GDR IASIS
Lyon

17 Fevrier 2025

Semi-Discrete Optimal Transport with 10^9 points … and beyond
Why and How?

Bruno Lévy

Inria - ParMA
Laboratoire de Mathématiques d’Orsay

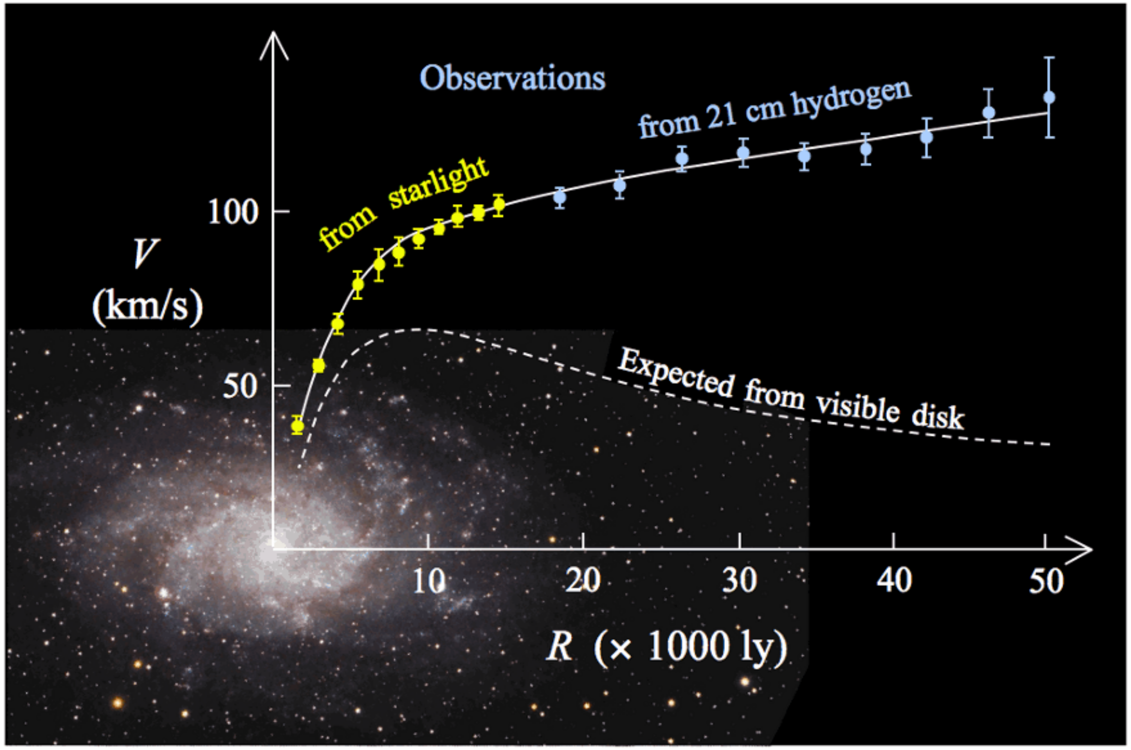
Overview

1. **Mysteries in the sky**
2. **Optimal Transport**
3. **Semi-Discrete**
4. **Scaling up**
5. **Red-shift distortion**
6. **Brenier-Monge-Ampere Gravitation**

1

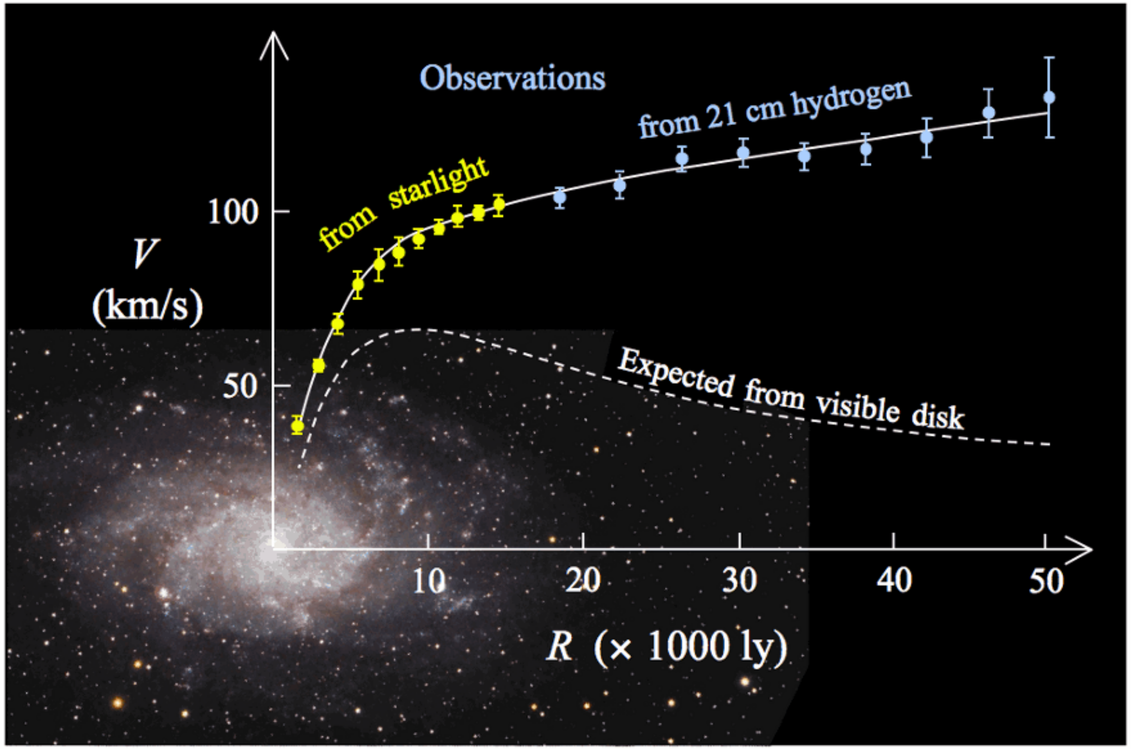
Mysteries in the sky

Mysteries in the sky



Vera Rubin - 1962

Mysteries in the sky

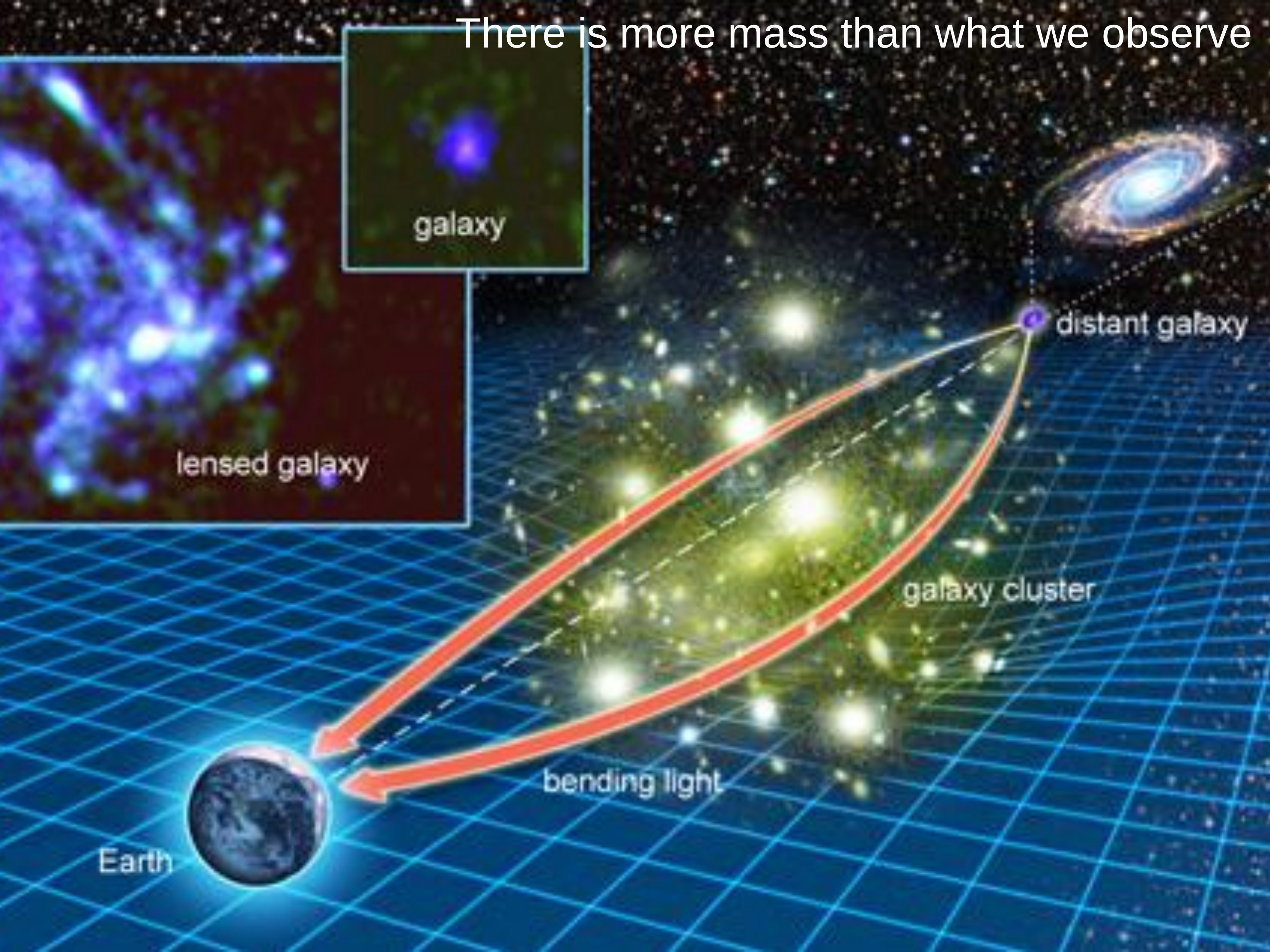


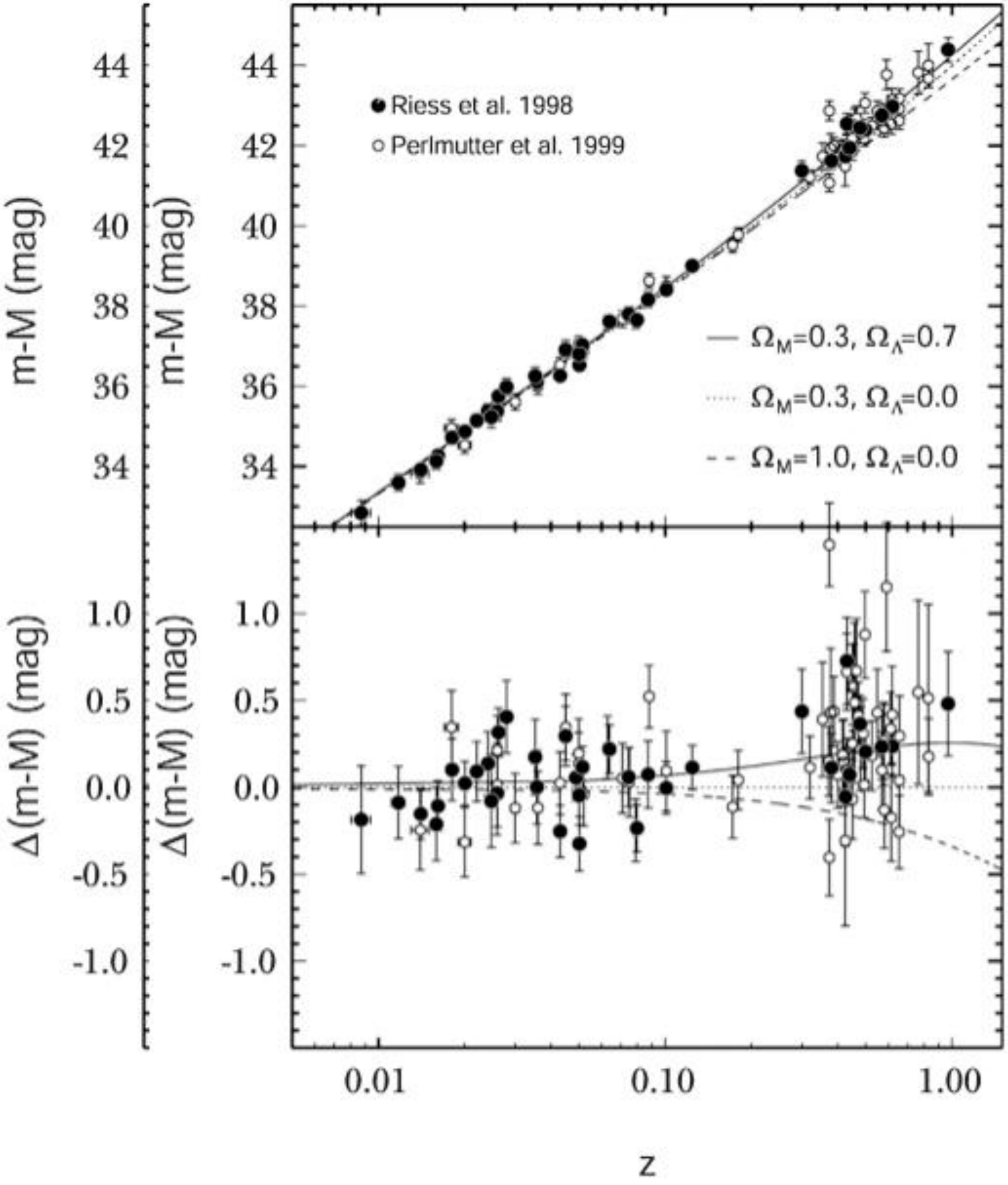
Vera Rubin - 1962

There is more mass than what we observe

There is more mass than what we observe

There is more mass than what we observe

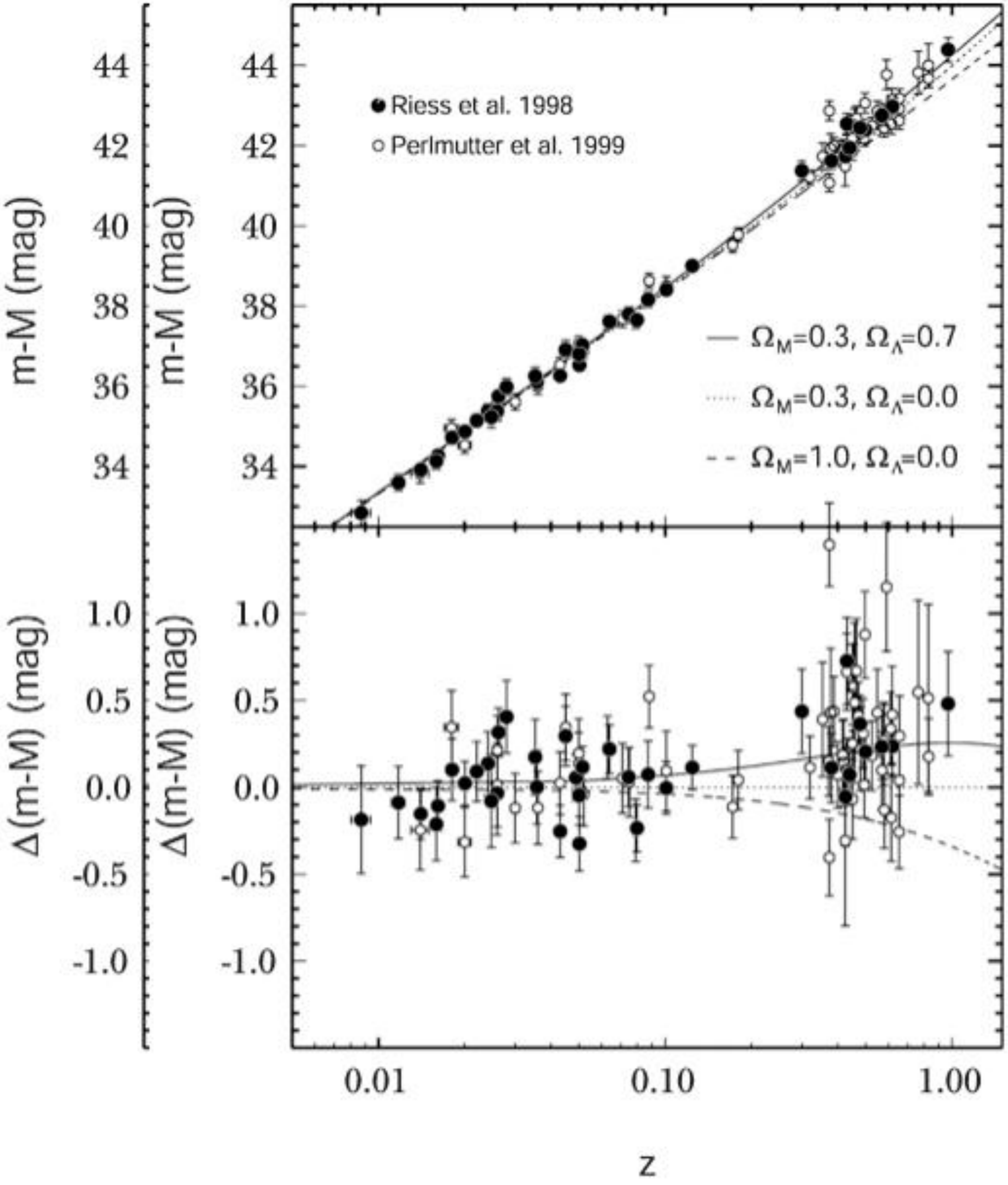




Type Ia supernovae “standard candles”

Permutter

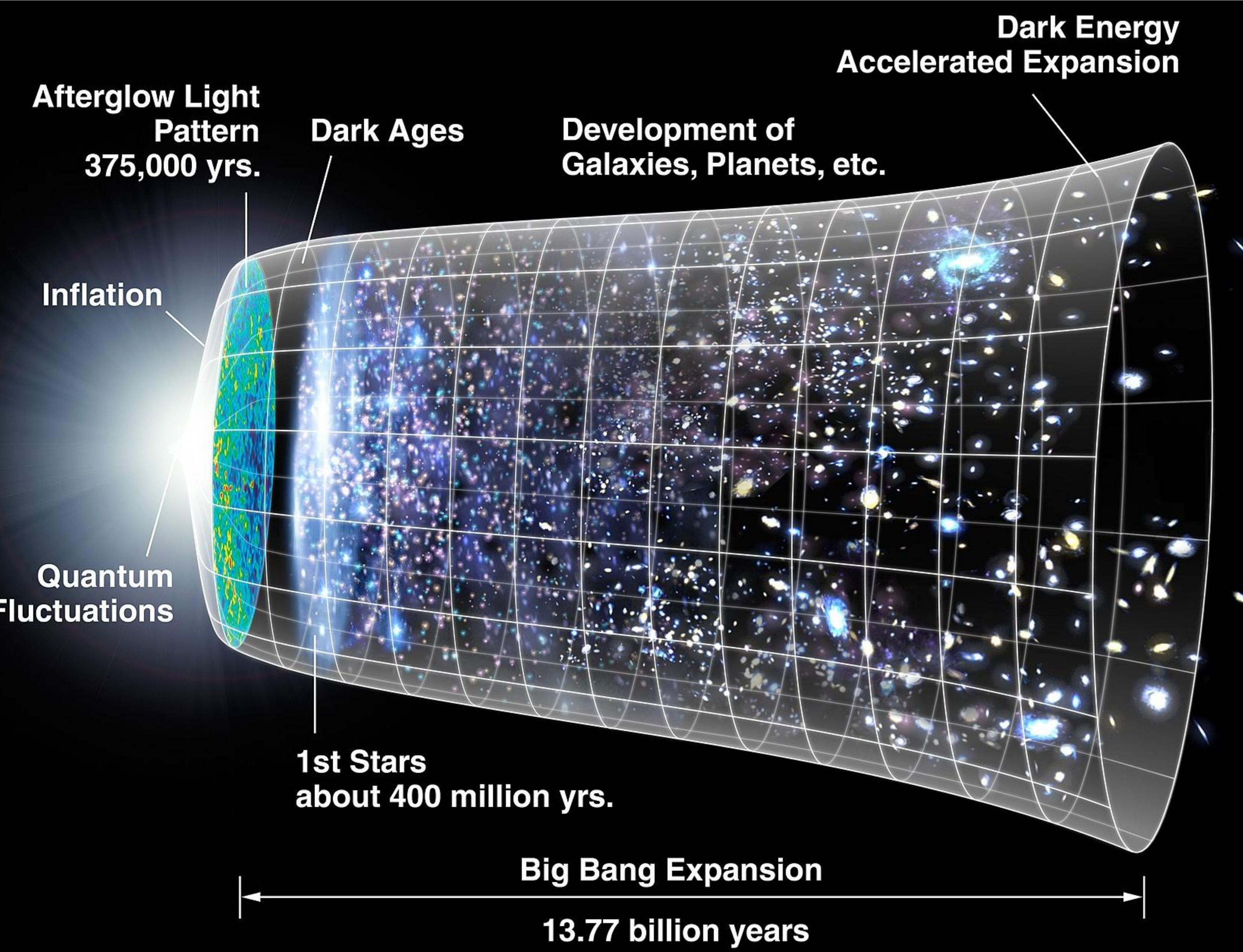
Riess



Type Ia supernovae “standard candles”

Permutter
Riess

The expansion of the Universe is accelerating.


