort to remove the singularity at  $\tau \rightarrow 0$  but also sufficient to render the problem well-posed:

$$\mathbf{v}_{in}(\mathbf{x}) + \nabla_{\mathbf{x}} \phi_g^{in} = 0 \quad \rho_{in} = 1$$

meaning that the reconstructed solution of the Euler-Poisson system has an initial velocity field equal to the gradient of the initial gravitational potential, while the initial density field must be rigorously uniform.

Under the hypothesis of collisionless matter, slaving also ensures that no multistreaming occurs, furtherly justifying the use of the Euler-Poisson equations.<sup>7</sup>

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<sup>7</sup>Otherwise the dynamics would be better described by the Vlasov-Poisson system.

As mentioned in [5], the slaving condition suggests the absence of *decaying mode*, as opposite to *growing mode*, which is assumed instead, since the time variable used in the previous and following equations is actually the *amplitude factor*  $\tau$ <sup>8</sup> of the growing mode.

The Reconstruction problem of the early dynamics of the Universe defined in (2) is now presented as the challenge of reconstructing a unique solution to this Hamiltonian system and, as a consequence, can be addressed with variational techniques.

Solutions to Hamiltonian systems are critical points for the action of the Lagrangian function

$$I = \frac{1}{2} \int_{[0,T]} dt \int_D \rho(t, dx) |\mathbf{v}(t, x)|^2 + |\nabla \phi_g(t, x)|^2 dx \quad (3)$$

Since the action is a convex functional in the variables  $(\rho, \rho \mathbf{v}, \phi_g)$  the critical point needs to be specifically a minimizer.

By performing the minimization of the action one will thus be able to find a solution in terms of an optimal transportation problem.

## 2.1 General formulation

Some crucial results, proved and widely discussed by G. Loeper [8], contributed to shaping the EUR problem within the Euler-Poisson dynamical frame into a mathematically rigorous one.

By introducing the domain  $D = [0, T] \times \mathbb{T}^d$ , given  $J = \rho \mathbf{v} \in \mathbb{R}^d$  and  $\rho \in \mathbb{R}^+$ , the functional  $I$  can be written as

$$\begin{aligned} \tilde{I}(\rho, J, \phi) = \sup_{c+m^2/2 \leq 0} & \left\{ \int_D c(t, x) d\rho(t, x) + m(t, x) \cdot dJ(t, x) \right\} + \\ & + \frac{1}{2} \int_D |\nabla \phi(t, x)|^2 dt dx \end{aligned} \quad (4)$$

where the supremum is taken over all  $(c, m) \in C(D) \times (C(D))^d$  with  $c \in \mathbb{R}$  and  $m \in \mathbb{R}^d$ . One can prove that (3) and (4) are the same functionals over  $] -\infty, +\infty[$ , with  $\rho$  being a measure on  $D$ ,  $\mathbf{v}$  being a  $d\rho$  measurable vector field and  $\phi$  a proper  $d\rho$  measurable function.

---

<sup>8</sup> $\tau$  is proportional to  $t^2/3$  in the Einstein-de Sitter universe.

It is possible to provide a variational formulation<sup>9</sup> of the EUR problem by combining the Euler-Poisson system defined in (2) and equation (4):

Minimize the action

$$I = \frac{1}{2} \int_0^T \int_{\mathbb{T}^d} \tau^{3/2} \left( |\mathbf{v}(\tau, x)|^2 d\rho(\tau, x) + |\nabla\phi(\tau, x)|^2 dx d\tau \right)$$

among all triples  $(\rho, J, \phi)$  that satisfy  $\rho \in C([0, T]; \mathcal{P}(\mathbb{T}^d) - w*)$ ,  $J \in (\mathcal{M}(D))^d$  and  $\nabla\phi \in L^2(D)$ , under the constraints

$$\rho(\tau = 0) = 1 \qquad \rho(\tau = T) = \rho_T$$

and those given by (2).

$\mathcal{P}(\mathbb{T}(D))$  is the set of probability measures on  $\mathbb{T}(D)$  and  $\mathcal{M}(D)$  indicates the set of bounded measures on the prescribed domain.

In addition to an *existence and uniqueness* theorem, as reported below, a *regularity* result was accomplished for the minimizer of the action  $\tilde{I}$  in (4).

**Theorem 1** *Existence & uniqueness*

Let  $\rho_0$  and  $\rho_T$  be two probability measures in  $L^{\frac{2d}{d+2}}(\mathbb{T}^d)$ .

There exists a unique triple  $(\rho, \rho\mathbf{v}, \phi) \in (\mathcal{M}(D)) \times (\mathcal{M}(D))^d \times L^2([0, T]; H^1(\mathbb{T}))$ , with  $\Delta\phi = \rho - 1$ , that minimizes the *E-P* problem.