Dark Energy
Accelerated Expansion
Afterglow Light
Pattern
375,000 yrs.
Dark Ages
Development of
Galaxies, Planets, etc.
Inflation
Quantum
Fluctuations
1st Stars
about 400 million yrs.
Big Bang Expansion
13.77 billion years

Mysteries in the sky

- There seems to be more matter than what we observe…

- The big-bang is big-banging faster than we thought …

Mysteries in the sky

- There seems to be more matter than what we observe…

“dark matter” (but we do not know what it is)

- The big-bang is big-banging faster than we thought …

“dark energy” (but we do not know what it is)

Shedding some light into the dark Universe

Models

Newton

No force $\Rightarrow$ everything moves along straight lines with constant speed

Force $\Rightarrow \mathbf{F} = m\mathbf{a}$

Gravity: $\mathbf{F} = -\mathcal{G}m_1m_2/d^2$

Shedding some light into the dark Universe

Models

Newton

No force $\Rightarrow$ everything moves along straight lines with constant speed

Force $\Rightarrow \mathbf{F} = m\mathbf{a}$

Gravity: $\mathbf{F} = -\mathcal{G} m_1 m_2 / d^2$

GR

Everything moves along « straight lines with constant speed »

Shedding some light into the dark Universe

Models

Newton

No force $\Rightarrow$ everything moves along straight lines with constant speed

Force $\Rightarrow \mathbf{F} = m\mathbf{a}$

Gravity: $\mathbf{F} = -\mathcal{G}m_1 m_2/d^2$

GR

Everything moves along « straight lines with constant speed »

$$G_{\mu\nu} = 8\pi\underset{\uparrow}{\mathcal{G}}T_{\mu\nu}$$

Mass and energy

Shedding some light into the dark Universe

Models

Newton

No force $\Rightarrow$ everything moves along straight lines with constant speed

Force $\Rightarrow \mathbf{F} = m\mathbf{a}$

Gravity: $\mathbf{F} = -\mathcal{G} m_1 m_2 / d^2$

GR

Everything moves along « straight lines with constant speed »

$$\underset{\uparrow}{G_{\mu\nu}} = 8\pi \underset{\uparrow}{\mathcal{G}} T_{\mu\nu}$$

Geometry (meaning of “straight lines with constant speed”)

Mass and energy

Shedding some light into the dark Universe

Models

Newton

No force $\Rightarrow$ everything moves along straight lines with constant speed

Force $\Rightarrow \mathbf{F} = m\mathbf{a}$

Gravity: $\mathbf{F} = -\mathcal{G} m_1 m_2 / d^2$

GR

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi\mathcal{G} T_{\mu\nu}$$

Geometry

“dark energy”

Mass and energy

Shedding some light into the dark Universe

Models

Newton

GR with lambda and cold dark matter (LCDM)

MOND (Modified Newton Dynamics)

MAG (Monge-Ampère grativation)

…

Shedding some light into the dark Universe

Models

Newton

LCDM

MOND

MAG

…

Observations

3D maps of the Universe (redshift acquisition surveys)

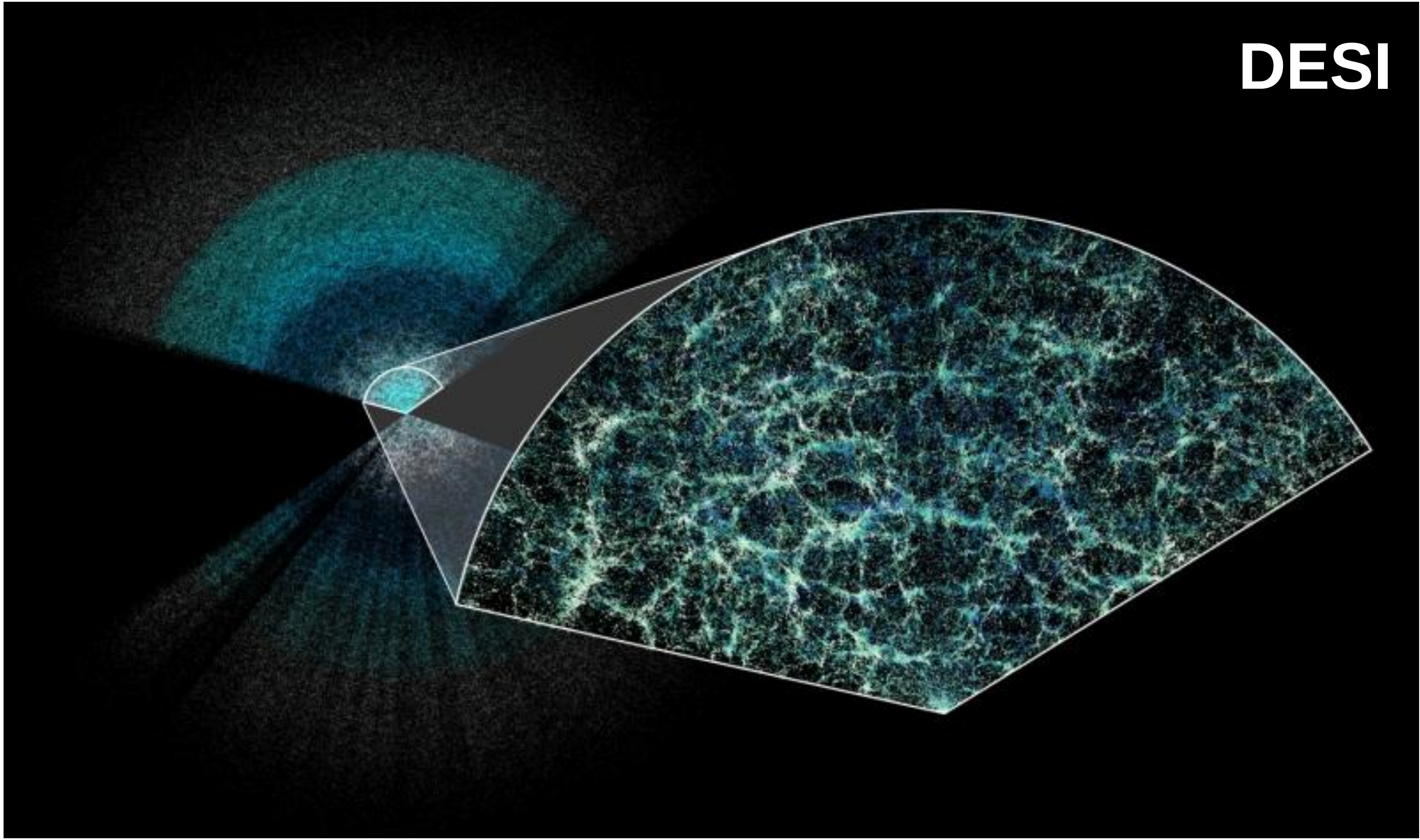
Shedding some light into the dark Universe

Models

Newton
LCDM
MOND
MAG
…

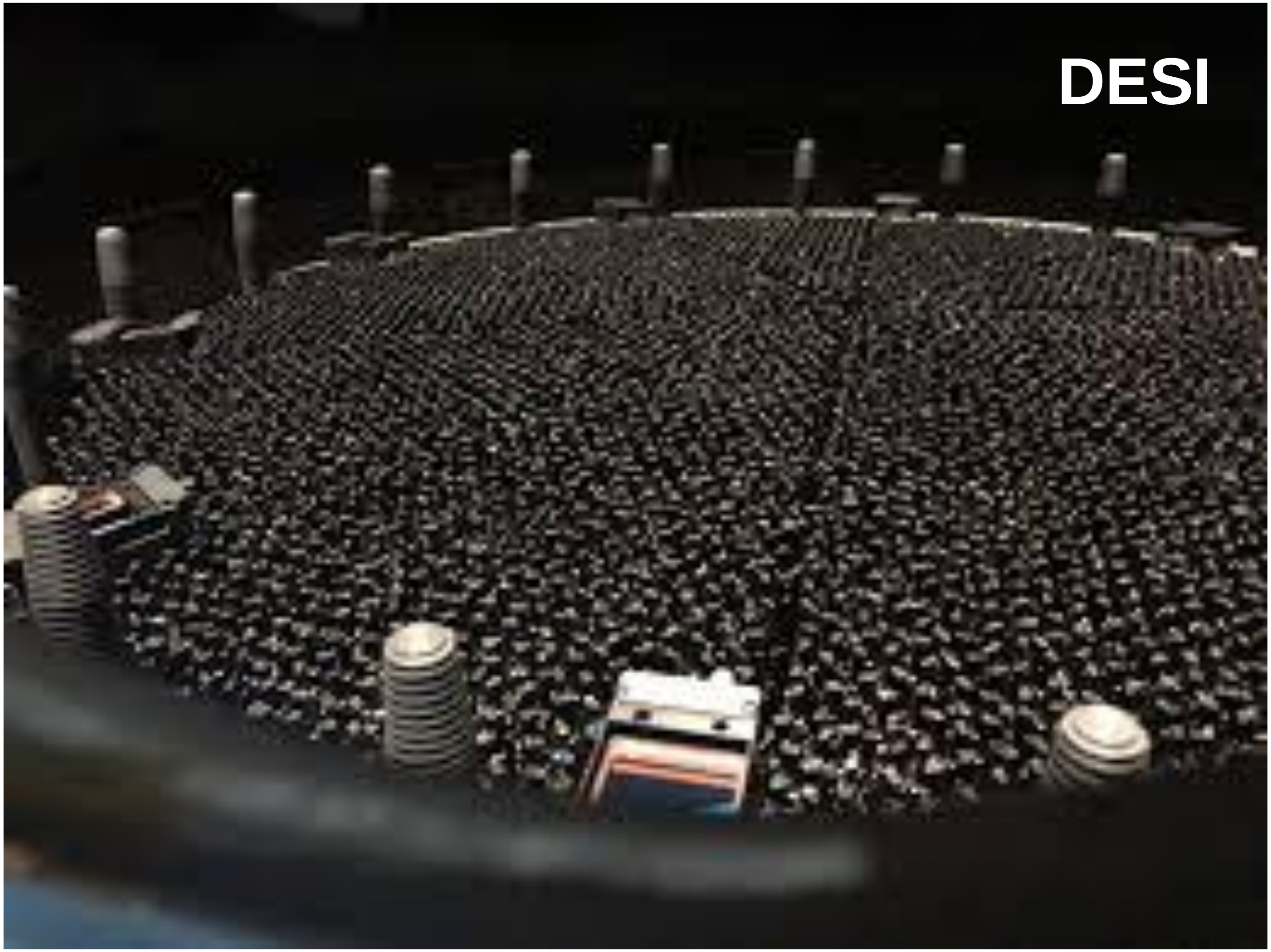
Observations

3D maps of the Universe (redshift acquisition surveys)



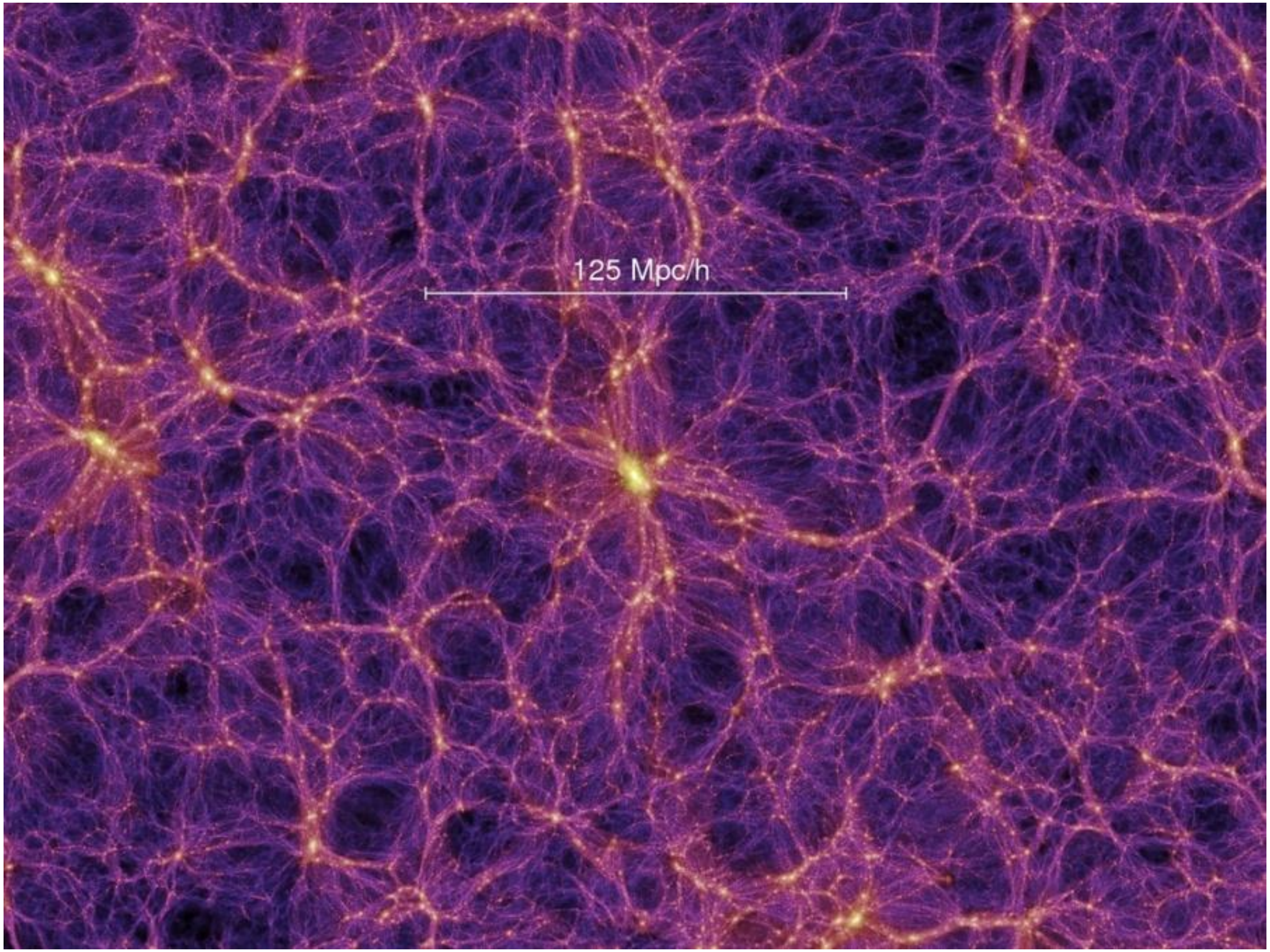
Shedding some light into the dark Universe

Shedding some light into the dark Universe



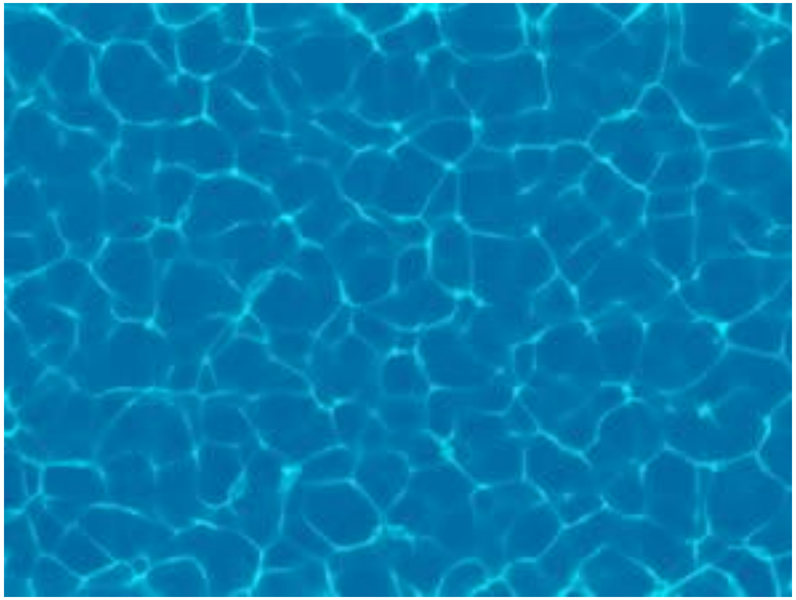
Shedding some light into the dark Universe

pc/h : parsec (= 3.2 light year)

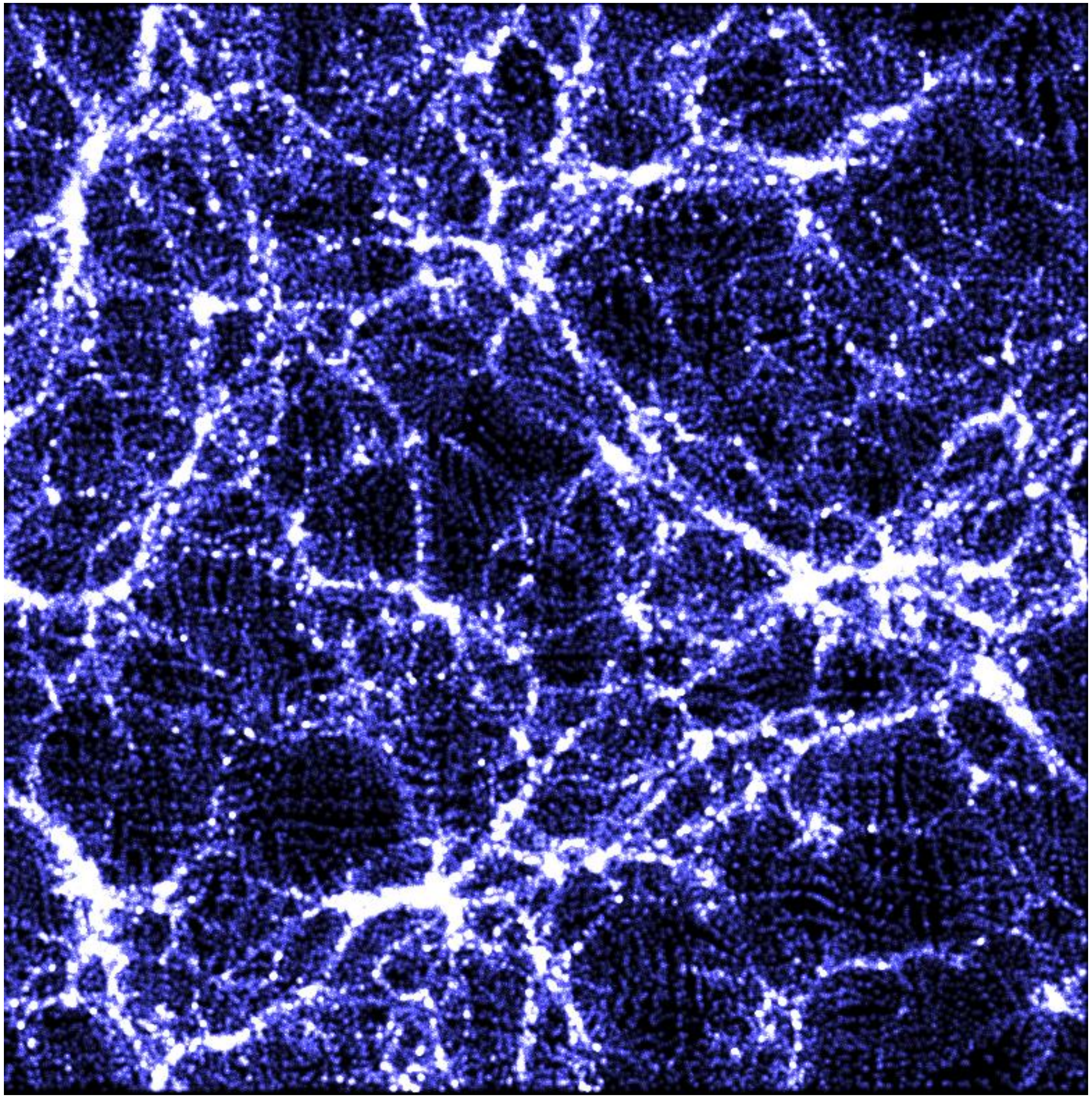


The millenium simulation project, Max Planck Institute fur Astrophysik

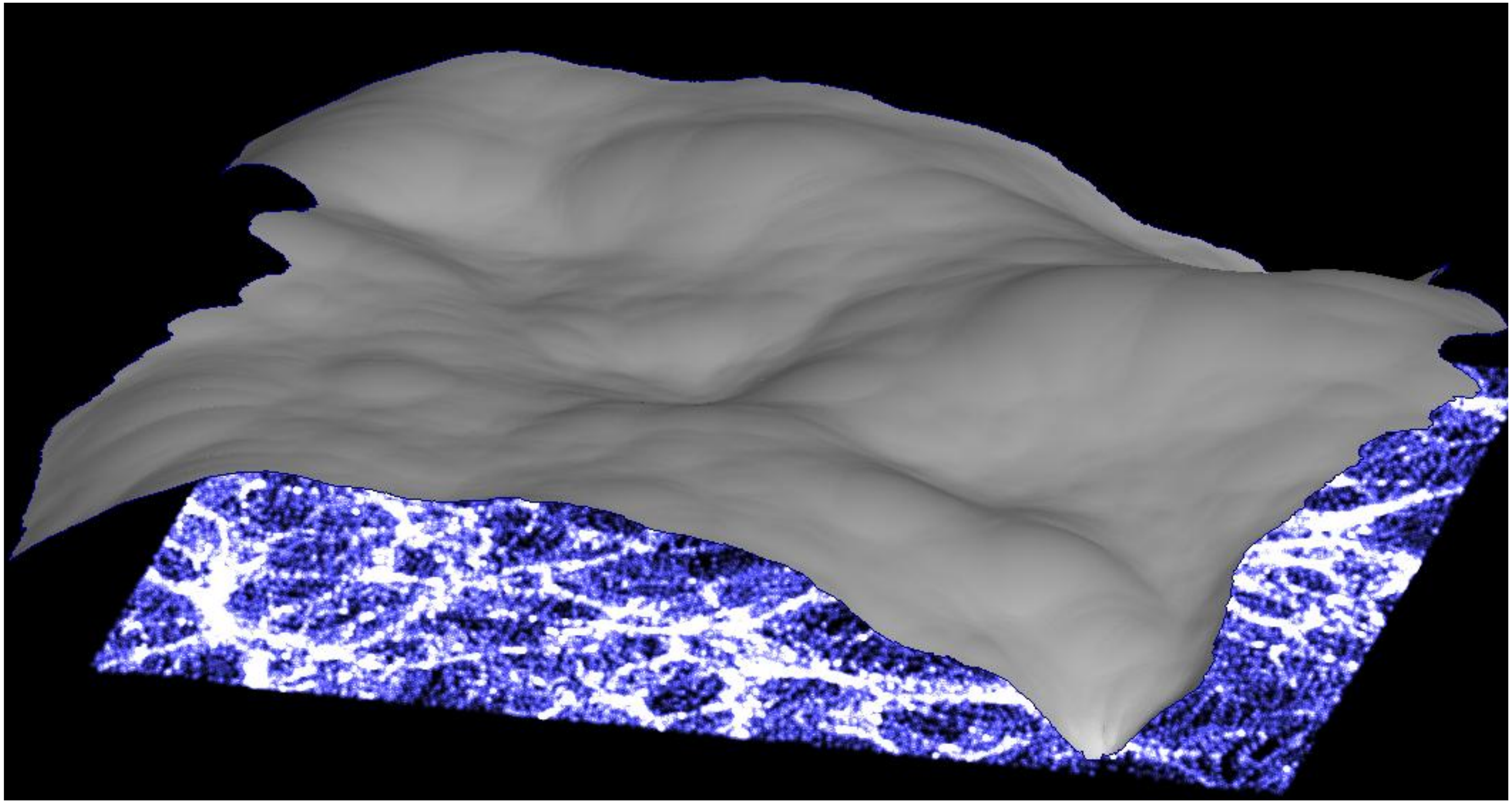
The Universal Swimming Pool



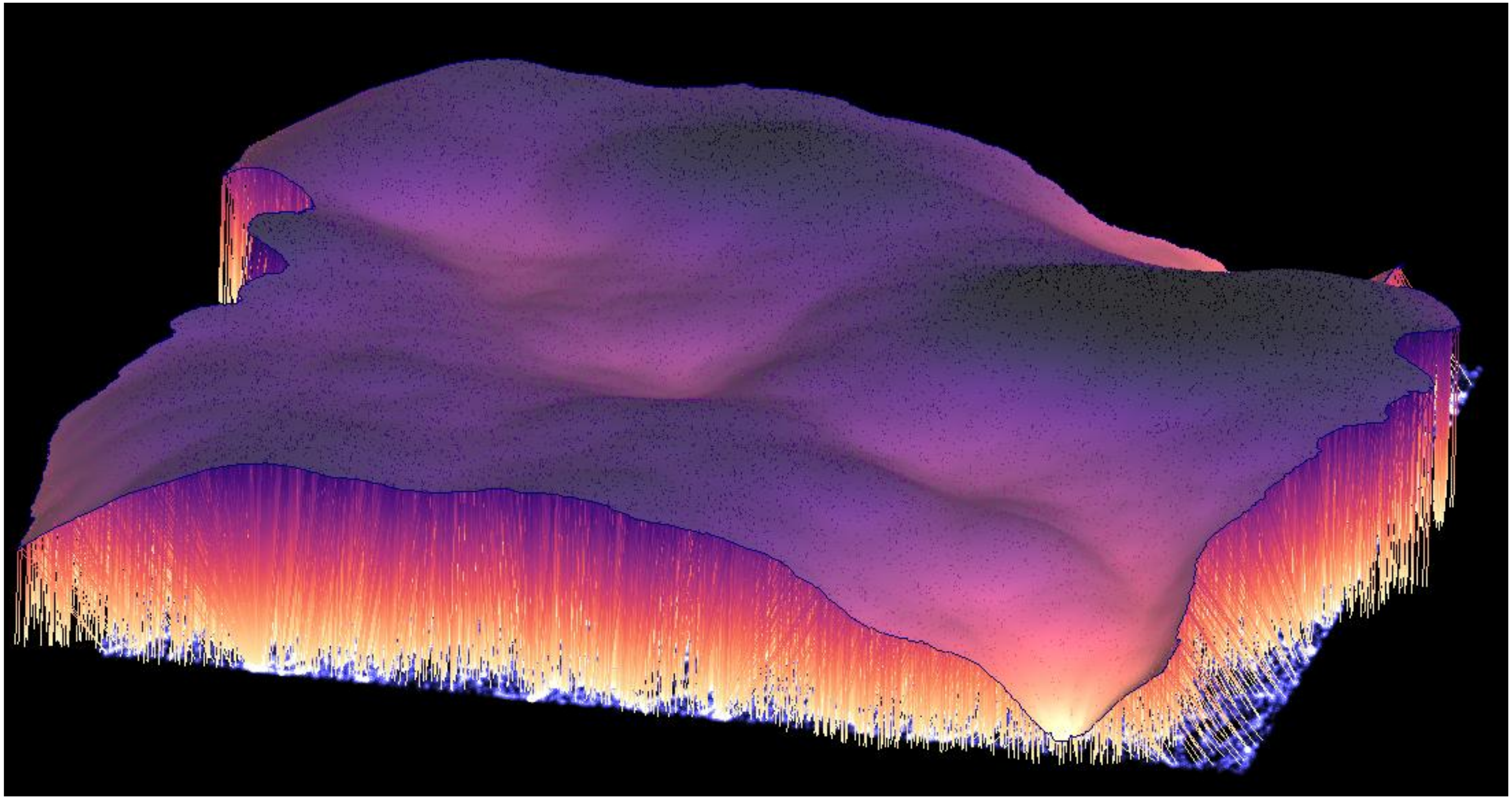
Caustics and displacement potential

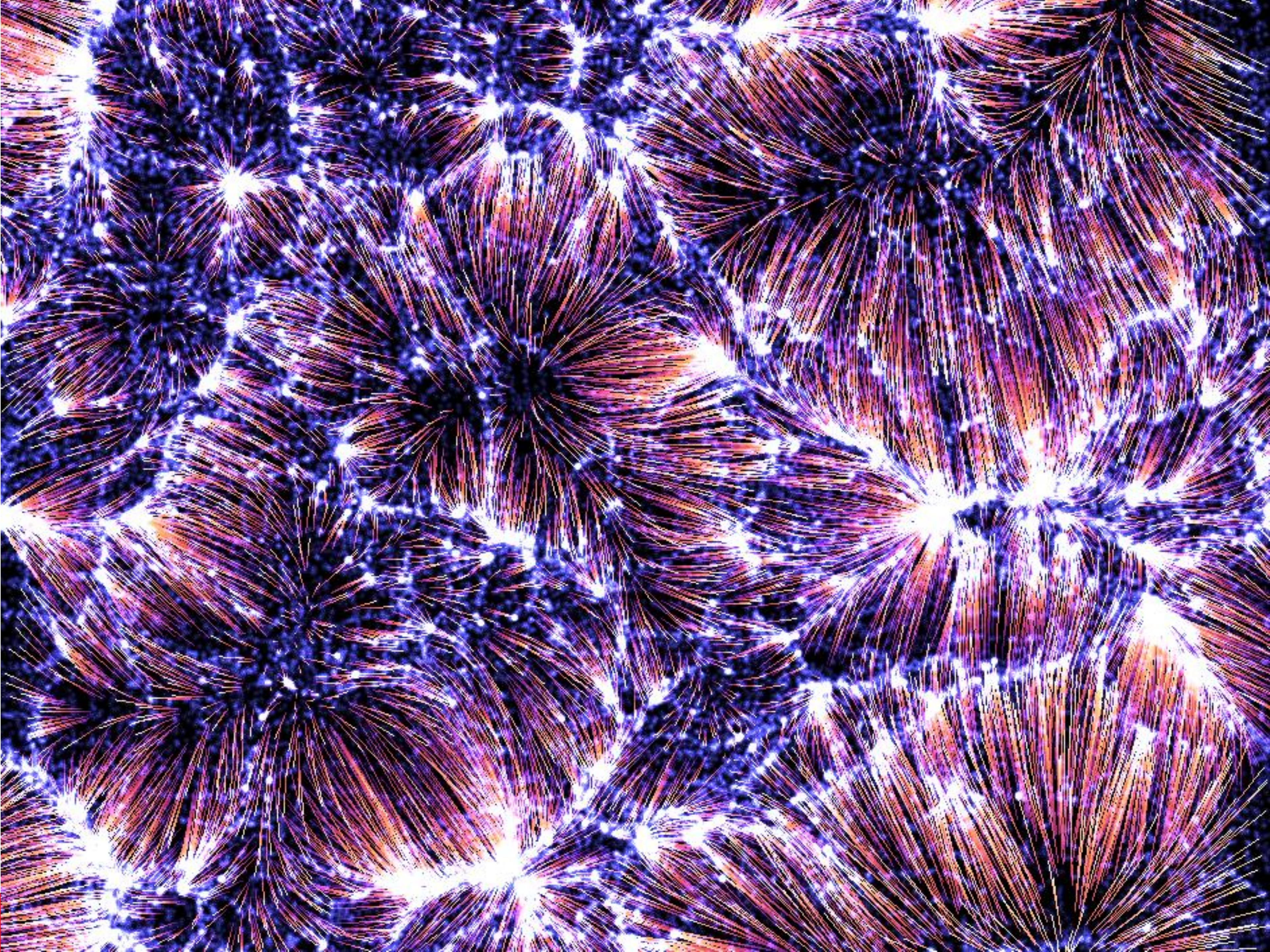


Caustics and displacement potential



Caustics and displacement potential





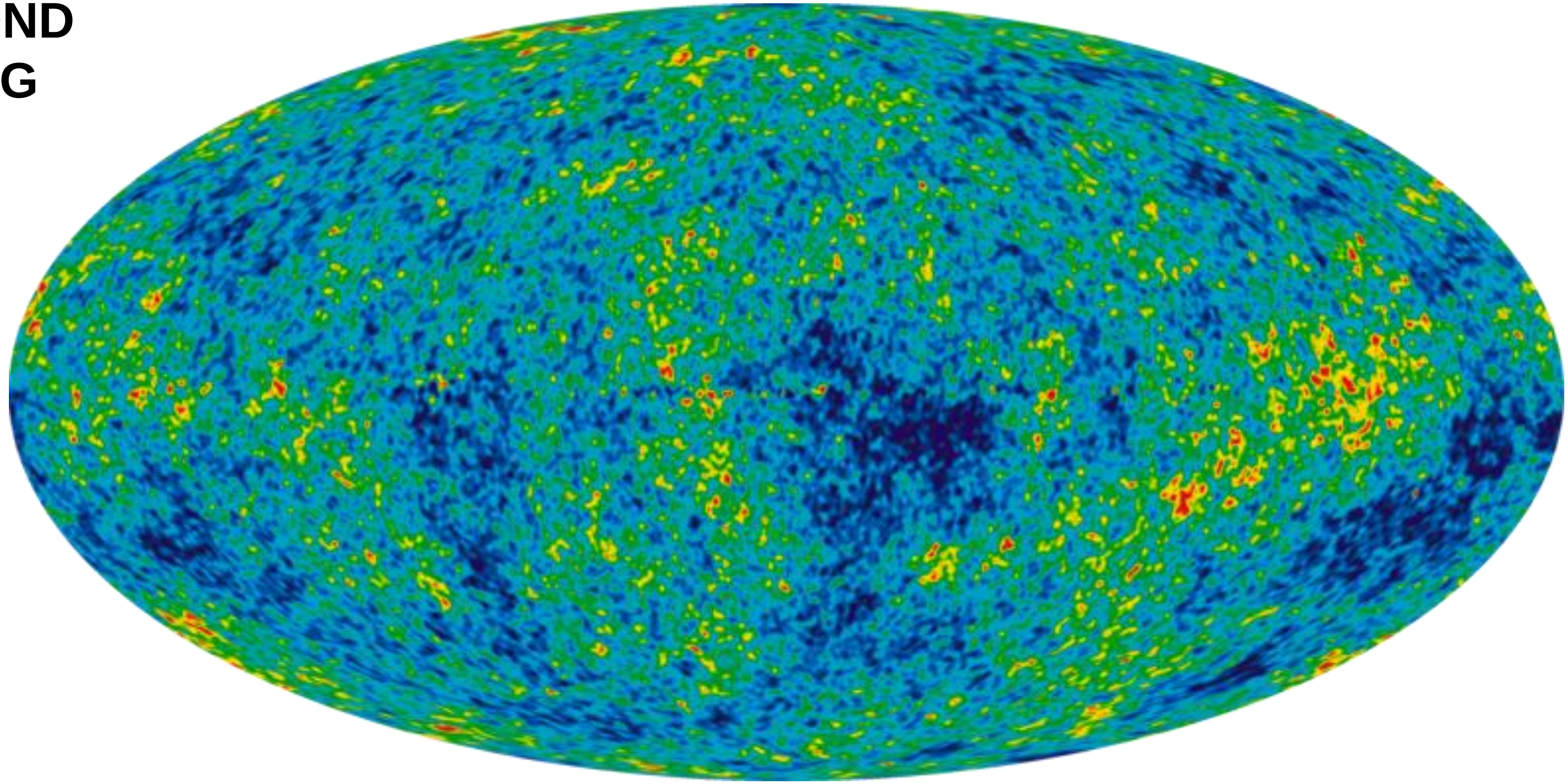
Shedding some light into the dark Universe

Models

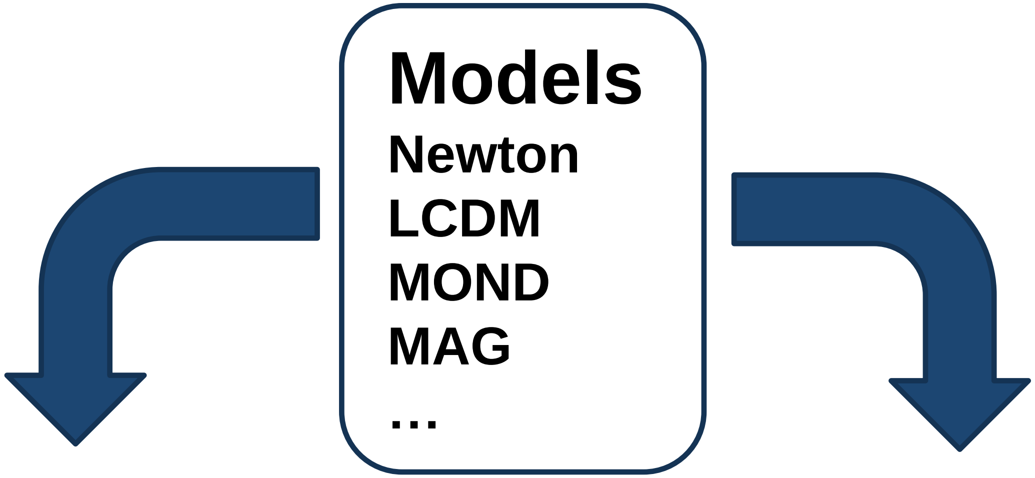
Newton
LCDM
MOND
MAG
…

Observations

Cosmic Microware Background



Connecting the present with the past



Models

Newton

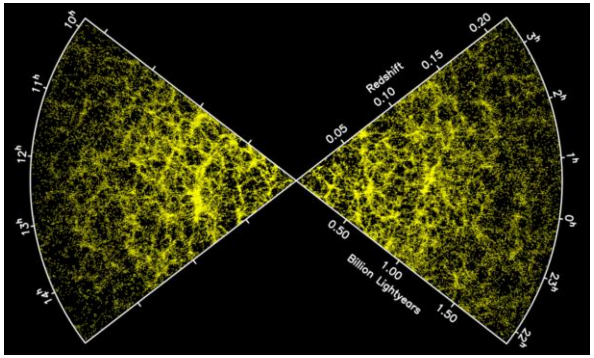
LCDM

MOND

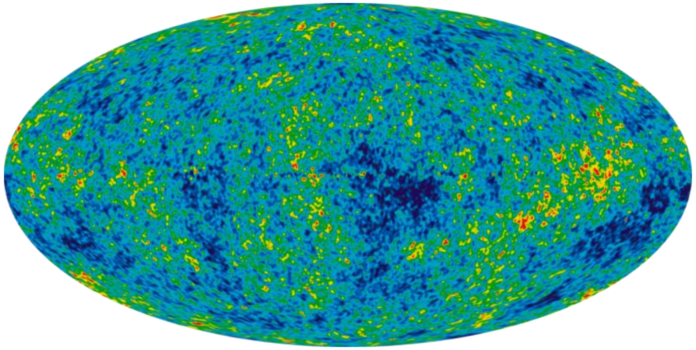
MAG

…

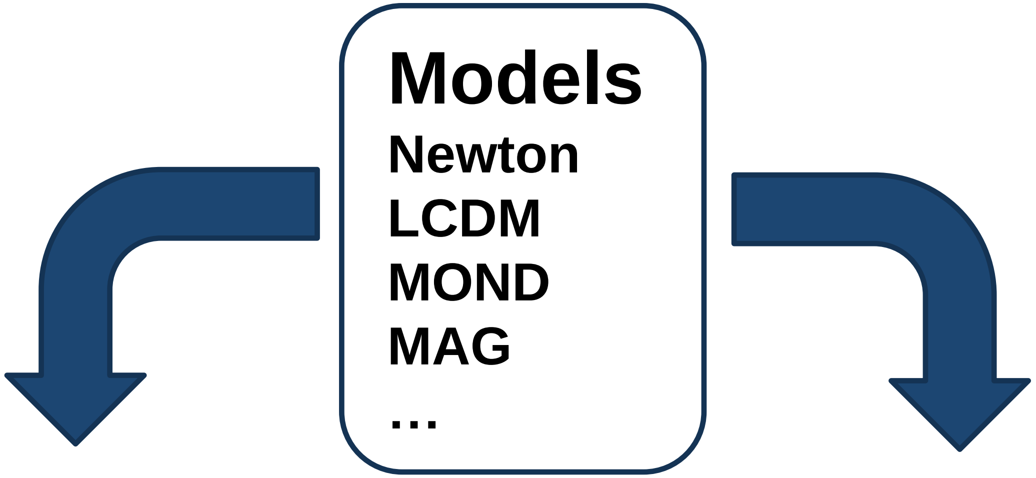
Now



13.7 billion years
(big bang + 380 000 years)