$(\rho, \mathbf{v}, \phi)$  is then a *weak solution*<sup>a</sup> of the Euler Poisson system and it is unique. Moreover

1. there exists  $\psi \in L^2_{loc}([0, T]; H^1(\mathbb{T}^d)) \cap L^\infty_{loc}([0, T] \times \mathbb{T}^d)$  such that  $\mathbf{v} = \nabla\psi d\rho$ .
2. any such extension satisfies

$$\int_{\mathbb{T}^d} \int_\tau^{T-\tau} |\mathbf{v}(t, x+y) - \mathbf{v}(t, x)|^2 d\rho(t, x) \leq C_\tau |y|^2$$

for all  $\tau \in ]0, T/2]$  and  $y \in \mathbb{R}^d$ .

3.  $\rho$  belongs to  $L^2_{loc}([0, T] \times \mathbb{T}^d) \cap C([0, T]; L^p)$  for any  $p \in [1, 3/2]$ .

---

<sup>a</sup>See **Appendix**.

<sup>9</sup>It will be referred to as the *E-P* problem from now on.

**Theorem 2** *Regularity*

If  $\rho_0$  and  $\rho_T$  are in  $L^{\frac{2d}{d+2}}$ , the unique solution  $(\rho, J, \phi)$  of the E-P problem has the following regularity properties:

1. The density  $\rho$  is in  $L_{loc}^\infty(]0, T[ \times \mathbb{T}^d) \cap C(]0, T[; L^k(\mathbb{T}^d))$  for every  $1 \leq k < \infty$ .

For every  $\tau \in ]0, T/2[$  there exists  $C_\tau$  such that for every  $t \in [\tau, T - \tau]$

$$\|\rho(t, \cdot)\|_{L^\infty(\mathbb{T}^d)} \leq C_\tau$$

and  $C$  such that

$$-C\left(1 + \frac{1}{t}\right) \leq \frac{d}{dt} \log(\|\rho(t, \cdot)\|_{L^k(\mathbb{T}^d)}) \leq C\left(1 + \frac{1}{T-t}\right)$$

Note that constants  $C_\tau$  and  $C$  do not depend on the choice one would make for  $\rho_0$  and  $\rho_T$ .

2. The velocity  $\mathbf{v} = \nabla\psi$  can be taken in  $L_{loc}^\infty(]0, T[ \times \mathbb{T}^d)$  and it is again not dependent on the choice one would make for  $\rho_0$  and  $\rho_T$ .
3. The functions

$$\int_{\mathbb{T}^d} [\rho]^k(t, x) dx \quad k \geq 1 \quad \int_{\mathbb{T}^d} [\rho \log \rho](t, x) dx$$

are convex with respect to the time variable.

4. The velocity potential  $\psi$  can be taken in  $W_{loc}^{1, \infty}(]0, T[ \times \mathbb{T}^d)$  to be a viscosity solution of equation

$$\partial_t \psi + \frac{1}{2} |\nabla \psi|^2 + \phi = 0$$

on every  $[s, t] \subset ]0, T[$ .

5. If  $\rho_T$  is in  $L^p(\mathbb{T}^d)$ ,  $p > d$ , then the previous condition can be extended up to  $t = T$ .

6. One can take  $\psi$  such that  $(\xi, \mathbf{q})(t, \mathbf{x}) = (-\psi, \phi)(T - t, \mathbf{x})$  is a viscosity solution of equation

$$\partial_t \xi + \frac{1}{2} |\nabla \xi|^2 + q = 0$$

on every  $[s, t] \subset ]0, T[$ .

7. For each  $t \in ]0, T[$  there exists a closed set  $S_t$  of full measure for  $\rho(t)$  such that  $\psi(t)$  is differentiable with respect to the space variable at every point of  $S_t$ .

For all  $t \in [\tau, T - \tau]$ ,  $\tau > 0$ , and all  $(x, y) \in S_t$  with  $|x - y| \leq \frac{1}{2}$

$$|\nabla \psi(t, x) - \nabla \psi(t, y)| \leq C(\tau) |x - y| \log \left( \frac{1}{|x - y|} \right).$$

Both existence and uniqueness of a minimizer of the action are so formulated, as a proposition, under the above mentioned constraints of the  $E$ - $P$  problem.

**Proposition** Under the assumption that  $\rho_0$  and  $\rho_T$  are in  $L^{\frac{2d}{d+2}}$ , there exists a unique minimizer  $(\rho, J, \nabla \phi) \in C([0, T]; \mathcal{P}(\mathbb{T}^d) - w^*) \times L^2(D)$  for the  $E$ - $P$  problem.

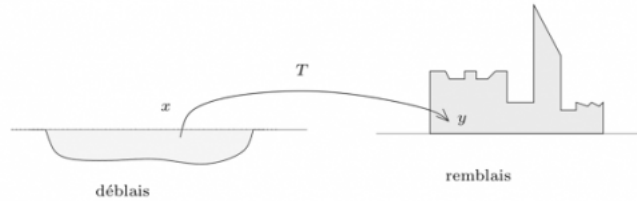
The proof of this result leads into mass transport theory, with the implementation of Kantorovich duality.

## 2.2 Mass transport theory

### 2.2.1 To the origins of the problem

The mass transportation problem, first formulated by Gaspard Monge in 1781 in a paper entitled *Théorie des déblais et des remblais*, is to search the optimal way, as the one that minimizes the cost, to move one given distribution of mass in the Euclidean space  $\mathbb{R}^3$  into a target distribution.