Connecting the present with the past



Models

Newton

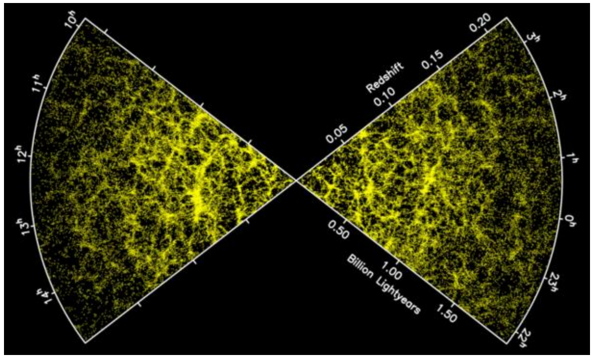
LCDM

MOND

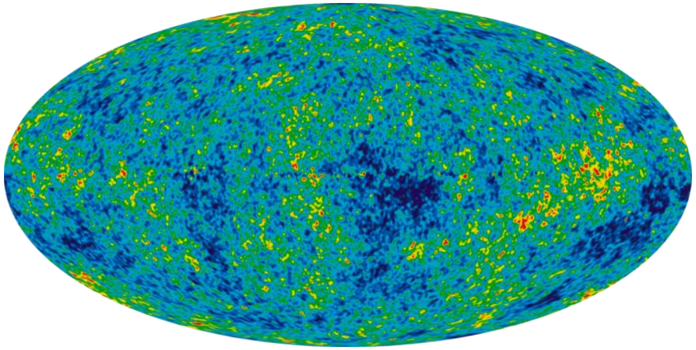
MAG

…

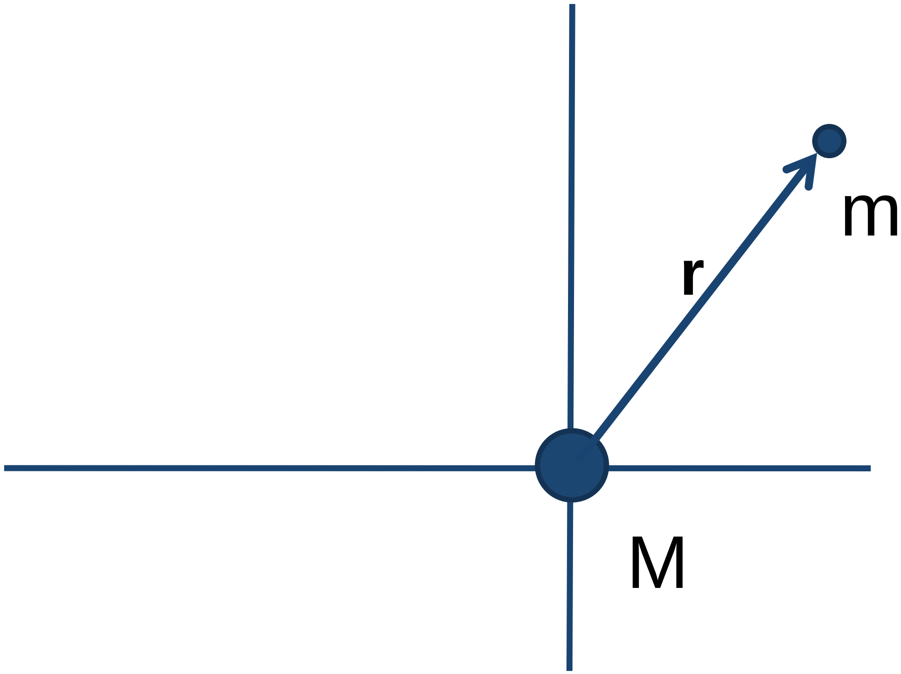
Now … 13.7 billion years



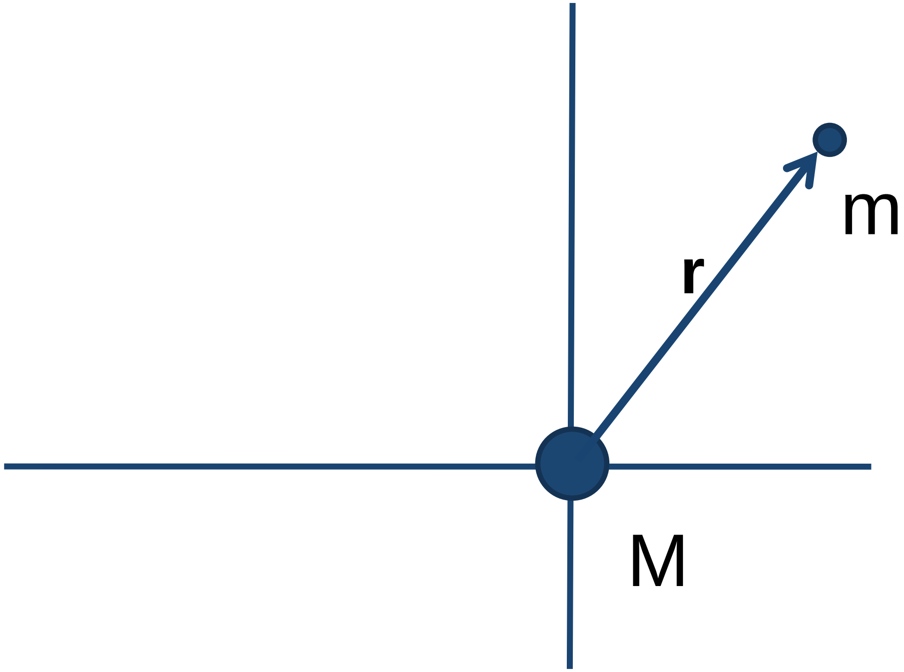
13.7 billion years
(big bang + 380 000 years)



The model

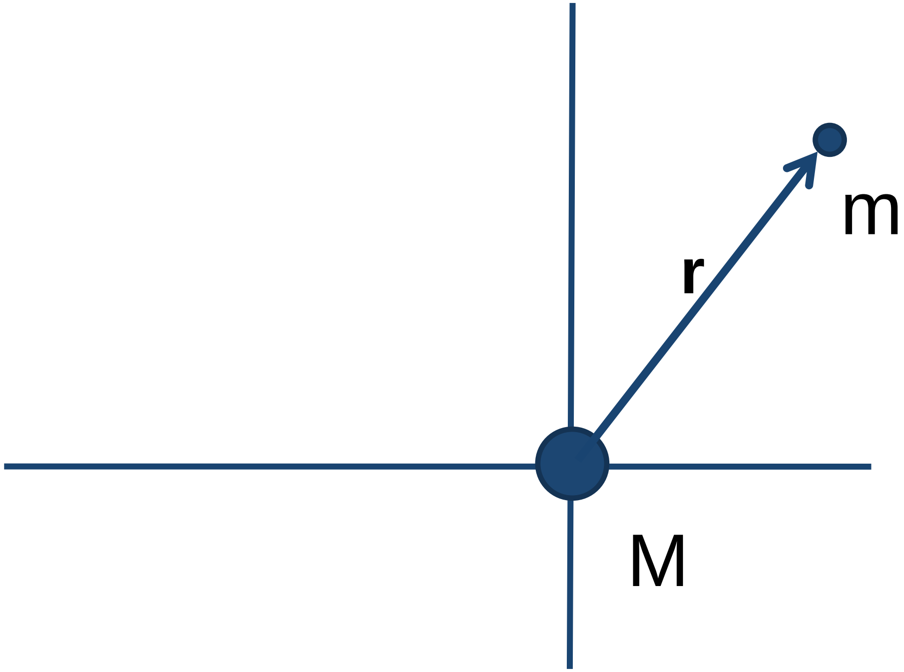


The model



$$\mathbf{F}(\mathbf{r}) = m\mathbf{G}(\mathbf{r}) = -m\mathcal{G}M\frac{\mathbf{r}}{||\mathbf{r}||^3}$$

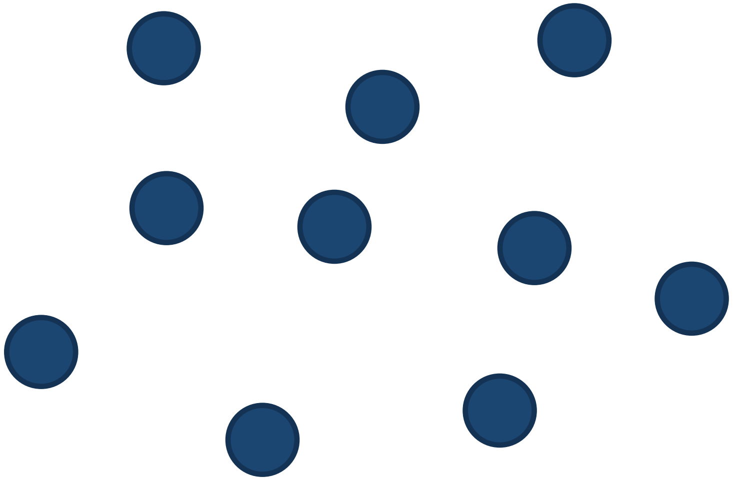
The model



$$\mathbf{F}(\mathbf{r}) = m\mathbf{G}(\mathbf{r}) = -m\mathcal{G}M\frac{\mathbf{r}}{\|\mathbf{r}\|^3}$$

$$\mathbf{G}(\mathbf{r}) = -\nabla\phi(\mathbf{r}) \quad ; \quad \phi(\mathbf{r}) = -m\mathcal{G}\frac{M}{\|\mathbf{r}\|}$$

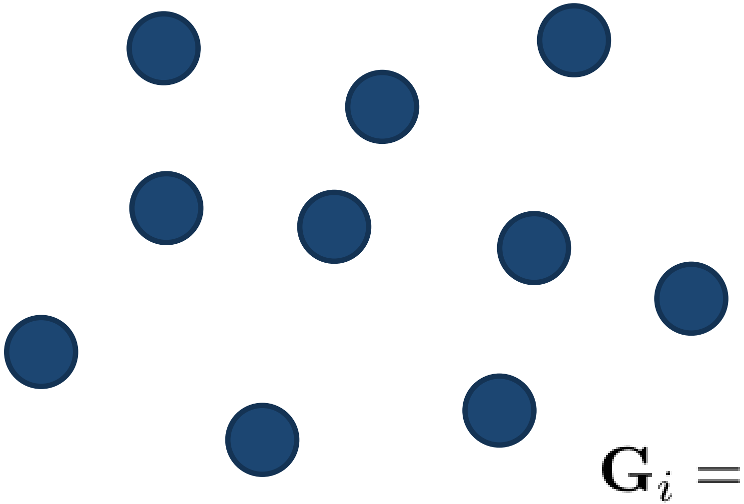
The model



$$\mathbf{F}_i = m_i \mathbf{G}_i$$

$$\mathbf{G}_i = -\mathcal{G} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|^3}$$

The model

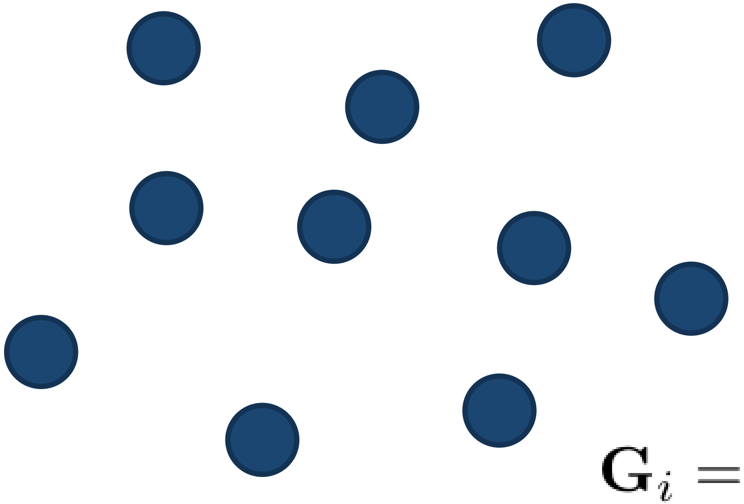


$$\mathbf{F}_i = m_i \mathbf{G}_i$$

$$\mathbf{G}_i = -\mathcal{G} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|^3}$$

$$\mathbf{G}_i = \nabla \phi_i \quad ; \quad \phi_i = -\mathcal{G} \sum_{\substack{j=1 \\ j \neq i}} \frac{m_j}{\|\mathbf{x}_i - \mathbf{x}_j\|}$$

The model



$$\mathbf{F}_i = m_i \mathbf{G}_i$$

$$\mathbf{G}_i = -\mathcal{G} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|^3}$$

$$\mathbf{G}_i = \nabla \phi_i \quad ; \quad \phi_i = -\mathcal{G} \sum_{\substack{j=1 \\ j \neq i}} \frac{m_j}{\|\mathbf{x}_i - \mathbf{x}_j\|}$$

$$\begin{cases} \frac{\partial^2 \mathbf{x}_i}{\partial t^2} & = & \nabla \phi_i \\ \phi_i & = & -\mathcal{G} \sum_{\substack{j=1 \\ j \neq i}} \frac{m_j}{\|\mathbf{x}_i - \mathbf{x}_j\|} \end{cases}$$

(F = ma)

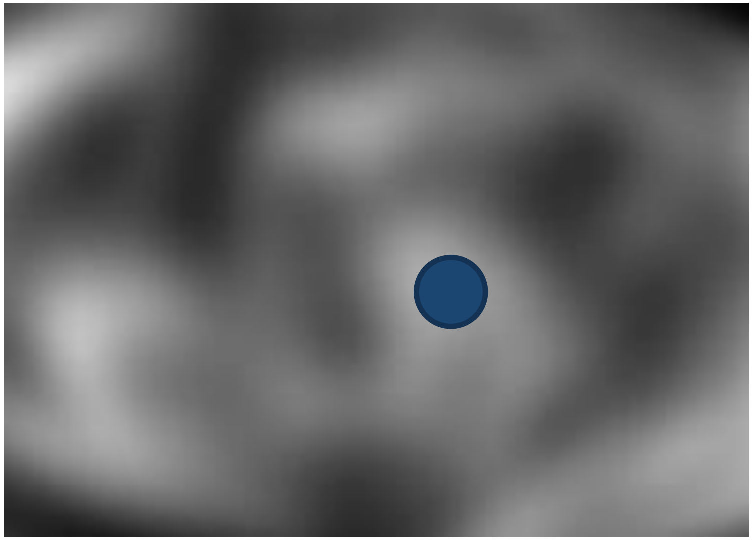
Gravity for a set of particles
(N-body)
Lagrangian coordinates

The model

$\rho(\mathbf{x}, t)$

Gravity for a density field ?
Eulerian coordinates

The model



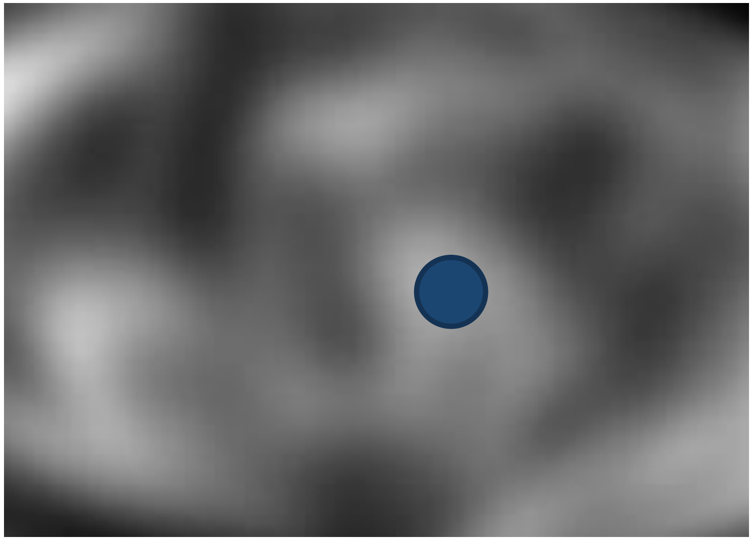
$$\rho(\mathbf{x}, t)$$

Gravity for a density field ?
Eulerian coordinates

(F=ma)

$$\mathbf{a}(\mathbf{x}, t) = \mathbf{G}(\mathbf{x}, t) = \nabla\phi(\mathbf{x}, t)$$

The model



$$\rho(\mathbf{x}, t)$$

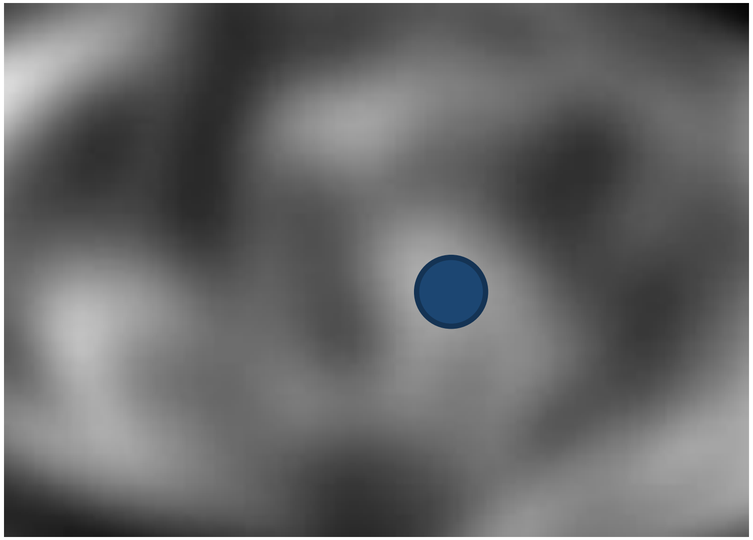
Gravity for a density field ?
Eulerian coordinates

(F=ma)

$$\mathbf{a}(\mathbf{x}, t) = \mathbf{G}(\mathbf{x}, t) = \nabla\phi(\mathbf{x}, t)$$

$$\phi(\mathbf{x}, t) = -\mathcal{G} \iiint_V \frac{\rho(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|} d\mathbf{y}$$

The model



$$\rho(\mathbf{x},t)$$

Gravity for a density field ?
Eulerian coordinates

(F=ma)

$$\mathbf{a}(\mathbf{x},t) = \mathbf{G}(\mathbf{x},t) = \nabla\phi(\mathbf{x},t)$$

$$\phi(\mathbf{x},t) = -\mathcal{G}\iiint_V \frac{\rho(\mathbf{y})}{\|\mathbf{x}-\mathbf{y}\|}d\mathbf{y}$$

Green function

$$\Delta f = g$$

$$f(\mathbf{x}) = \iiint_V K(\mathbf{x},\mathbf{y})g(\mathbf{y})d\mathbf{y}$$

$$K(\mathbf{x},\mathbf{y}) = -\frac{1}{4\pi}\frac{1}{\|\mathbf{x}-\mathbf{y}\|}$$

The model

$$\rho(\mathbf{x}, t)$$

Gravity for a density field ?
Eulerian coordinates

$$\Delta\phi = 4\pi\mathcal{G}\rho$$

(F=ma)

$$\mathbf{a}(\mathbf{x}, t) = \mathbf{G}(\mathbf{x}, t) = \nabla\phi(\mathbf{x}, t)$$

$$\phi(\mathbf{x}, t) = -\mathcal{G}\iiint_V \frac{\rho(\mathbf{y})}{\|\mathbf{x}-\mathbf{y}\|} d\mathbf{y}$$

Green function

$$\Delta f = g$$

$$f(\mathbf{x}) = \iiint_V K(\mathbf{x}, \mathbf{y}) g(\mathbf{y}) d\mathbf{y}$$

$$K(\mathbf{x}, \mathbf{y}) = -\frac{1}{4\pi}\frac{1}{\|\mathbf{x}-\mathbf{y}\|}$$

The model

$\rho(\mathbf{x}, t)$

Gravity for a density field ?
Eulerian coordinates

(F=ma)

$$\mathbf{a}(\mathbf{x}, t) = \mathbf{G}(\mathbf{x}, t) = \nabla\phi(\mathbf{x}, t)$$

$$\boxed{\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}} \quad = \quad \nabla\phi$$

Velocity field

Correction term
(convective derivative)

$$\Delta\phi = 4\pi\mathcal{G}\rho$$

The model

$$\rho(\mathbf{x}, t)$$

Gravity for a density field ?
Eulerian coordinates

(F=ma)

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} \quad = \quad \nabla \phi$$

$$\Delta \phi = 4\pi \mathcal{G} \rho$$

The model

$\rho(\mathbf{x}, t)$

Gravity for a density field ?
Eulerian coordinates

(F=ma)

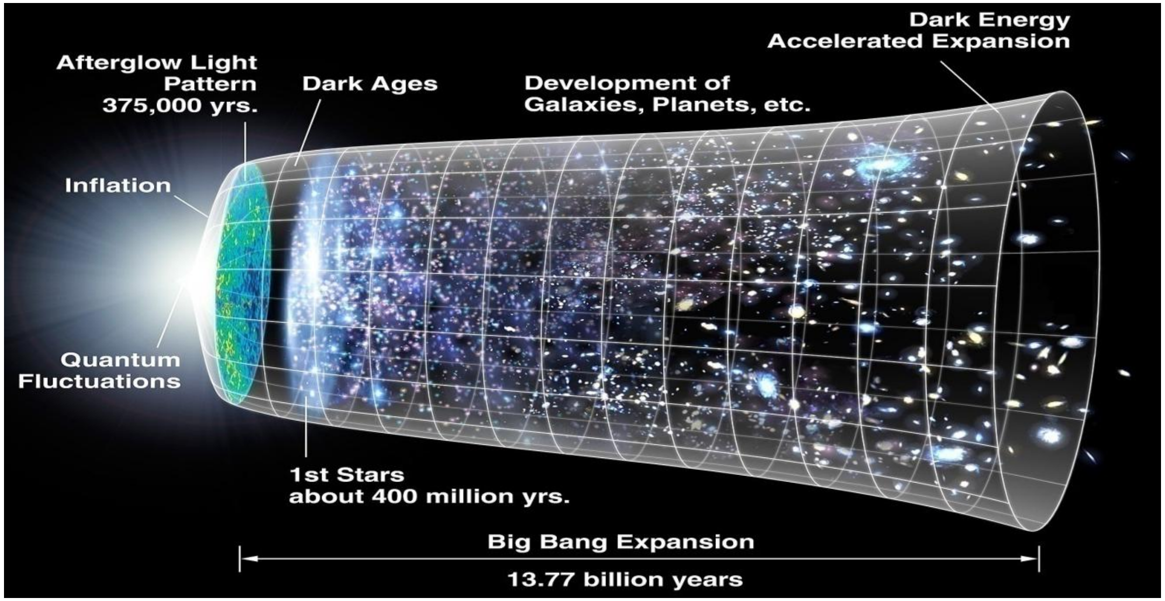
$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} \quad = \quad \nabla\phi$$