Monge's original criterion to do so as efficiently as possible was to minimize the average distance of transportation.



What is the optimal way of moving soil into building a fortress?

The elementary work to move a *mass molecule*  $x$  into  $T(x)$  is given by  $|x - T(x)|$ , so that the total work is

$$\int_{\text{déblais}} |x - T(x)| dx$$

Monge's query is then to find the minimum work over an admissible transport map  $T$ , i.e. a map that maps *déblais* into *remblais*.

It is convenient to consider the topic within the framework of metric spaces:

- $(X, d)$  is a metric space;
- $f^+, f^-$  are two probabilities on  $X$ , corresponding respectively to *déblais* and *remblais*;
- $T$  is an admissible transport map if  $T\#f^+ = f^-$ .

Consequently, Monge's problem takes the form

$$\min \left\{ \int_X d(x, T(x)) dx, T \text{ admissible} \right\}$$

and does not admit a solution in general when  $f^+, f^-$  are singular, since in that case the class of admissible transport maps could be empty.

In 1942 the mathematician and economist Leonid Kantorovich provided a generalization of the problem, actually solvable in more than one dimension, by allowing the mass distribution to *split* in the product space, where more than one position in the fills -*remblais*- could be associated with a position in the cuts -*déblais*-<sup>10</sup>.

Kantorovich developed the groundbreaking techniques of duality in optimization theory and linear programming, which were successfully employed in the resolution of this *relaxed* version of the problem.

<sup>10</sup>In other words, he *allowed multistreaming*.



In the 90's mass transportation theory was eventually brought together with the Monge-Ampère equation when the french mathematician Yann Brenier formally proved that the optimization problem, assuming quadratic cost<sup>11</sup>, amounts to an elliptic Monge-Ampère equation.

As extensively discussed in [11], Brenier considers the case in wich  $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$  and the cost would be  $c(x, y) = |x - y|^2/2$ , proving the following theorem.

Let  $\mu$  and  $\nu$  be two compactly supported probability measures on  $\mathbb{R}^n$ . If  $\mu$  is absolutely continuous with respect to the Lebesgue measure, then

1. there exists a unique solution  $T$  to the optimal transport problem with cost  $c(x, y) = |x - y|^2/2$ ;
2. there exists a convex function  $u : \mathbb{R}^n \rightarrow \mathbb{R}$  such that the optimal map  $T$  is given by  $T(x) = \nabla u(x)$  for  $\mu$ -a.e.  $x \in \mathbb{R}^n$

Furthermore, if  $\mu(dx) = f(x)dx$  and  $\nu(dy) = g(y)dy$ , then  $T$  is differentiable  $\mu$ -a.e. and

$$|\det(\nabla T(x))| = \frac{f(x)}{g(T(x))} \quad \text{for } \mu\text{-a.e. } x \in \mathbb{R}^n$$

For a broad discussion of the regularity results of optimal transport maps deriving from this theorem refer to [11].

### 2.3 Zel'dovich approximation

In the early 70's the astronomer Yakov B. Zel'dovich published his work on gravitational instability introducing a simplification of the problem known as the *Zel'dovich approximation*. Assuming the Zel'dovich approximation, the pursuit of a solution for the reconstruction problem doesn't rely on the mathematically rigorous framework considered in the previous section. Consider equation

$$D_\tau^2 \mathbf{x} = -\frac{3}{2\tau} (D_\tau \mathbf{x} + \nabla_{\mathbf{x}} \phi_g)$$

in place of the Poisson equation. Here  $\mathbf{x}(\mathbf{q}, \tau)$  is the Lagrangian map, crucially assumed to be equal to the gradient of a convex potential, as mentioned before.

At  $\tau = 0$  the Hubble drag term and the gravitational force cancel exactly and still do so to leading order in any dimension for small  $\tau$ <sup>12</sup>.

<sup>11</sup>In the previous works on the topic the cost was assumed to be linear, i.e. directly proportional to the distance.

<sup>12</sup>Consequence of the slaving condition.

The Zel'dovich approximation removes any restriction in time: the acceleration  $D_\tau^2 \mathbf{x}$  just vanishes for all  $\tau$ .

The spatial structure of the initial perturbations is described by the potential vector field, the same convex potential that satisfies  $\mathbf{x} = \nabla_q \Phi$  takes the form

$$\Phi(\mathbf{q}, \tau) \equiv \frac{|\mathbf{q}|^2}{2} - \tau \phi_g^{in}(\mathbf{q}) \quad (5)$$

As long as the potential  $\Phi$  is convex, the map  $\mathbf{x}(\mathbf{q}, \tau)$  is essentially invertible. From the physical point of view, the same assumption corresponds to the absence of multistreaming<sup>13</sup> To be more precise, the Zel'dovich approximation itself is not enough to completely rule out multistreaming: a variant, known as *adhesion model*, was introduced by S.N. Gurbatov and A.I. Saichev in 1984, that makes use of a multidimensional Burger's equation

$$\partial_\tau \mathbf{v} + (\mathbf{v} \cdot \nabla_x) \mathbf{v} = \nu \nabla_x^2 \mathbf{v} \quad (6)$$

in the *inviscid* limit in which viscosity  $\nu$  tends to zero<sup>14</sup>.

Zel'dovich approximation had the potential of predicting how the first structures are formed but it does not tell us what happens after the formation of the first shocks. The viscosity term introduced on the right side of equation (6) would prevent particle orbit crossing, thus preserving shocks after they form. This allows us to track the unfolding of the cosmic web to much later times than Zel'dovich approximation is capable of.

If considering the Lagrangian formulation given above, adhesion model is obtained by replacing  $\Phi(\mathbf{q}, \tau)$  by its *convex hull*<sup>15</sup> in the variable  $\mathbf{q}$ .

Even though the adhesion model appears to be defective when it comes to conservation of momentum in more than one dimension, it is still, as the  $N$ -body simulations show, in a better agreement with observations than the Zel'dovich approximate model.

## 2.4 The Monge-Ampère equation

The assumption that the Lagrangian map is derived from a convex potential leads to a pair of Monge–Ampère equations, one for this very potential and another for its Legendre transform.

<sup>13</sup>Having more than one velocity at a given point.

<sup>14</sup>Note that it's  $\nu \rightarrow 0$  and not  $\nu = 0$  for which it would simply go back to Zel'dovich approximation.

<sup>15</sup>See **Appendix**.

Starting from a general definition, the Monge–Ampère equation in its classical form is given by a nonlinear second-order partial differential equation

$$[\det u]^2 = f(\mathbf{x}, u, \nabla u) \quad \text{in } \Omega,$$

where  $\Omega \subset \mathbb{R}^n$  is some open set,  $u : \Omega \rightarrow \mathbb{R}$  is a convex function, and  $f : \Omega \times \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^+$  is given. As a result, the equation prescribes the product of the eigenvalues of the Hessian matrix of  $u$ , the convexity of which is a necessary condition to make the equation degenerate elliptic and achieve the regularity results mentioned in the previous subsection.

Going back to the EUR frame, since in the adopted notation the initial quasi-uniform mass distribution has unit density, mass conservation inevitably implies that, for a prescribed density field  $\rho_0(\mathbf{x})$

$$\rho_0(\mathbf{x}) d^3 \mathbf{x} = d^3 \mathbf{q}$$

In terms of the Jacobian matrix  $\nabla_{\mathbf{q}} \mathbf{x}$

$$\det \nabla_{\mathbf{q}} \mathbf{x} = \frac{1}{\rho_0(\mathbf{x}(\mathbf{q}))}$$

Under assumption (5) over the potential, one will get to the final form

$$\det(\nabla_{x_i} \nabla_{x_j} \Theta(\mathbf{x})) = \rho_0(\mathbf{x})$$

The function  $\Theta(\mathbf{x}) = \max_{\mathbf{q}} \mathbf{x} \cdot \mathbf{q} - \Phi(\mathbf{q})$  is the Legendre transform of the potential  $\Phi$  and subsequently the convex potential of the inverse map.

Mass conservation can be thus rewritten as

$$\det(\nabla_{x_i} \nabla_{x_j} \Theta(\mathbf{x})) = \rho_0(\mathbf{x}) \quad (7)$$

i.e. the much-awaited elliptic Monge–Ampère equation<sup>16</sup>.

#### 2.4.1 Weak formulation

When dealing with actual mass concentration in the present distribution of matter, the density field at the right member of equation (7) acquires a singular component and smoothness of the potential  $\Theta$  is in jeopardy.

Nonetheless, by requiring mass conservation in its integrated form

$$\int_{D_E} \rho_0(\mathbf{x}) d^3 \mathbf{x} = \int_{\nabla_x \Theta(D_E)} d^3 \mathbf{q}$$

<sup>16</sup>Monge–Ampère equation for self-gravitating matter may be viewed as a non-linear generalization of a Poisson equation, to which it reduces if the fluctuations from initial position are very small.

with  $D_E$  being the arbitrary domain of variable  $\mathbf{x}$  in the Eulerian space and  $\mathbf{q}(D_E)$  its image in the Lagrangian space, a *weak formulation* of the Monge-Ampère equation is provided.

Smoothness and uniqueness of the solution are guaranteed in this form, as long as the mass distributions themselves are smooth and occupy bounded and convex domains.

## 2.5 MAK

Piecing together the notions that have been introduced, the Monge-Ampère-Kantorovich method developed [4] and in [5], makes use of a variational reformulation of (7).

When the cost to mass transportation problem is a quadratic function of the distance, the purpose of finding a potential Lagrangian map with prescribed initial and present mass density fields reduces to finding the minimizer to the functional

$$I = \int_{D_{in}} \frac{|\mathbf{x}(\mathbf{q}) - \mathbf{q}|^2}{2} d^3 \mathbf{q} = \int_{D_0} \frac{|\mathbf{x} - \mathbf{q}(\mathbf{x})|^2}{2} \rho_0(\mathbf{x}) d^3 \mathbf{x}$$

Solution  $\mathbf{q} \rightarrow \mathbf{x}(\mathbf{q} = \nabla \Theta(\mathbf{q}))$  must satisfy condition (7).

A variational proof of the equivalence is given in [5].