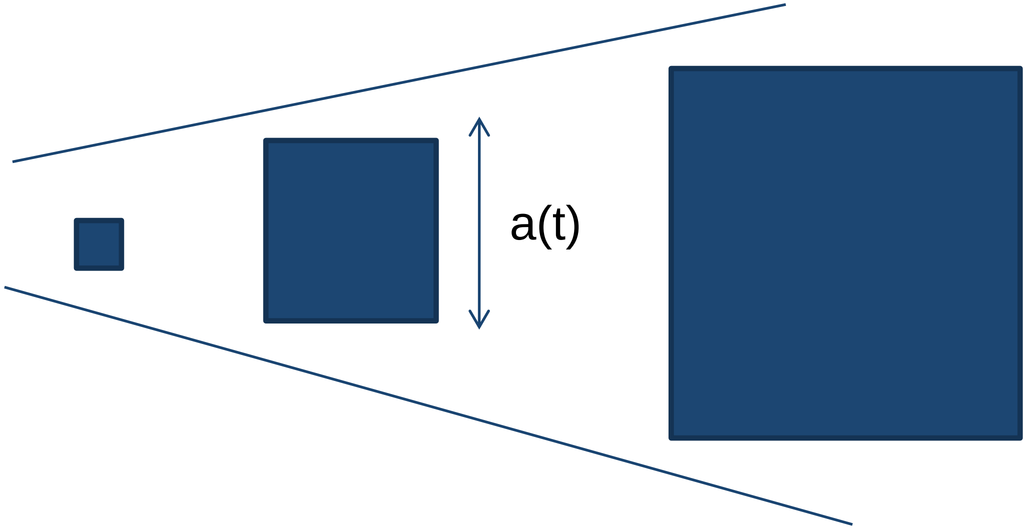
$$\Delta\phi = 4\pi\mathcal{G}\rho$$

$$\partial_t \rho + \nabla \cdot (\rho\mathbf{u}) \quad = \quad 0$$

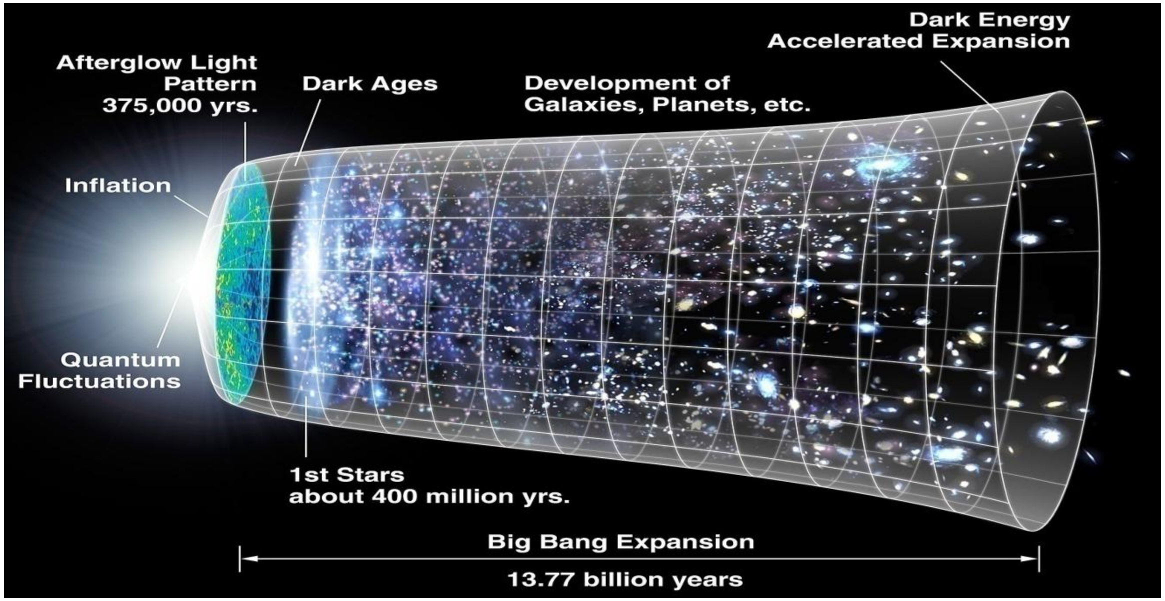
(Mass conservation *continuity eqn*)

The model


Dark Energy Accelerated Expansion
Afterglow Light Pattern 375,000 yrs.
Dark Ages
Development of Galaxies, Planets, etc.
Inflation
Quantum Fluctuations
1st Stars about 400 million yrs.
Big Bang Expansion
13.77 billion years


a(t)

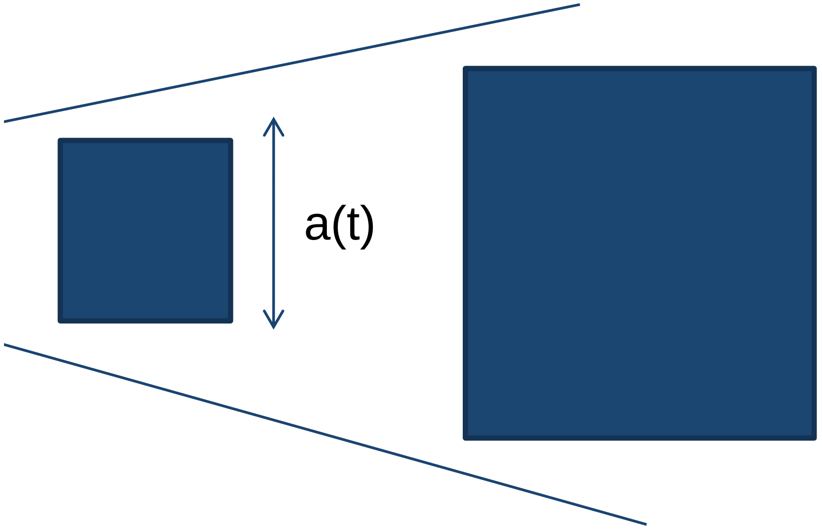
The model



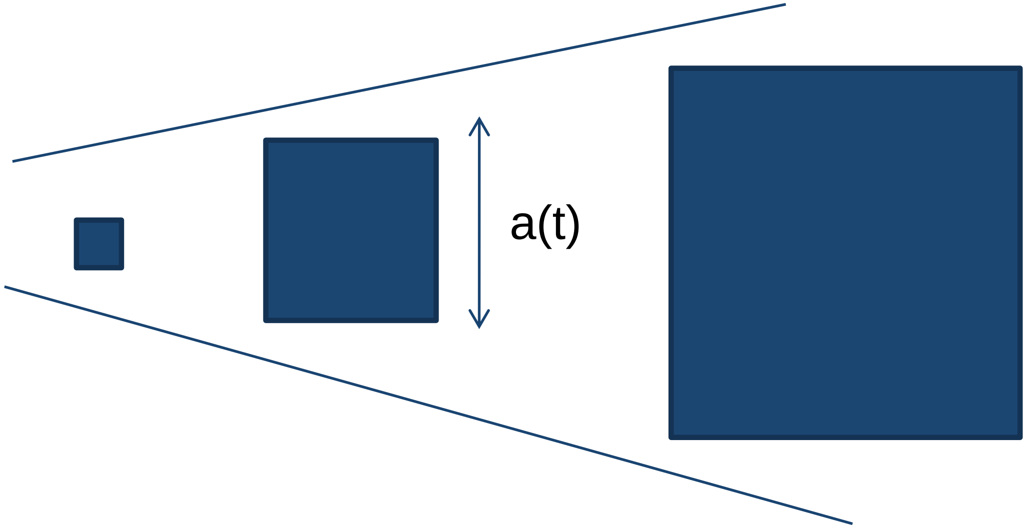
$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\left(\rho + \frac{3p}{c^2}\right) + \frac{\Lambda c^2}{3}$$

FRIEDMANN EQUATIONS

$$\frac{\dot{a}^2 + kc^2}{a^2} = \frac{8\pi G\rho + \Lambda c^2}{3}$$



The model

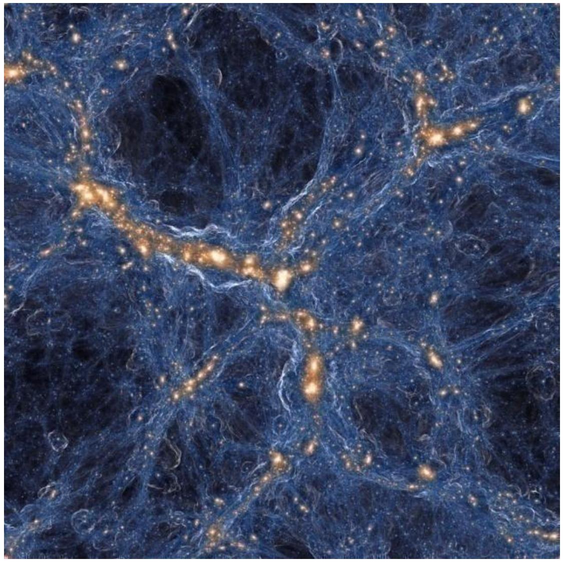


$$\begin{cases} \partial_\tau \mathbf{v} + (\mathbf{v}\cdot\nabla_x)\mathbf{v} = -\boxed{\frac{3}{2\tau}}(\nabla_x\phi + \boxed{\mathbf{v}}) \\ \partial_\tau \rho + \nabla_x \cdot (\rho\mathbf{v}) = 0 \\ \Delta\phi = 4\pi\mathcal{G}\frac{\rho - 1}{\tau} \end{cases}$$

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem

Initial condition (homogeneous)

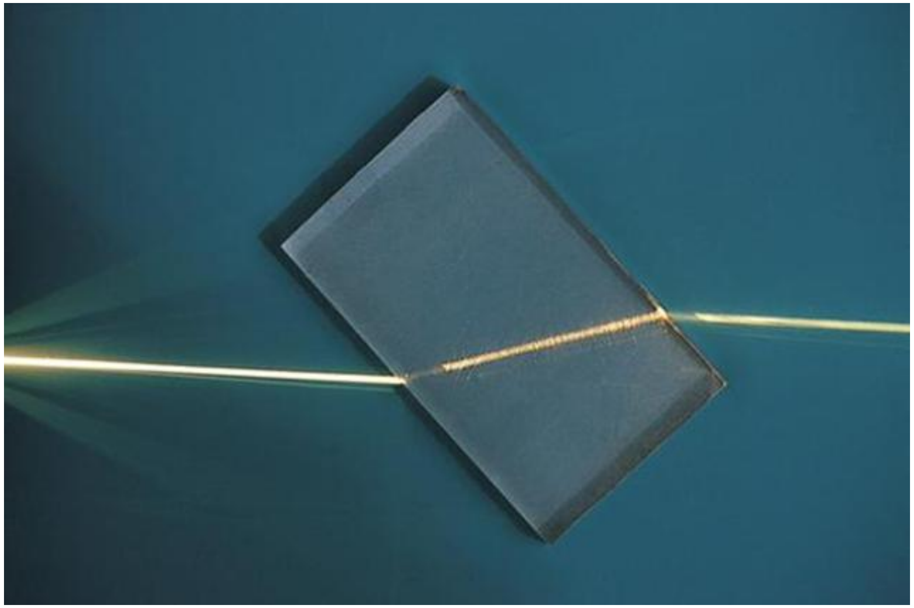


Redshift acquisition survey

$$\begin{cases} \partial_\tau \mathbf{v} + (\mathbf{v} \cdot \nabla_x)\mathbf{v} = -\dfrac{3}{2\tau}(\nabla_x \phi + \mathbf{v}) \\ \partial_\tau \rho + \nabla_x \cdot (\rho \mathbf{v}) = 0 \\ \Delta \phi = 4\pi \mathcal{G} \dfrac{\rho - 1}{\tau} \end{cases}$$

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

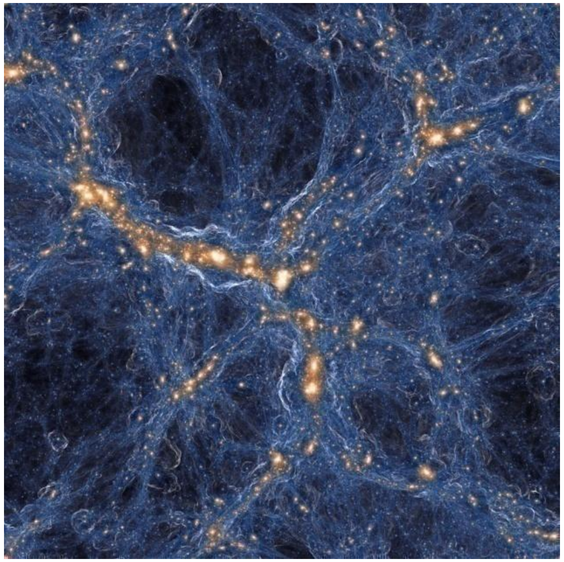
The inverse problem – least action



[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – least action

Initial condition (homogeneous)



Redshift acquisition survey

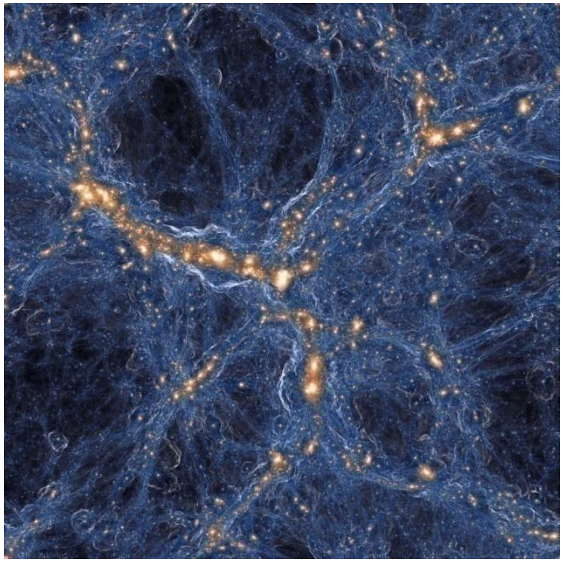
$$I = \frac{1}{2}\int_{\tau_I}^{\tau_F}\int_V \quad (\rho|\mathbf{v}|^2 + \frac{3}{2}|\nabla_x\phi|^2)\tau^{3/2} \quad d^3\mathbf{x}\, d\tau$$

$$\rho(.,\tau_I) = \rho_I(.) = 1 \quad ; \quad \rho(.,\tau_F) = \rho_F(.)$$

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – least action

Initial condition (homogeneous)



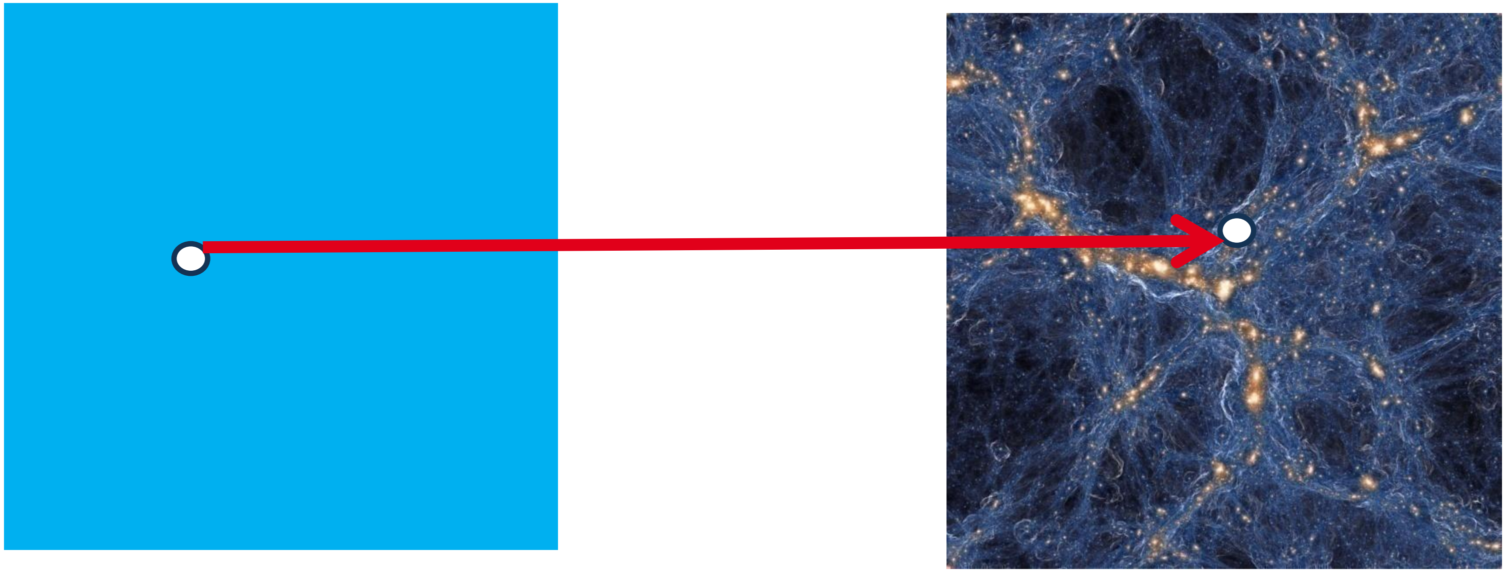
Redshift acquisition survey

$$I = \frac{1}{2} \int_{\tau_I}^{\tau_F} \int_V \quad \rho |\mathbf{v}|^2 \quad d^3\mathbf{x} \; d\tau$$

$$\rho(.,\tau_I) = \rho_I(.) = 1 \quad ; \quad \rho(.,\tau_F) = \rho_F(.)$$

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – Benamou-Brenier thm



Initial condition (homogeneous)

Redshift acquisition survey

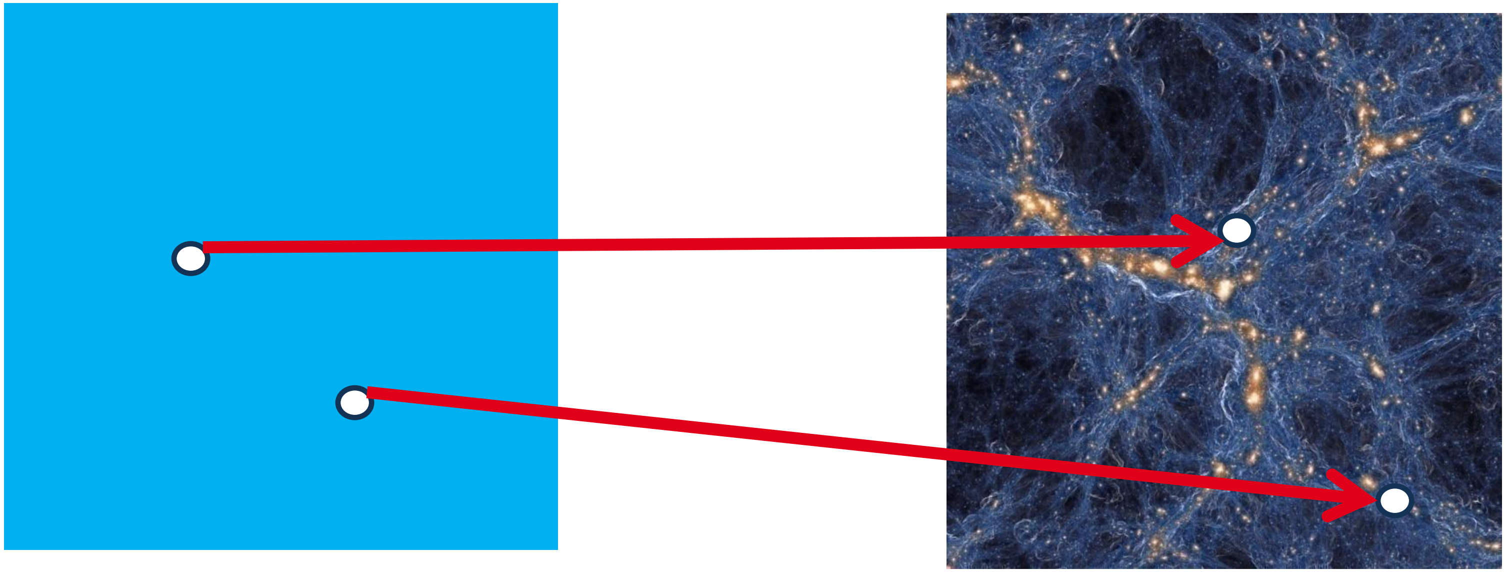
Everybody moves along a straight line at constant speed

$$I = \frac{1}{2}\int_{\tau_I}^{\tau_F}\int_V \quad \rho|\mathbf{v}|^2 \quad d^3\mathbf{x}\, d\tau$$

$$\rho(.,\tau_I) = \rho_I(.) = 1 \quad ; \quad \rho(.,\tau_F) = \rho_F(.)$$

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – Benamou-Brenier thm



Initial condition (homogeneous)

Redshift acquisition survey

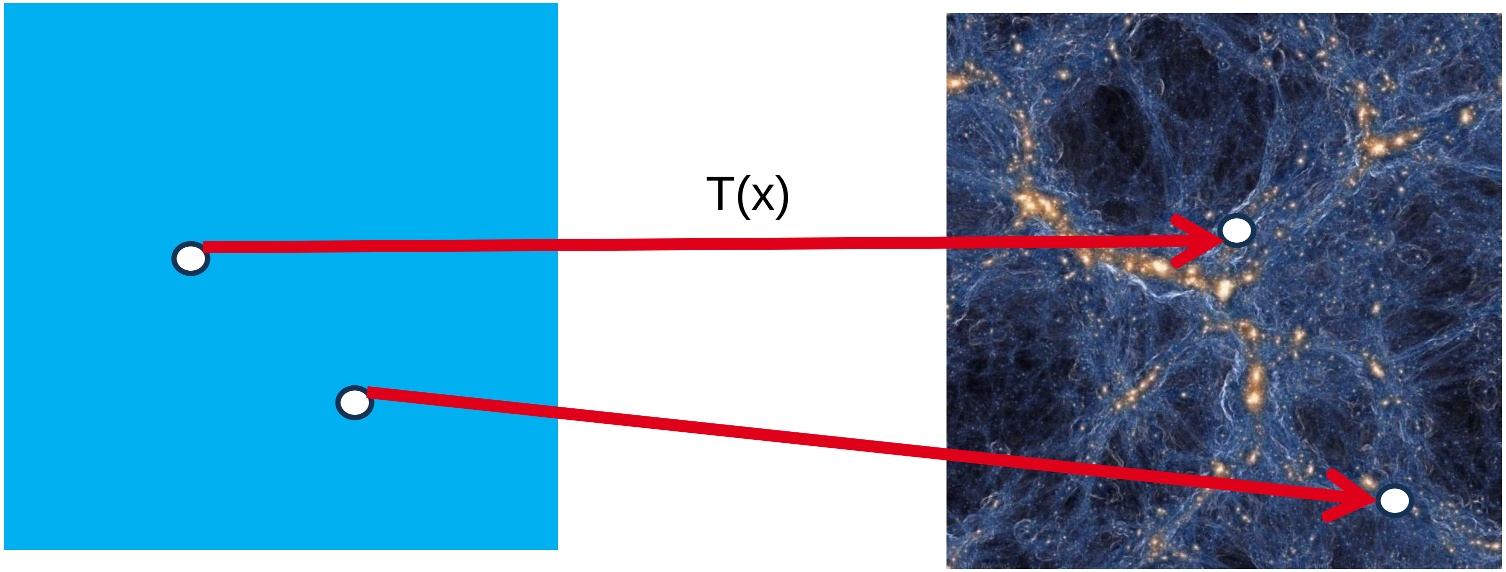
Which point corresponds to which point ?