### 2.5.1 the Assignment problem

Once the mass distribution is converted into an ensemble of  $N$  particles, cost minimization becomes what is known as an *assignment problem* in optimization theory: find the unique one-to-one pairing of a set of  $N$  initial points  $\mathbf{q}_i$  and  $N$  final points  $\mathbf{x}_i$  that provides minimization of the *discrete* action

$$I_{discr} = \sum_{i=1}^N |\mathbf{x}_i - \mathbf{q}_{j(i)}|^2$$

Taking this further step, complexity of the algorithms used for  $N$ -body simulations is close to  $N^3$  for arbitrary cost functions and notably reduced if cost is assumed to be quadratic.

## 3 the Monge-Ampère gravitational model

The Monge-Ampère gravitational model presented by Y. Brenier in [9] consists of a modified Euler-Poisson system, in which the linear Poisson equation is substituted by the fully non-linear Monge-Ampère equation.

Remarkably enough, the resulting model allows exact solutions for the Zel'dovich approximation. It is noted that the way the problem has been addressed by G. Loeper provides only solutions to the Euler-Poisson system without concentrations, a restraint that Brenier is able to overcome, modifying the action in order to obtain minimizers that would not be necessarily concentration free. Brenier employs the theory of self-dual lagrangians developed by N. Ghoussoub, whose work on Self-dual Partial Differential Systems is cited among the references in [9].

### 3.1 MAG

The definition of the MAG model is given by taking the Hilbert space

$$H = L^2(D, R^d)$$

of all Lebesgue square-integrable maps from  $D$  to  $R^d$ . The subset of all the Lebesgue measure-preserving maps  $s$  of  $D$  will be

$$S = \left\{ s \in H, \int_D f(s(a)) da = \int_D f(a) da, \quad \forall f \in C(R^d) \right\}$$

The dynamical system

$$\beta^{-2} \frac{d}{dt} \left( \alpha^2(t) \frac{dx}{dt} \right) = (\nabla_H \Phi)[x] = x - \pi[x]$$

displays the scaling parameters  $\alpha(t) = t^{\frac{3}{4}}$  and  $\beta(t) = t^{-\frac{1}{4}} \sqrt{3/2}$  from the theory of General Relativity, as required by the physical context. The other notable variables are the given potential  $\Phi$  and  $\pi[x]$ , the latter defined as the closest point to  $x$  on  $S$ . The potential is assumed to be defined in the form

$$\Phi[\tilde{x}] = \inf \left\{ \frac{\|\tilde{x} - s\|^2}{2} ; s \in S \right\}$$

For the extensive discussion of the abstract framework see [9].

In order to formulate the MAG model in Eulerian coordinates one can introduce, given a solution  $t \rightarrow \mathbf{x}(t)$ , the following measures

$$\begin{aligned} \rho(t, dx) &= \int_D \delta(x - \tilde{x}(t, a)) da \\ \nu(t, x) \rho(t, dx) &= \int_D \partial_t x(t, a) \delta(a - \tilde{x}(t, a)) da \end{aligned}$$

respectively valued in  $\mathbb{R}$  and  $\mathbb{R}^d$ .

By using optimal transportation theory one will get to the following set of partial differential equations

$$\begin{aligned}\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \partial_t (\alpha^2 \rho \mathbf{v}) + \nabla \cdot (\alpha^2 \rho \mathbf{v} \otimes v) &= -\beta^2 \rho \nabla \phi_g \\ \rho &= \det(I + D_x^2 \phi_g)\end{aligned}\tag{8}$$

where  $(\rho, \mathbf{v}, \phi)(t, \mathbf{x}) \in \mathbb{R}_+ \times \mathbb{R}^D \times \mathbb{R}$ ,  $(t, \mathbf{x}) \in \mathbb{R} \times \mathbb{R}^d$

The fully non-linear Monge-Ampère equation, the third equation in system (8), if used to replace the linear Poisson equation encountered above provides a model that is correspondingly a non-linear correction of the original *E-P* classical model.

Note that, in one dimension, the two perfectly overlap.

### 3.2 Modified action

By exploring the self-dual form of the action, it becomes clear that any solution of the gradient flow equation

$$\frac{dX}{dt} = (\nabla_H \Phi)[X] = X - (\nabla_H \Pi)[X]\tag{9}$$

always represents a minimizer of the action. Each solution  $X(t)$  to (9) in the Hilbert space is a Lipschitz continuous function of  $t$  and right-differentiable  $\forall t$ . The self-dual formulation<sup>17</sup> of a modified action is set to be

$$\hat{A}_{[t_0, t_1]}[X] = \int_{t_0}^{t_1} \frac{1}{2} \left\| \frac{dX}{dt} - X + d^0 \Pi[X] \right\|^2 dt$$

For the EUR problem, it can be rewritten as

$$A = \int_{t_0}^{t_1} \alpha(t)^2 \left\| \frac{dX}{dt} \right\|^2 + \beta(t)^2 \left\| \nabla_H \Phi[X(t)] \right\|^2 dt$$

By performing integration by part under the assumption that

$$\frac{d}{dt} (\alpha(t) \beta(t)) = \lambda \beta(t)^2$$

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<sup>17</sup>  $d^0 \Pi[X]$  is uniquely defined and denotes the element of  $\partial \Pi[x]$  with minimal norm.

the same action can be expressed as

$$A = BT + \int_{t_0}^{t_1} \left\| \alpha(t) \frac{dX}{dt} - \mu \beta(t) \nabla_H \Phi[X(t)] \right\|^2 dt$$

with  $BT$  being a boundary term depending only on  $X(t_1)$  and  $X(t_0)$ ,  $\mu$  taken such that  $\mu^2 + \mu\lambda + 1 = 1$ .

The gradient flow equation that allows concentrations is

$$t \frac{dX(t+0)}{dt} = X(t) - d^0 \Pi[X(t)] \quad (10)$$

Equation (10) also implies the biggest dissipation of kinetic energy during the concentration process<sup>18</sup>. The ultimate expression that is suggested for the EUR problem according to MAG model is eventually given by

$$\hat{A} = \int_{t_0}^{t_1} t^{-\frac{1}{2}} \left\| t \frac{dX}{dt} - X + d^0 \Pi[X] \right\|^2 dt$$

### 3.2.1 ZA solutions

Brenier extends the discussion to those solutions to the gradient flow equation (10) that coincide in fact with the approximate Zel'dovich formula

$$X(q, \tau) = q - \tau \nabla \phi_g^{in}(q) \quad (11)$$

where  $q$  is the material coordinate that labels the mass particle at time  $\tau$  and  $\phi_g^{in}$  regards the behaviour of the density field at early stages.

These special solutions come from the fact that any map  $X \in H$  has a unique rearrangement  $X^* \in K$ , with  $K \subset H$  being the set of all points  $X$  that admit  $\mathbb{1}$  as a closest point on  $S$ .

It can be mathematically formulated as

$$\int_D \delta(x - X^*(q)) dq = \int_D \delta(x - X(q)) dq$$

For the seeked solutions (10) reduces to a linear ODE

$$\nabla_H \Phi[X(t)] = X(t) - \mathbb{1}$$

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<sup>18</sup>This specific aspect could be matter of discussion from a physical point of view.

leading explicitly to

$$X(q, t) = q + \frac{t}{t_0}(\nabla\phi(t_0, q) - q) = q + \frac{t}{t_0}(X(t_0, q) - q) \quad (12)$$

given the fact that if  $X$  belongs to  $K$  then  $X(t, q) = \nabla\psi(t, q)$ , with  $\psi(t, q)$  convex in  $q$ . Equation (12) coincides with equation (11), providing an indirect validation of the model.

### 3.3 Discretization

Following the ideas discussed above, a one-dimensional algorithm is designed and acts as a link between the mathematical model and the  $N$ -body numerical simulations.

The modified action that has been introduced is now taken in a *time-discrete* version, starting from the gradient flow equation (10).

One would naturally choose

$$X_{n+1} = X_n(1 + \theta_n) - \nabla_H \Pi[X_n] \theta_n + \eta_n$$

where  $X_n$  is an approximation of  $X(t)$  at the  $n^{\text{th}}$  time-step  $T_n$ ,  $n = 0, \dots, N$ ,  $T_0 = t_0$ ,  $T_N = t_1$  and

$$\Theta_n = \left[ \frac{T_{n+1}}{T_n} - 1 \right] \rightarrow 0.$$

The last term  $\eta_n$  represents an arbitrary small perturbation that guarantees that  $X_n$  is a point of differentiability of  $\Pi$ ,  $\forall n$ .

From such time-discrete scheme a time-discrete version of the modified action is defined as well

$$\sum_{n=0}^{N-1} r_n \|X_{n+1} - X_n(1 + \theta_n) + \pi[X_n] \theta_n\|^2 \quad r_n = \frac{T_n^{3/2}}{T_{n+1} - T_n}$$

Nevertheless, the original EUR problem does not involve the  $X_n$  variables, but rather the corresponding probability measures.

In order to address the loss of information that would be caused,  $X_0$  and  $X_N$  are rearranged with convex potentials  $X_0^\#$  and  $X_N^\#$ .

If  $X_n = Y_n \circ s_n$ ,  $Y_n = X_n^\# \in K$ ,  $s_n = \pi[X_n] \in S$  is the closest point in  $S$  to  $X_n$ .

The time-discrete version of the gradient flow naturally turns into

$$Y_{n+1} \circ s_{n+1} = (Y_n(1 + \Theta_n) - \Theta_n \mathbb{1}) \circ s_n$$



As a consequence, the time-discrete EUR problem within the MAG frame is now an issue of minimization of

$$\sum_{n=0}^{N-1} r_n \| Y_{n+1} \circ s_{n+1} - (Y_n(1 + \theta_n) - \theta_n \mathbb{1}) \circ s_n \|^2$$

By introducing the quadratic *Wasserstein distance*<sup>19</sup> the problem once again takes new form, as the minimization in  $Y_n \in K$  of

$$\sum_{n=0} d_W(Y_{n+1}, Y_n(1 + \theta_n) - \theta_n \mathbb{1})^2$$

### 3.3.1 Fully discrete LAP

The Least Action Principle (LAP) comes in a scheme in which not only the time variable but also the space variable is discrete. The continuous domain  $D$  is replaced with  $L$  disjoint subdomains  $D_i$  of Lebesgue measure  $1/L$ , with  $i = 1, \dots, L$ .