$$I = \frac{1}{2}\int_{\tau_I}^{\tau_F}\int_V \rho|\mathbf{v}|^2 \quad d^3\mathbf{x}\; d\tau$$

$$\rho(.,\tau_I) = \rho_I(.) = 1 \quad ; \quad \rho(.,\tau_F) = \rho_F(.)$$

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – Benamou-Brenier thm



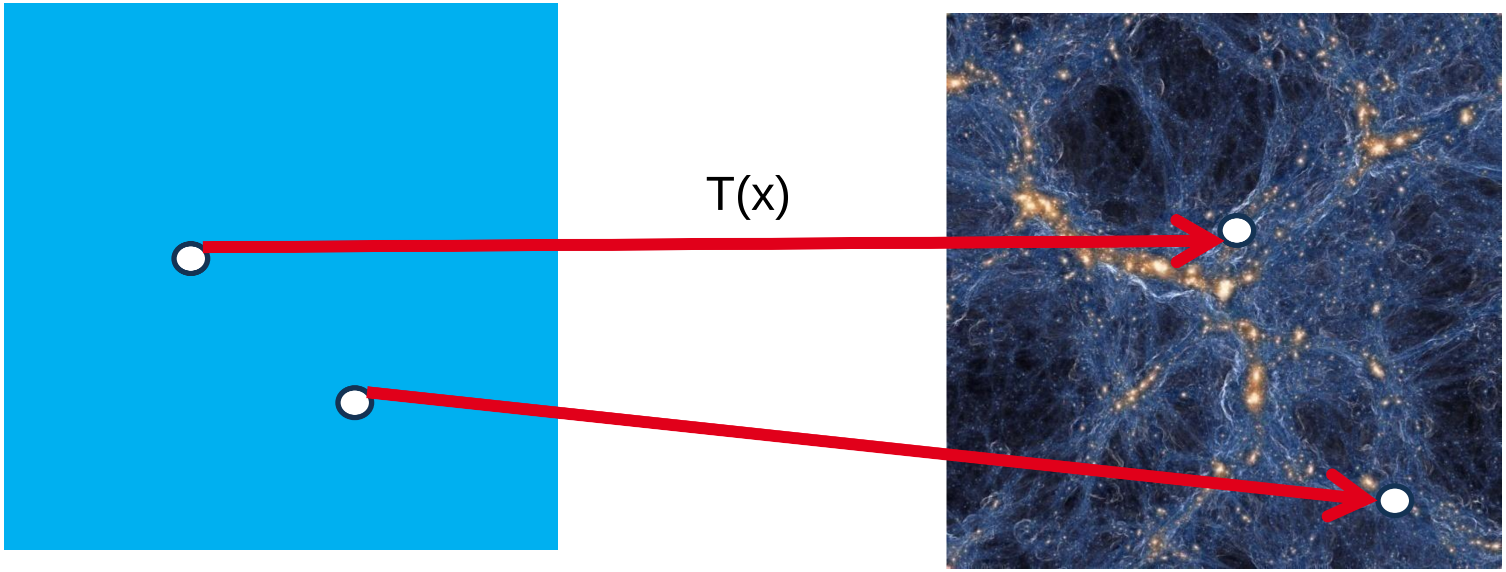
Initial condition (homogeneous)

Redshift acquisition survey

Which point corresponds to which point ?

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – Benamou-Brenier thm



Initial condition (homogeneous)

Redshift acquisition survey

Minimize

$$A(\rho,v) = (t_2 - t_1) \int_{t_1}^{t_2} \int_V \rho(x,t)\, \|v(t,x)\|^2 dxdt$$

s.t. $\rho(t_1,.) = \rho_1$; $\rho(t_2,.) = \rho_2$; $\frac{d\,\rho}{dt} = - \mathrm{div}(\rho v)$

$$\Longleftrightarrow$$

Optimal transport

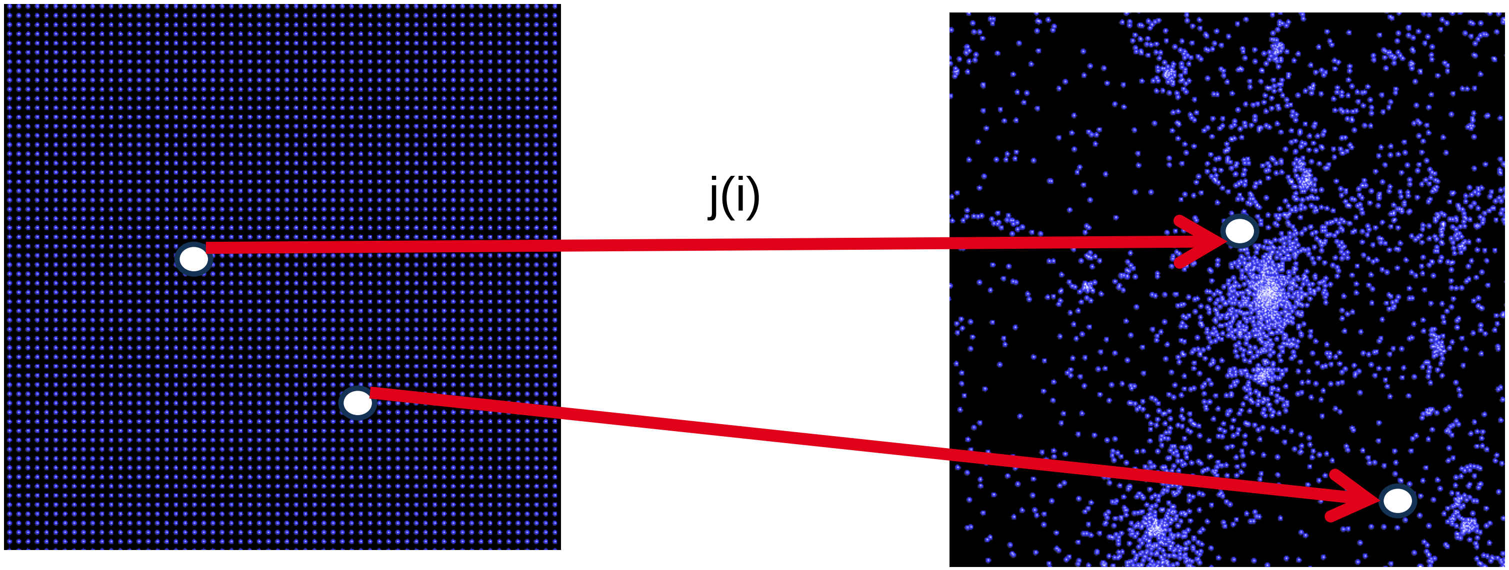
Minimize C(T) =

$$\int_V \rho_1(x) \| \; x - T(x) \, \|2 \; dx$$

s.t. T is measure-preserving

[Frisch, Matarrese, Mohayaee, Sobolevski 2002 (Nature)]
[Brenier, Frish, Henon, Loeper, Matarrese, Mohayaee, Sobolevskii 2003]

The inverse problem – Benamou-Brenier thm



Initial condition (homogeneous)

Redshift acquisition survey

Optimal transport

Minimize

$$A(\rho,v) = (t_2-t_1)\int_{t_1}^{t_2}\int_{V} \rho(x,t)\,||v(t,x)||^2 dxdt$$

s.t. $\rho(t_1,.) = \rho_1$; $\rho(t_2,.) = \rho_2$; $\frac{d\rho}{dt} = -\,\mathrm{div}(\rho v)$

⟺

Minimize C(T) =

$$\sum || \; x_i - y_{j(i)} \; ||^2 \, dx$$

2

Optimal Transport

Part. 2 Optimal Transport – Monge's problem

(X;µ)

(Y;v)

Two measures µ, v such that $\int_X d\mu(x) = \int_Y dv(x)$

Part. 2 Optimal Transport – Monge's problem

$(X;\mu)$

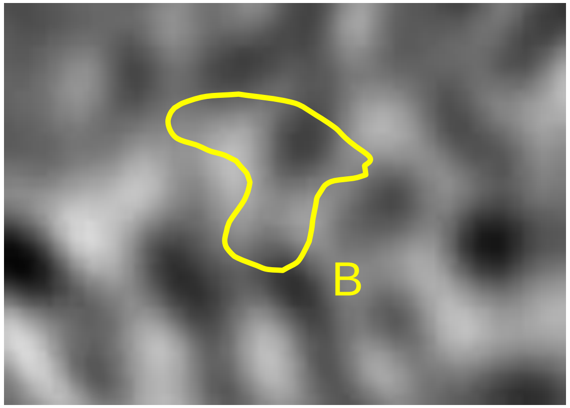
$(Y;\nu)$

A map T is a ***transport map*** between μ and ν if

$$\mu(T^{-1}(B)) = \nu(B) \text{ for any Borel subset } B \text{ of } Y$$

Part. 2 Optimal Transport – Monge’s problem

$(X;\mu)$

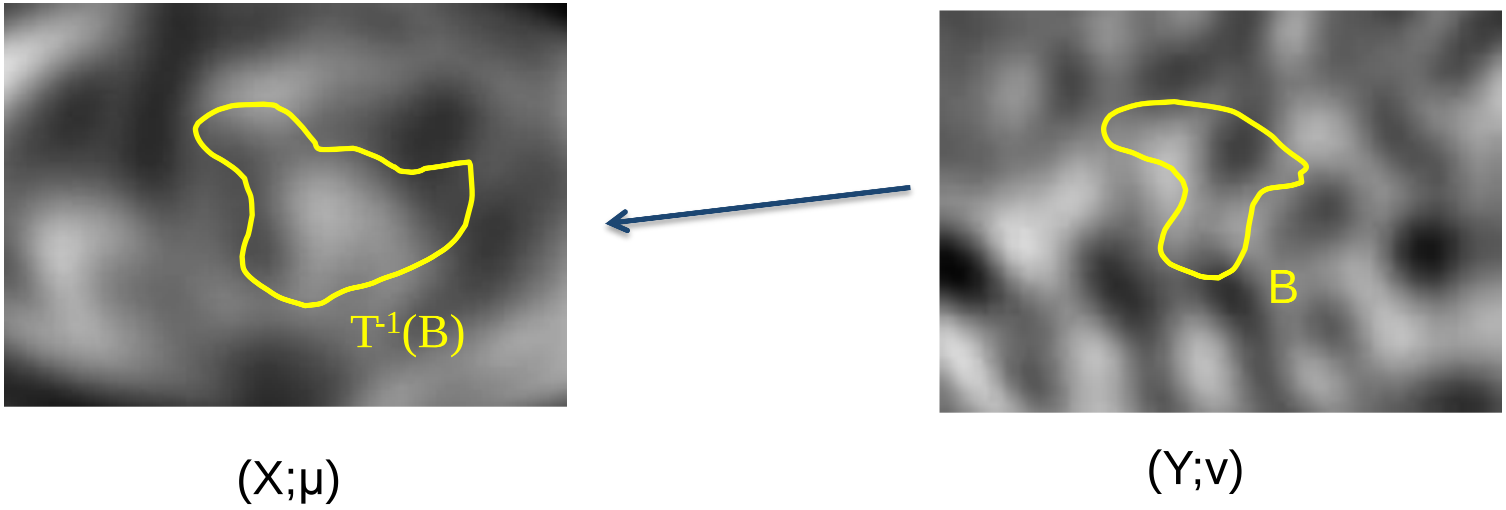


$(Y;\nu)$

A map T is a ***transport map*** between μ and ν if

$\mu(T^{-1}(B)) = \nu(B)$ for any Borel subset B

Part. 2 Optimal Transport – Monge’s problem



A map T is a ***transport map*** between μ and ν if
$\mu(T^{-1}(B)) = \nu(B)$ for any Borel subset B

Part. 2 Optimal Transport – Monge's problem

$(X;\mu)$

$(Y;\nu)$

A map T is a ***transport map*** between μ and ν if

$\mu(T^{-1}(B)) = \nu(B)$ for any Borel subset B

(or $\nu = T\#\mu$ the ***pushforward*** of μ)

Part. 2 Optimal Transport – Monge’s problem

(X;μ)

(Y;v)

Monge’s problem:

Find a transport map T that minimizes $C(T) = \int_X || x - T(x) ||^2 d\mu(x)$

Part. 2 Optimal Transport – Monge's problem

Monge's problem:

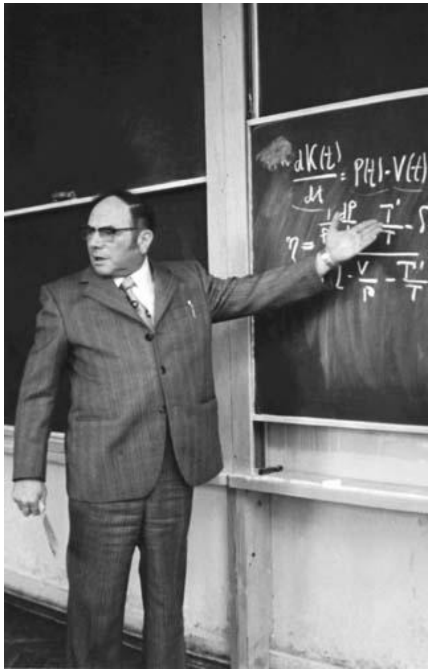
Find a transport map T that minimizes $C(T) = \int_X || x - T(x) ||^2 d\mu(x)$

- Difficult to study
- Constraint (T is a transport map) is complicated
- If μ has an atom (isolated Dirac),
  it can only be mapped to another Dirac
  (T needs to be a map)

Part. 2 Optimal Transport – Kantorovich

Monge's problem:

Find a transport map T that minimizes $C(T) = \int_X \| x - T(x) \|^2 d\mu(x)$



***Kantorovich's problem* (1942):**

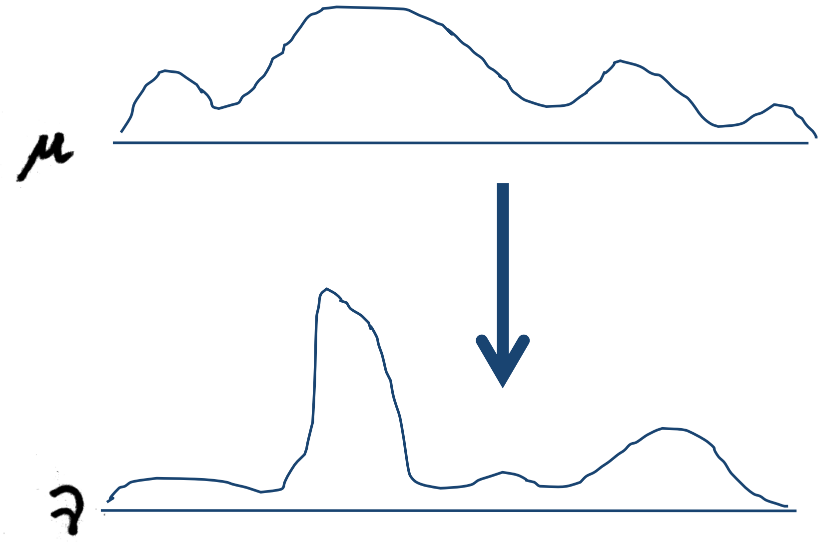
Find a measure γ defined on X x Y

such that $\int_{x \text{ in } X} d\gamma(x,y) = d\nu(y)$

and $\int_{y \text{ in } Y} d\gamma(x,y) = d\mu(x)$

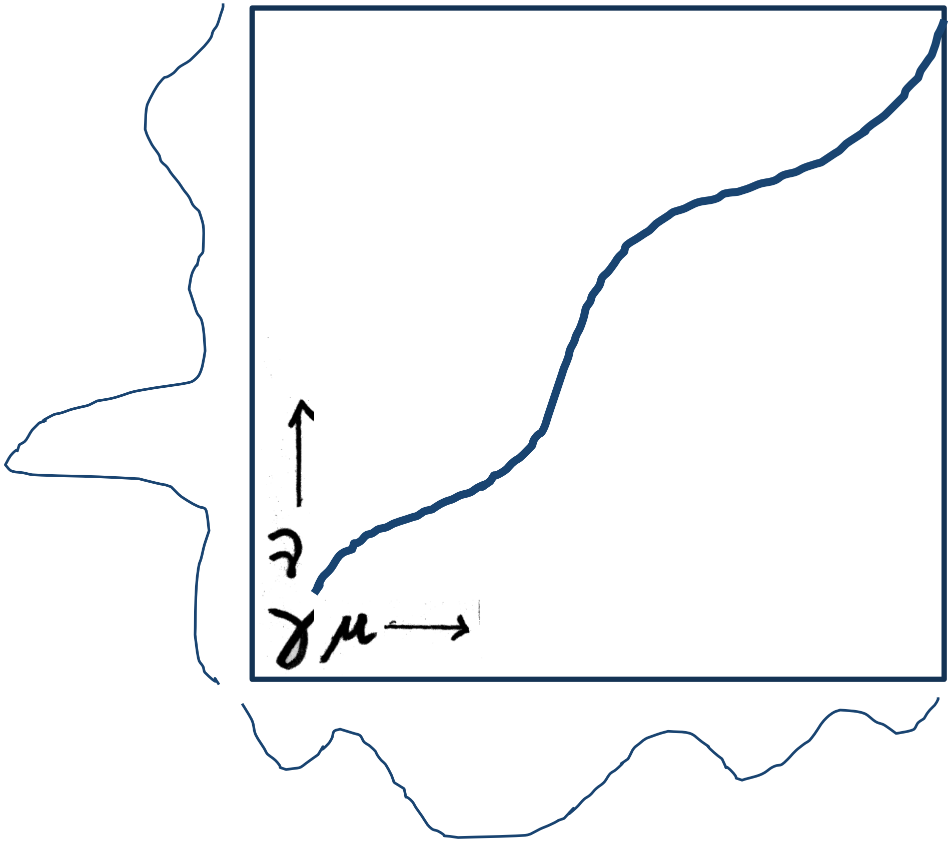
that minimizes $\iint_{X \times Y} \| x - y \|^2 d\gamma(x,y)$