$H$  is consequently taken as the euclidean space  $(\mathbb{R}^d)^L$  provided with a euclidean norm  $\|\cdot\|$ .  $S$  contains all permutations  $s$  of the  $L$  first integers and satisfies the group property of invariance for the norm.

The minimization problem is furtherly reduced to the minimization of the following

$$\sum_{n=0}^{N-1} r_n \| Y_{n+1} - (Y_n(1 + \theta_n) - \theta_n Id) \circ \sigma_{n+1} \|^2$$

as  $Y_0$  and  $Y_N$  are fixed in  $K$ , the latter corresponding to the cone of all sequences  $Y_i$  such that

$$\sum_i Y_i \cdot (a_i - a_{s_i}) \geq 0$$

Solution to the minimization problem is shown in [9], making use of Gauss-Seidel type iterations.

In order to validate the model, the time-discrete scheme is then successfully employed by Y. Brenier to solve the *initial value problem* (IVP), in one and multi-dimensions, alongside with the time-discrete least action principle.

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<sup>19</sup>See **Appendix**.

## 4 Numerical applications

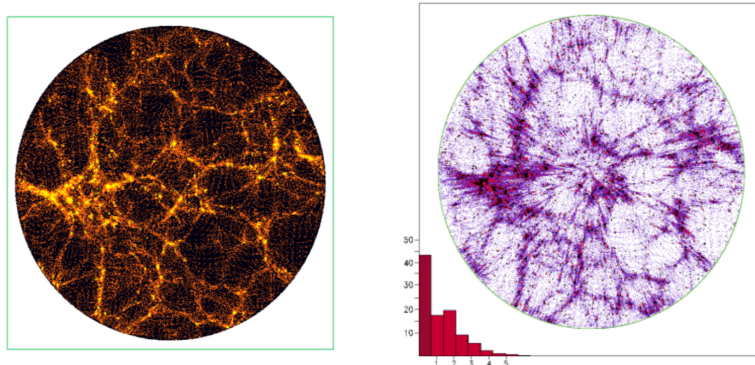
### 4.1 Testing MAK

Taking up on the Monge-Ampère-Kantorovich (MAK) gravitational model, that was briefly discussed in section 2.5, the following images show the  $N$ -body simulation output used for testing the MAK reconstruction method.

The distribution of dark matter is taken as a discrete *ensemble* of  $N$  particles of identical mass. The reconstruction reduces to evaluating the actual pairing between initial and final positions of these particles, according to Newtonian gravitational dynamics<sup>20</sup>.

On the left is the projection on the  $x$ - $y$  plane of a 10% amount of about  $200h^{-1}\text{Mpc}$ , where all highlighted points refer to Reconstruction failing by more than  $6.25h^{-1}\text{Mpc}$ <sup>21</sup>.

On the right is the projection of the same simulation box tested specifically with a redshift-space variant of MAK reconstruction. A comparison between the two shows that MAK is reliable with respect of redshift systematic errors.



### 4.2 Testing MAG

Following the discretization of the algorithm a few numerical simulations are performed, visually presented and discussed in section 6 of [9].

The considered time interval is divided into 60 equal steps, during which the trajectories of 51 particles are followed and reconstructed, resulting into an almost perfect matching between the reconstructed solution and the IVP problem for the MAG equations.

<sup>20</sup>Assuming periodic boundary conditions.

<sup>21</sup>That would happen more frequently in high density regions.

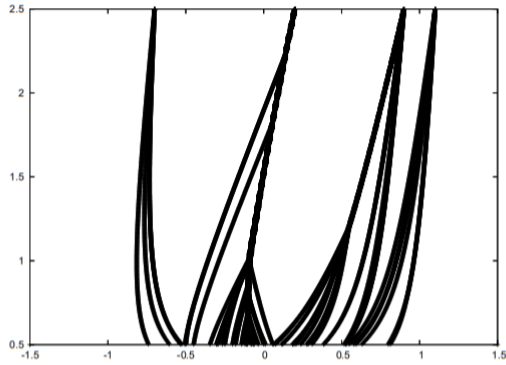


FIGURE 1. Case 1/reconstruction

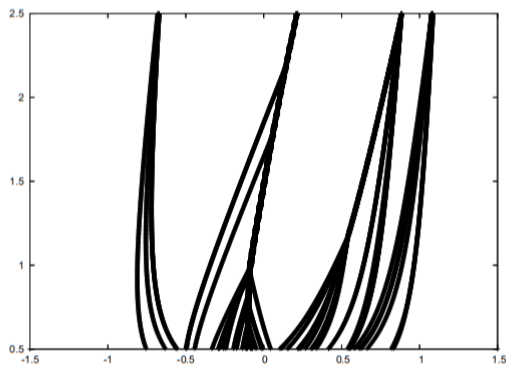


FIGURE 2. Case 1/initial value problem (IVP) after reconstruction

## 5 Conclusions

In these few pages, certainly a lot fewer than those needed to fully explore the issue we're addressing, the attempt is to give a glimpse, a rather general overview of the ideas that were conceived in order to find a solution to the Early Universe Reconstruction (EUR) problem.