Part. 2 Optimal Transport – Kantorovich



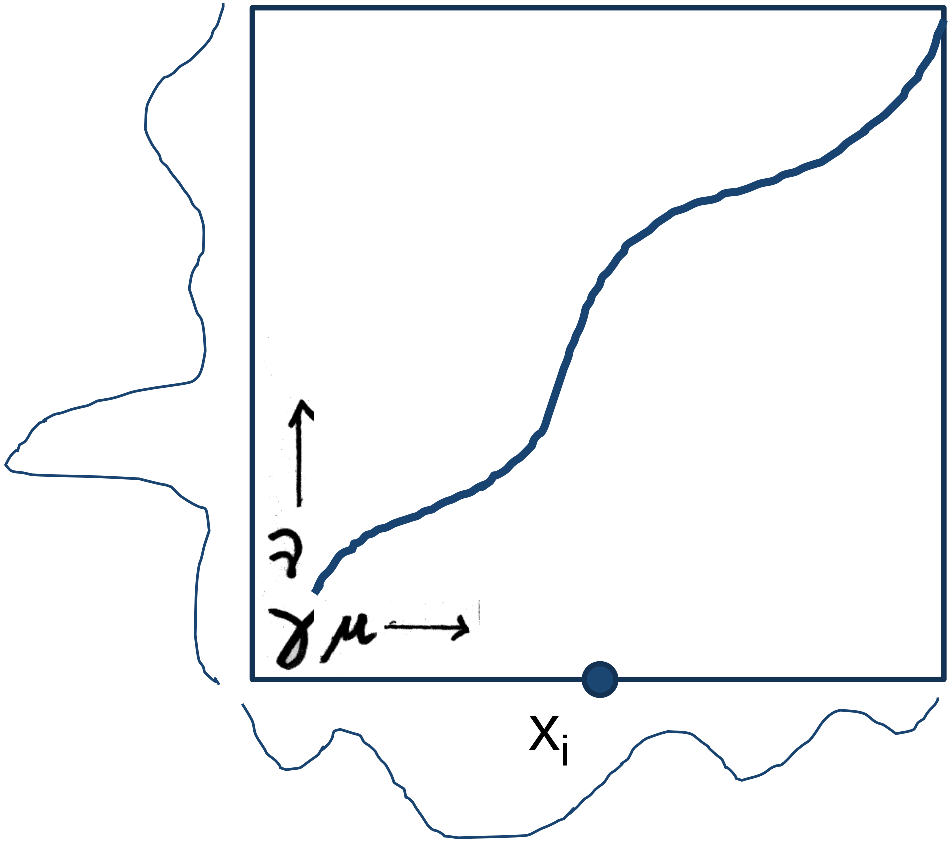
Transport plan – example in 1D

Part. 2 Optimal Transport – Kantorovich



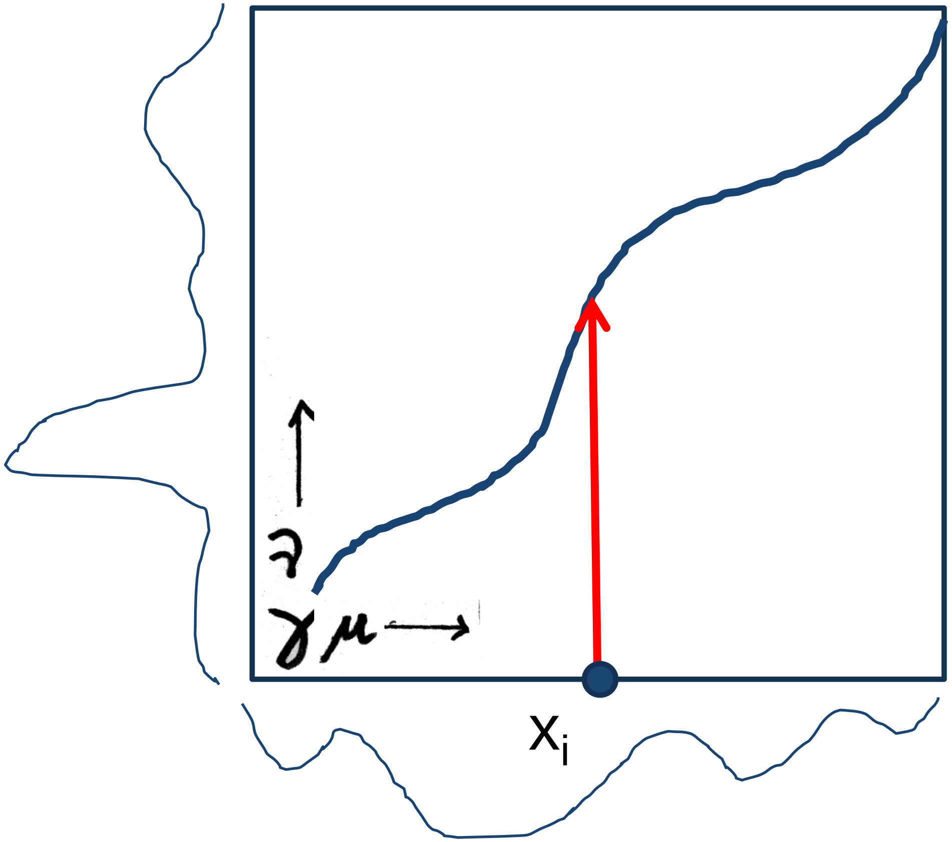
Transport plan – example in 1D

Part. 2 Optimal Transport – Kantorovich



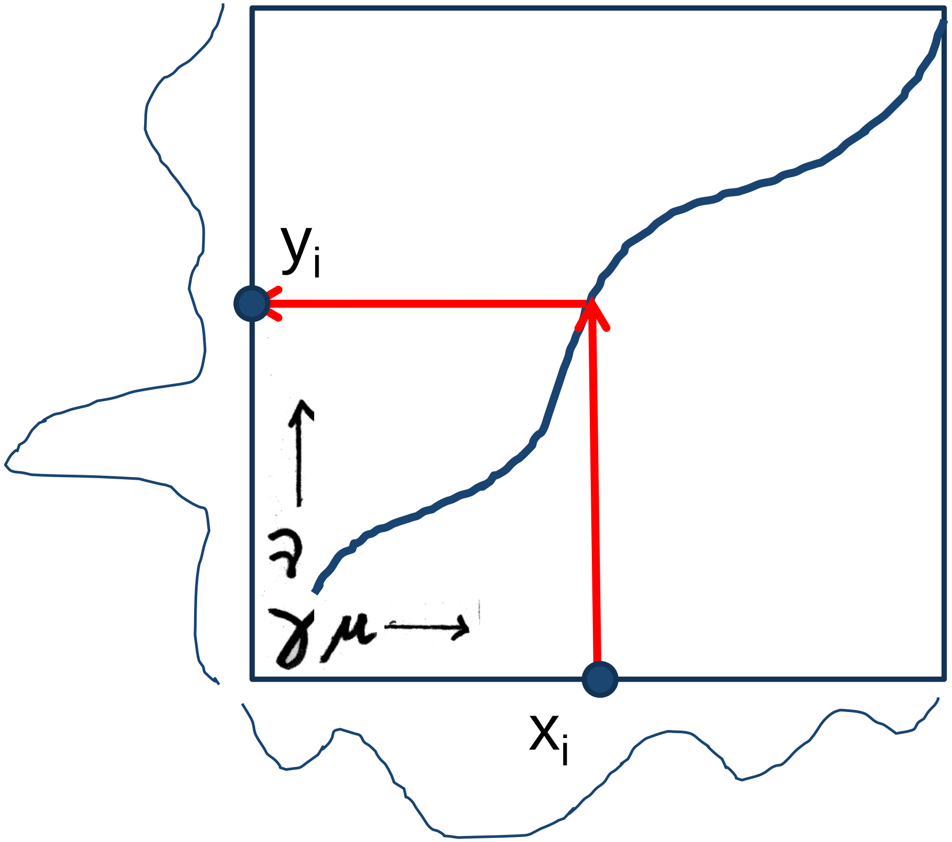
Transport plan – example in 1D

Part. 2 Optimal Transport – Kantorovich



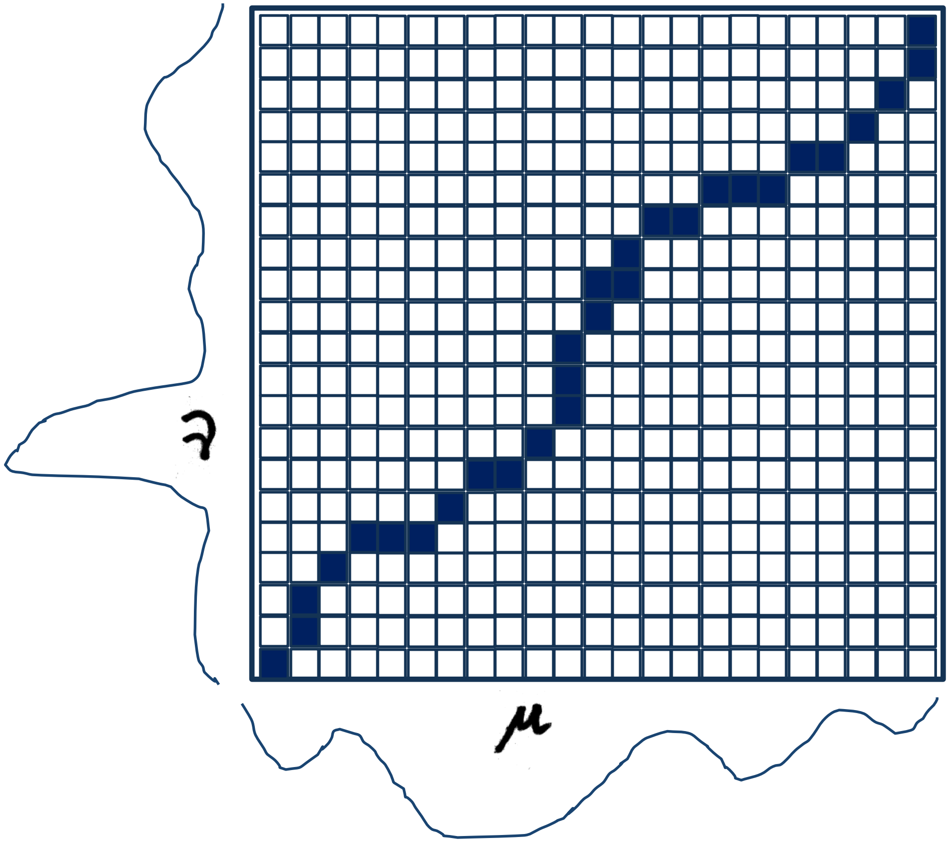
Transport plan – example in 1D

Part. 2 Optimal Transport – Kantorovich



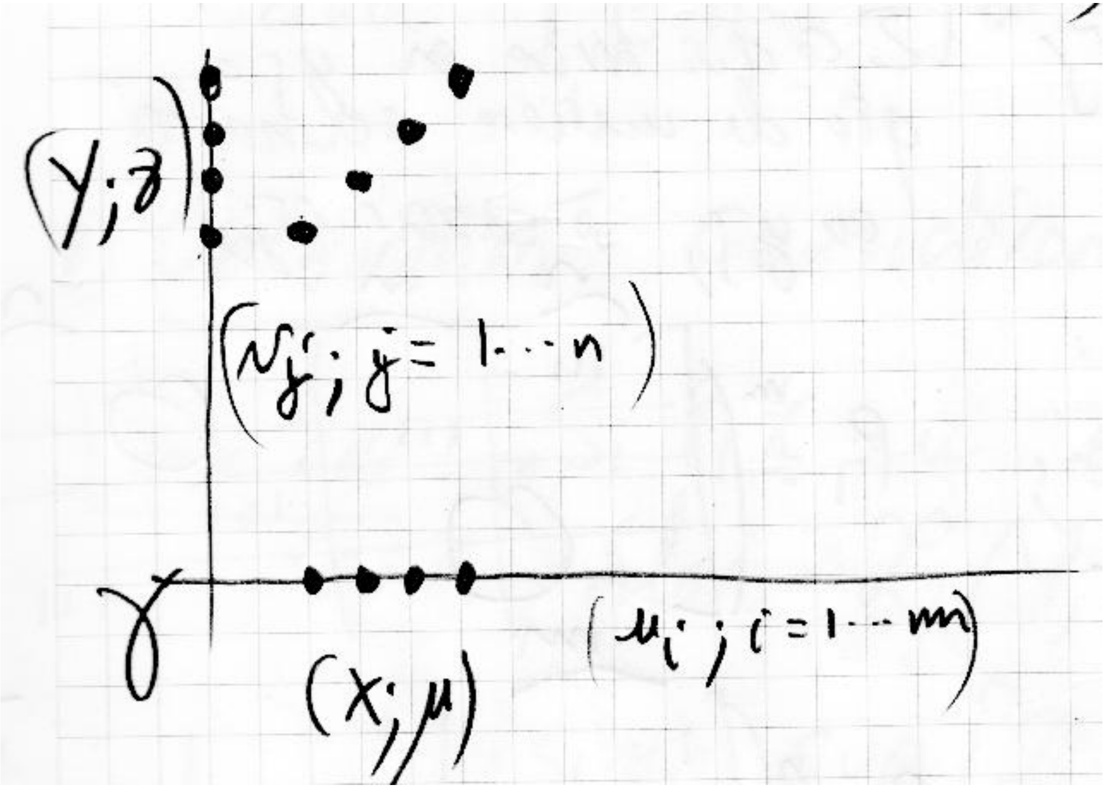
Transport plan – example in 1D

Part. 2 Optimal Transport – Kantorovich



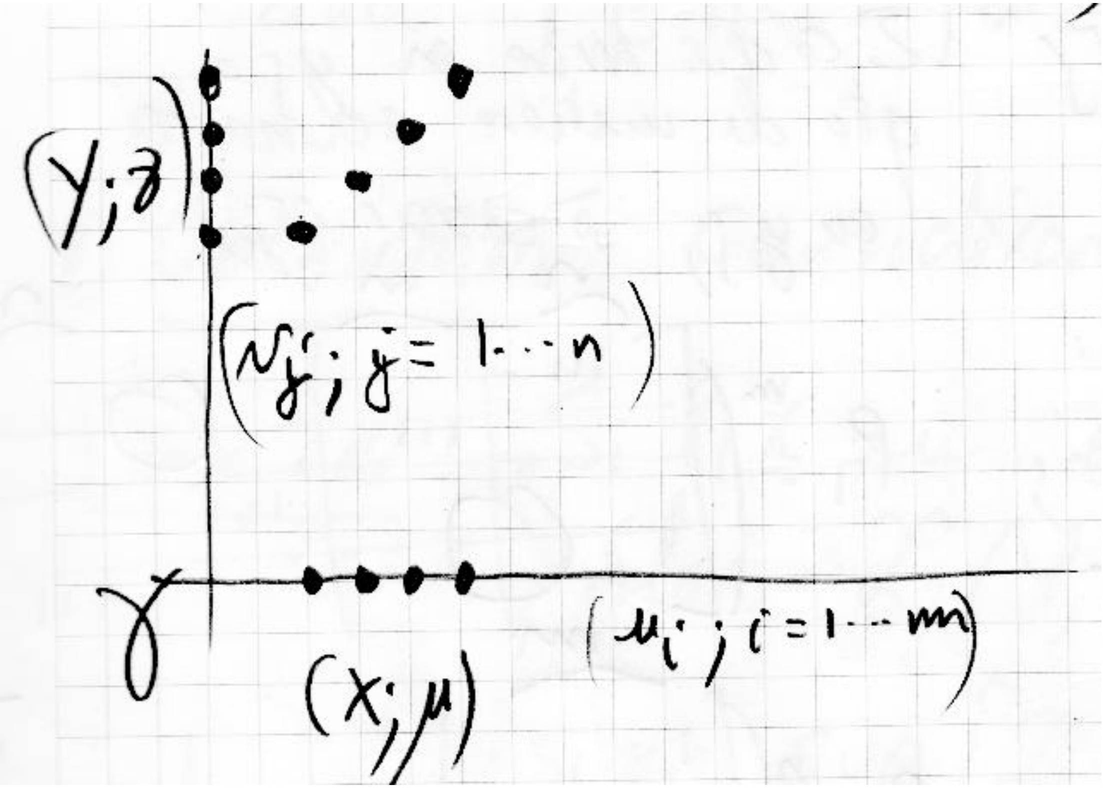
Transport plan – example in 1D

Part. 2 Optimal Transport – Duality



Duality is easier to understand with a discrete version
Then we’ll go back to the continuous setting.

Part. 2 Optimal Transport – Duality

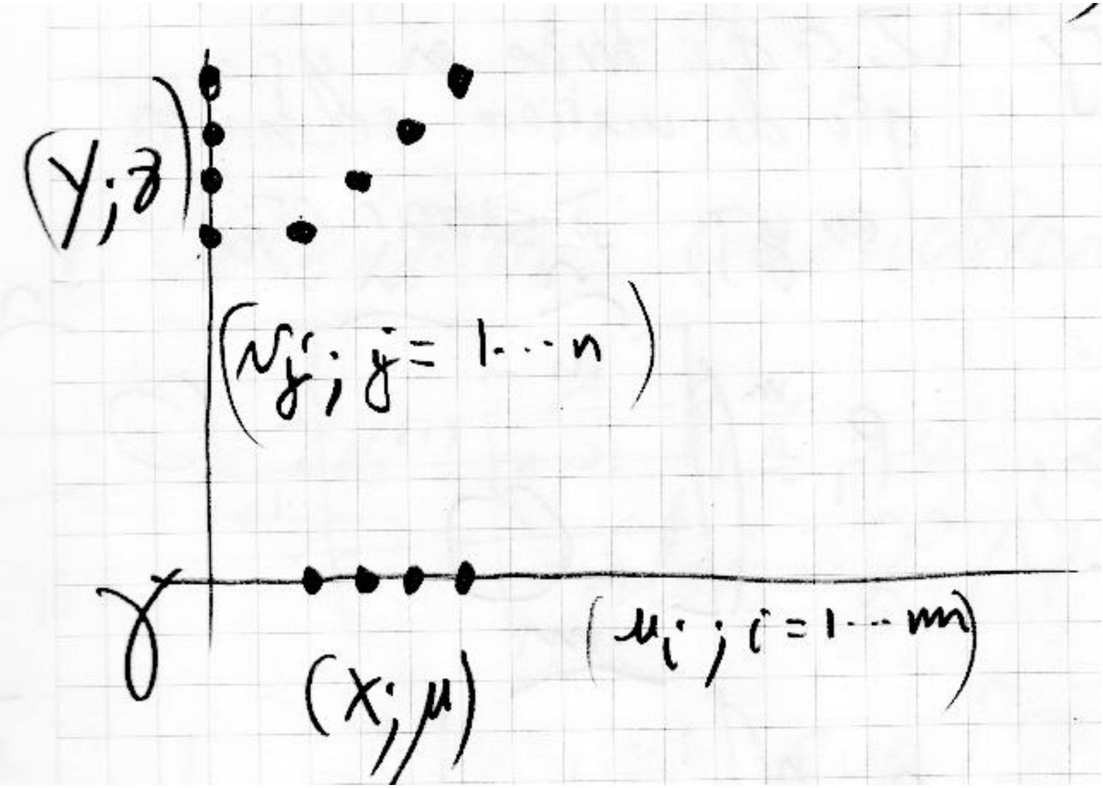


(DMK):

$$\text{Min} \ \langle c, \gamma \rangle$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Part. 2 Optimal Transport – Duality



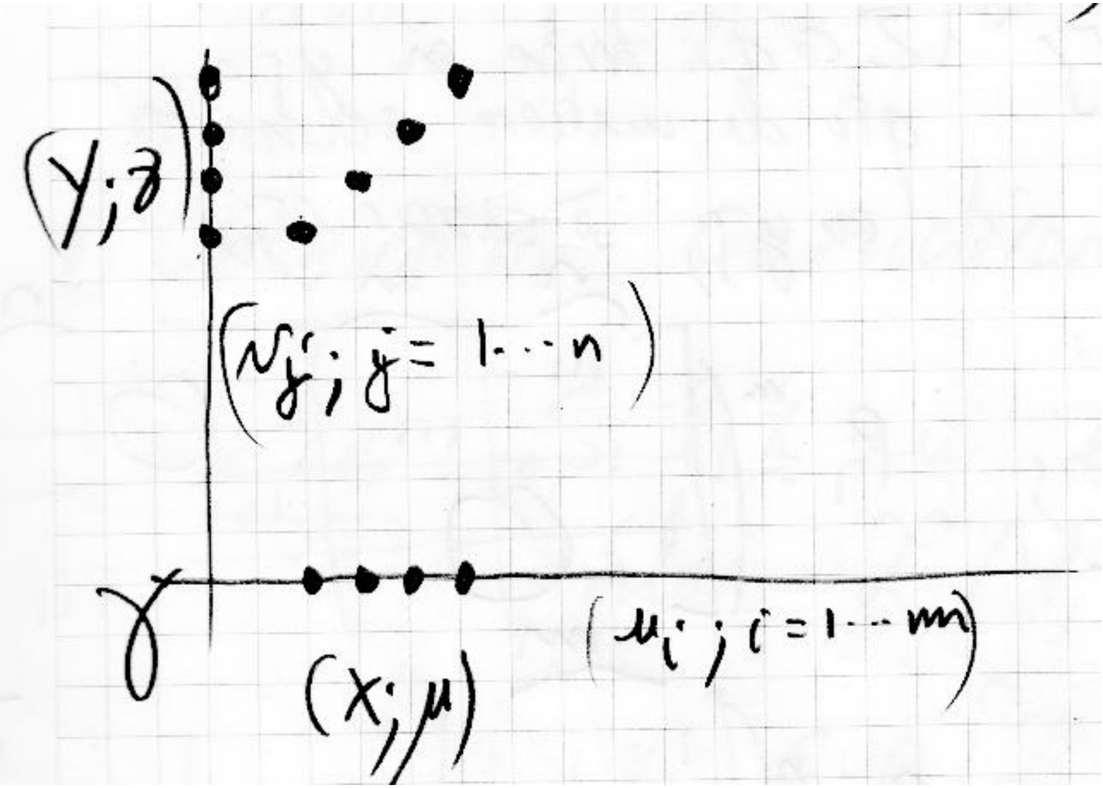
(DMK):

$$\text{Min } \langle c, \gamma \rangle$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\in \mathrm{IR}^{mn}}{\gamma} = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \ldots \\ \gamma_{1n} \\ \gamma_{22} \\ \ldots \\ \gamma_{2n} \\ \ldots \\ \ldots \\ \gamma_{mn} \end{bmatrix}$$