The apparatus and tools of optimal transport theory and the Monge-Ampère equation, in some way rediscovered for this purpose, end up having crucial roles in the hunt for an answer.

From the historical contextualization that has been made it becomes

clear that the issue has caught the attention of both cosmologists and mathematicians, whose efforts and research would converge right into building an efficient model, an algorithm capable of tracing and piecing together the path on which matter has been moving through billions of years.

Among the best developed models in the field the Monge-Ampère-Kantorovich (MAK) model [5] stands out, as it is the first one that engages with the EUR problem as a *well-posed* problem having a *unique* solution.

We've been then mainly focusing on Yann Brenier's formulation of the Monge-Ampère Gravitational (MAG) model, that makes use of the least action principle to design a one-dimensional algorithm, in which mass concentrations are included by employing gradient flow theory.

The efficiency of the algorithm is proved by the Zel'dovich solutions on one side and by the numerical simulations on the other.

It is worthy to mention, among the most recent publications around the MAK method, the work of B. Levy, R. Mohayaee and S. von Hausegger [13], as they were able to efficiently run  $N$ -body simulations with a *semidiscrete* optimal transport algorithm (SDMAK) over a continuous density field, partitioned into *Laguerre cells*<sup>22</sup>. The SDMAK successfully reconstructs the initial positions of up to  $\mathcal{O}(10^7)$  particles in a matter of hours, recovering subtle features of the initial power spectrum, such as the baryonic acoustic oscillations.

It is great indeed to watch this major topic regarding our cosmos, along with its many facets, slowly clear up in front of us, as we move forward towards future goals.

Large 3D surveys will make increasingly detailed reconstruction of early density fluctuations possible, giving some solid base to verify important assumptions that has been made about them.

On a theoretical level, researchers will probably commit to developing a viable multi-dimensional algorithm, as well as investigating the relative accuracy of Newtonian and Monge-Ampère gravitational models in relation to General Relativity.

Besides, there are many unexpected and significant applications of both optimal transport theory and the Monge-Ampère-Kantorovich problem, applications that completely depart from the cosmological frame of work.

As it is deftly presented in [12], the version of Monge's optimal transport problem later repropesed by L. Kantorovich opened the way to an appropriate variational theory that applies to living systems, able to prescribe the optimal stationary distribution of metabolites throughout the arterial network. The *reconstruction* of the whole dynamic is well-crafted and its efficiency is

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<sup>22</sup>An individual region in a *Laguerre* diagram.

confirmed by Kleiber's phenomenological law<sup>23</sup>.

The same mathematical machinery can be used to describe the way trees get their nutrition through their roots, in an *optimal* way.

It is not hard to imagine how all the research that still has to come around the subject might open doors on even more fascinating worlds, revealing a *fil rouge* that connects, behind the scenes, the structure and the history of our Universe to the simplest breathing entity that is part of it.

## 6 Appendix

- **weak solution** A triple  $(\rho, v, \phi)$  is a weak solution for the E-P problem if

1.  $\rho \in L^2([0, T]; H^{-1}(\mathbb{T}^d)) \cap C([0, T]; \mathcal{P}(\mathbb{T}^d) - w*)$ ,  $v \in L^2(D, d\rho)$ ,
2. for any  $\psi = (\psi^j)_{j \in [1..d]} \in (C_c^\infty([0, T] \times \mathbb{T}^d))^d$ , we have

$$\int_{[0, T] \times \mathbb{T}^d} \partial_t \psi \cdot v d\rho + D\phi : v \otimes v d\rho - \psi \cdot \nabla \phi + D\psi : \nabla \phi \otimes \nabla \phi - \frac{1}{2} (\nabla \cdot \psi) |\nabla \phi|^2 = 0$$

3. for any  $\psi \in C^\infty([0, T] \times \mathbb{T}^d)$

$$\int_{[0, T] \times \mathbb{T}^d} \partial_t \psi d\rho + \nabla \psi \cdot v d\rho = \int_{\mathbb{T}^d} \rho_T \psi|_{t=T} - \int_{\mathbb{T}^d} \rho_0 \psi|_{t=0}$$

$$\int_{[0, T] \times \mathbb{T}^d} (d\rho - 1) \psi + \nabla \phi \cdot \nabla \psi = 0$$

- **convex hull** The convex hull of the function  $\Phi(q)$ , the latter being the velocity potential in the Zel'dovich approximation, is defined as the largest convex function for which the graph lies below that of  $\Phi(q)$ .
- **Wasserstein distance** The Wasserstein (or Monge-Ampère) quadratic distance on  $H$  is defined as

$$d_W(X, \tilde{X}) = \inf\{ \|X \circ s - \tilde{X} \circ \tilde{s}\|, s, \tilde{s} \in S\}$$

<sup>23</sup>Kleiber's law states that  $B \propto M^{\frac{3}{4}}$ , B being the basal metabolic rate in mammals, M the metabolite.

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