Part. 2 Optimal Transport – Duality



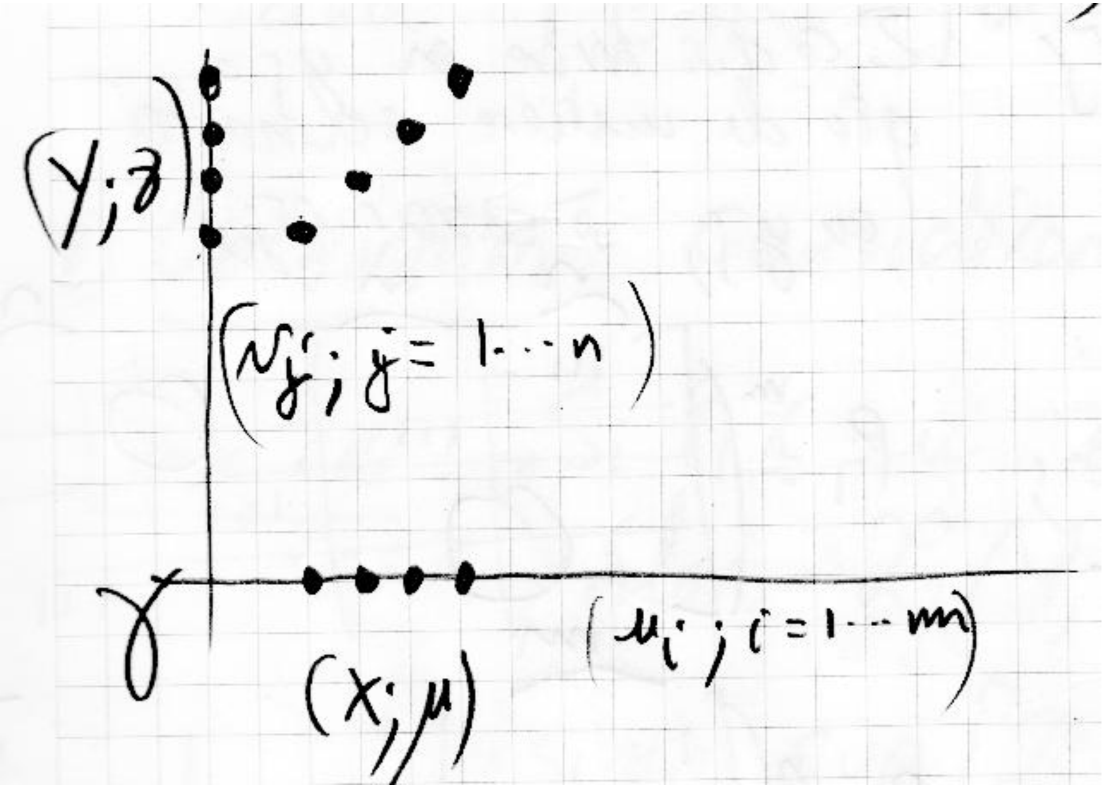
(DMK):

$$\text{Min } \langle c, \gamma \rangle$$

$$s.t. \begin{cases} P_1\,\gamma = u \\ P_2\,\gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\in \mathrm{IR}^{mn}}{c} = \begin{bmatrix} c_{11} \\ c_{12} \\ \ldots \\ c_{1n} \\ c_{22} \\ \ldots \\ c_{2n} \\ \ldots \\ \ldots \\ c_{mn} \end{bmatrix} \qquad \underset{\in \mathrm{IR}^{mn}}{\gamma} = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \ldots \\ \gamma_{1n} \\ \gamma_{22} \\ \ldots \\ \gamma_{2n} \\ \ldots \\ \ldots \\ \gamma_{mn} \end{bmatrix}$$

Part. 2 Optimal Transport – Duality



(DMK):

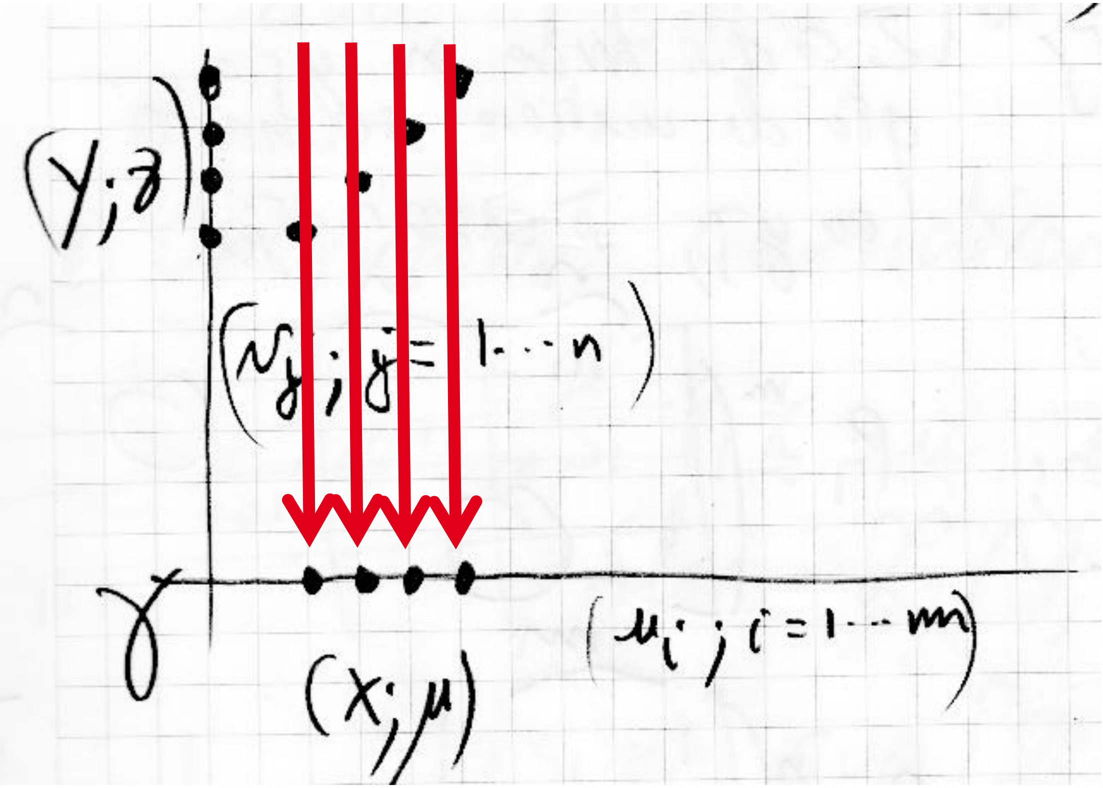
$$\text{Min} \ \langle c, \gamma \rangle$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \in \mathrm{IR}^{mn} \qquad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix} \in \mathrm{IR}^{mn}$$

$$c_{ij} = || x_i - y_j ||^2$$

Part. 2 Optimal Transport – Duality



(DMK):

Min $<c, \gamma>$

mn X m →

$$\text{s.t.} \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \end{bmatrix} c_{mn} \qquad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \end{bmatrix} \gamma_{mn}$$

$\in IR^{mn}$ $\qquad$ $\in IR^{mn}$

$c_{ij} = || x_i - y_j ||^2$ →

Part. 2 Optimal Transport – Duality

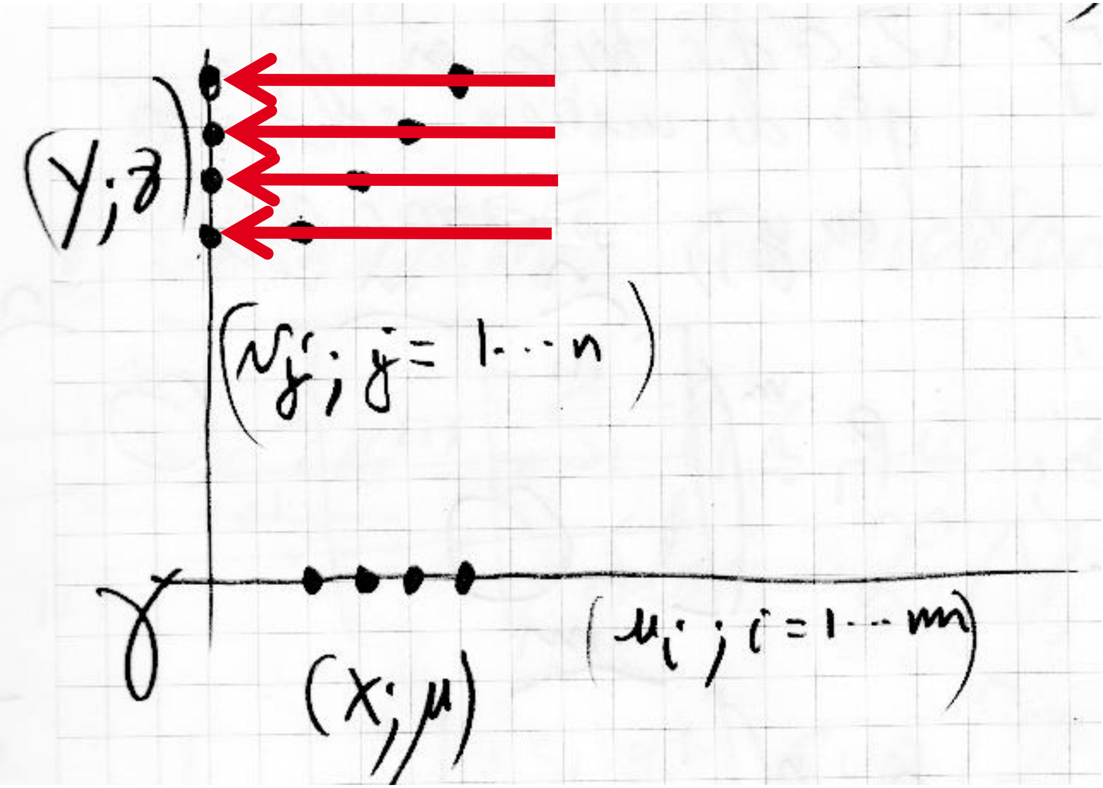
(DMK):

$$\text{Min}\ \langle c, \gamma \rangle$$

mn X m

$$\text{s.t.}\ \begin{cases} P_1\,\gamma = u \\ \mathbf{P_2}\,\gamma = v \\ \gamma \geq 0 \end{cases}$$

mn X n

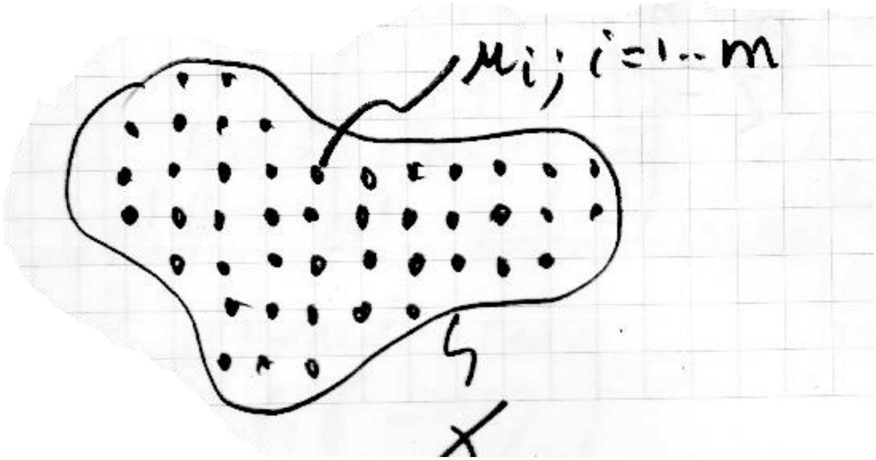


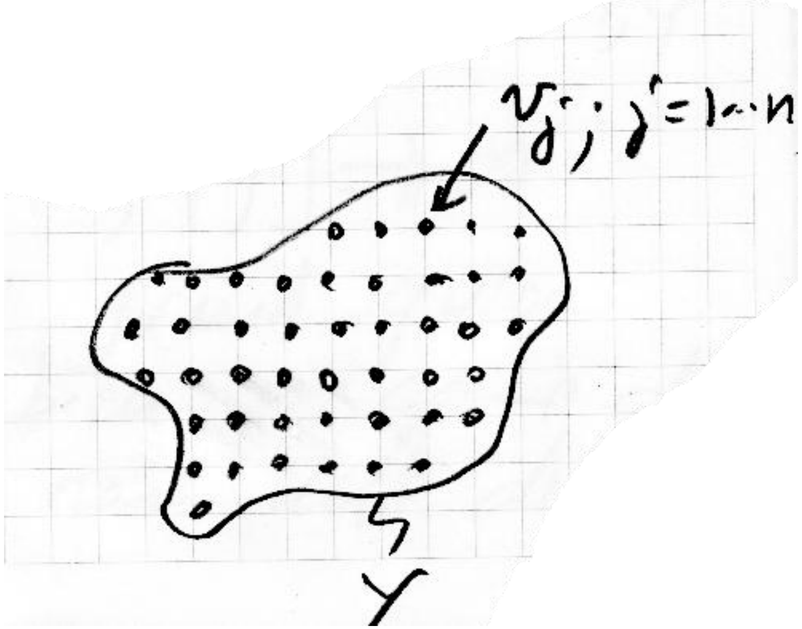
$$c = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \qquad \gamma = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix}$$

$c \in \mathrm{IR}^{mn}$ $\quad$ $\gamma \in \mathrm{IR}^{mn}$

$$c_{ij} = \|\, x_i - y_j \,\|^2$$

Part. 2 Optimal Transport – Duality





(DMK):

$$\text{Min} \ \langle c, \gamma \rangle$$

$$\text{s.t.} \ \begin{cases} \overset{mn \times m}{P_1} \gamma = u \\ \underset{mn \times n}{P_2} \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\in \mathrm{IR}^{mn}}{c} = \begin{bmatrix} c_{11} \\ c_{12} \\ \dots \\ c_{1n} \\ c_{22} \\ \dots \\ c_{2n} \\ \dots \\ \dots \\ c_{mn} \end{bmatrix} \qquad \underset{\in \mathrm{IR}^{mn}}{\gamma} = \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \dots \\ \gamma_{1n} \\ \gamma_{22} \\ \dots \\ \gamma_{2n} \\ \dots \\ \dots \\ \gamma_{mn} \end{bmatrix}$$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \ \ <c, \gamma>$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

< u, v > denotes the dot product between u and v

Consider $\mathcal{L}(\varphi,\psi) = <c, \gamma> - <\varphi, P_1 \gamma - u> - <\psi, P_2 \gamma - v>$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Consider $\mathcal{L}(\varphi,\psi) = \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle$

Remark: $\sup_{\substack{\varphi \in \mathbb{R}^m \\ \psi \in \mathbb{R}^n}} [\, \mathcal{L}(\varphi,\psi) \,] = \langle c, \gamma \rangle$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

Part. 2 Optimal Transport – Duality

(DMK):

Min $<c, \gamma>$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Consider $\mathcal{L}(\varphi,\psi) = <c, \gamma> - <\varphi, P_1 \gamma - u> - <\psi, P_2 \gamma - v>$

Remark: $\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}}[\mathcal{L}(\varphi,\psi)] = < c, \gamma>$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

$= +\infty$ otherwise

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } <c, \gamma>$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Consider $\mathcal{L}(\varphi,\psi) = <c, \gamma> - <\varphi, P_1 \gamma - u> - <\psi, P_2 \gamma - v>$

$$\text{Remark: } \underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}}[\, \mathcal{L}(\varphi,\psi)\,] = < c, \gamma> \text{ if } P_1 \gamma = u \text{ and } P_2 \gamma = v$$

$$= +\infty \text{ otherwise}$$

$$\text{Consider now: } \underset{\gamma \geq 0}{\text{Inf}} \Big[\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}}[\, \mathcal{L}(\varphi,\psi)\,] \Big]$$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \ \langle c, \gamma \rangle \quad s.t. \ \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Consider $\mathcal{L}(\varphi,\psi) = \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle$

Remark: $\operatorname{Sup}_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\ \mathcal{L}(\varphi,\psi)\ ] = \langle c, \gamma \rangle$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

$= +\infty$ otherwise

Consider now: $\operatorname{Inf}_{\gamma \geq 0} \left[\operatorname{Sup}_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\ \mathcal{L}(\varphi,\psi)\ ] \right] = \operatorname{Inf}_{\substack{\gamma \geq 0 \\ P_1 \gamma = u \\ P_2 \gamma = v}} [\ \langle c, \gamma \rangle\ ]$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \quad < c, \gamma >$$

$$s.t. \quad \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

Consider $\mathcal{L}(\varphi,\psi) = < c, \gamma > - < \varphi, P_1 \gamma - u > - < \psi, P_2 \gamma - v >$

Remark: $\sup\limits_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\ \mathcal{L}(\varphi,\psi)\ ] = < c, \gamma >$ if $P_1 \gamma = u$ and $P_2 \gamma = v$

$= +\infty$ otherwise

Consider now: $\inf\limits_{\gamma \geq 0} \Big[\sup\limits_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\ \mathcal{L}(\varphi,\psi)\ ] \Big] = \inf\limits_{\substack{\gamma \geq 0 \\ P_1 \gamma = u \\ P_2 \gamma = v}} [\ < c, \gamma >\ ]$ **(DMK)**

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\operatorname*{Inf}_{\gamma \geq 0} \Big[\operatorname*{Sup}_{\substack{\varphi \in IR^m \\ \psi \in IR^n}} [\langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle] \Big]$$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min } \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\gamma \geq 0}{\text{Inf}} \Big[\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}} [\langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle] \Big]$$

Exchange Inf Sup

$$\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}} \Big[\underset{\gamma \geq 0}{\text{Inf}} [\langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle] \Big]$$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \ \ \langle c, \gamma \rangle$$

$$s.t. \ \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\text{Inf}\Big[\text{Sup}[\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle \ ] \Big]$$

$\gamma \geq 0$ $\varphi \in IR^m$
$\psi \in IR^n$

Exchange Inf Sup

$$\text{Sup}\Big[\text{Inf}[\ \langle c, \gamma \rangle - \langle \varphi, P_1 \gamma - u \rangle - \langle \psi, P_2 \gamma - v \rangle \ ] \Big]$$

$\varphi \in IR^m$ $\gamma \geq 0$
$\psi \in IR^n$

Expand/Reorder/Collect

$$\text{Sup}\Big[\text{Inf}[\ \langle \gamma, c - P_1^t \varphi - P_2^t \psi \rangle + \langle \varphi, u \rangle + \langle \psi, v \rangle \ ] \Big]$$

$\varphi \in IR^m$ $\gamma \geq 0$
$\psi \in IR^n$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \ <c, \gamma>$$

$$s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\gamma \geq 0}{\text{Inf}} \Big[\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}}[\ <c, \gamma> - <\varphi, P_1 \gamma - u> - <\psi, P_2 \gamma - v>] \Big]$$

Exchange Inf Sup

$$\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}} \Big[\underset{\gamma \geq 0}{\text{Inf}}[\ <c, \gamma> - <\varphi, P_1 \gamma - u> - <\psi, P_2 \gamma - v>] \Big]$$

Expand/Reorder/Collect

$$\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}} \Big[\underset{\gamma \geq 0}{\text{Inf}}[\ < \gamma, c - P_1^t \varphi - P_2^t \psi > + <\varphi, u> + <\psi, v>] \Big]$$

Interpret

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \ \langle c, \gamma \rangle \quad s.t. \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\substack{\varphi \ \in IR^m \\ \psi \ \in IR^n}}{\text{Sup}} \Big[\underset{\gamma \geq 0}{\text{Inf}} \Big[< \gamma, c - P_1^t \varphi - P_2^t \psi > + <\varphi, u> + <\psi, v> \Big] \Big]$$

Interpret

$$\underset{\substack{\varphi \ \in IR^m \\ \psi \ \in IR^n \\ P_1^t \varphi + P_2^t \psi \leq c}}{\text{Sup}} \Big[<\varphi, u> + <\psi, v> \Big] \qquad \textbf{(DDMK)}$$

Part. 2 Optimal Transport – Duality

(DMK):

$$\text{Min} \ \langle c, \gamma \rangle$$

$$s.t. \ \begin{cases} P_1 \gamma = u \\ P_2 \gamma = v \\ \gamma \geq 0 \end{cases}$$

$$\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n}}{\text{Sup}}\Big[\underset{\gamma \geq 0}{\text{Inf}}\big[< \gamma, c - P_1^t \varphi - P_2^t \psi > + <\varphi, u> + <\psi, v> \big] \Big]$$

Interpret

$$\underset{\substack{\varphi \in IR^m \\ \psi \in IR^n \\ P_1^t \varphi + P_2^t \psi \leq c}}{\text{Sup}}\Big[<\varphi, u> + <\psi, v> \Big]$$

(DDMK)

$\varphi_i + \psi_j \leq c_{ij} \quad \forall (i,j)$

Part. 2 Optimal Transport – Kantorovich dual

Kantorovich's problem:

Find a measure γ defined on X x Y
such that $\int_{x \text{ in } X} d\gamma(x,y) = d\mu(x)$
and $\int_{y \text{ in } Y} d\gamma(x,y) = d\nu(x)$

that minimizes $\iint_{X \times Y} || x - y ||^2 d\gamma(x,y)$

Dual formulation of Kantorovich's problem (Continuous):

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½|| x - y ||^2$
that maximize $\int_X \varphi d\mu + \int_Y \psi d\nu$

Part. 2 Optimal Transport – c-conjugate functions

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½|| x - y ||^2$

that maximize $\int_X \varphi(x) d\mu + \int_Y \psi(y) d\nu$

Part. 2 Optimal Transport – c-conjugate functions

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½\| x - y \|^2$

that maximize $\int_X \varphi(x) d\mu + \int_Y \psi(y) d\nu$

If we got two functions φ and ψ that satisfy the constraint

Then it is possible to obtain a better solution by replacing ψ with φ^c defined by:
For all y, $\varphi^c(y) = \inf_{x \text{ in } X} ½\| x - y \|^2 - \varphi(y)$

- φ^c is called the **c-conjugate** function of φ
- If there is a function φ such that $\psi = \varphi^c$ then ψ is said to be **c-concave**
- If ψ is c-concave, then $\psi^{cc} = \psi$

Part. 2 Optimal Transport – c-conjugate functions

Dual formulation of Kantorovich's problem:

Find two functions φ in $L^1(\mu)$ and ψ in $L^1(\nu)$
Such that for all x,y, $\varphi(x) + \psi(y) \leq ½\| x - y \|^2$

that maximize $\int_X \varphi(x)d\mu + \int_Y \psi(y)d\nu$

If we got two functions φ and ψ that satisfy the constraint

Then it is possible to obtain a better solution by replacing ψ with φ^c defined by:
For all y, $\varphi^c(y) = \inf_{x \text{ in } X} ½\| x - y \|^2 - \varphi(y)$

- φ^c is called the **c-conjugate** function of φ
- If there is a function φ such that $\psi = \varphi^c$ then ψ is said to be **c-concave**
- If ψ is c-concave, then $\psi^{cc} = \psi$

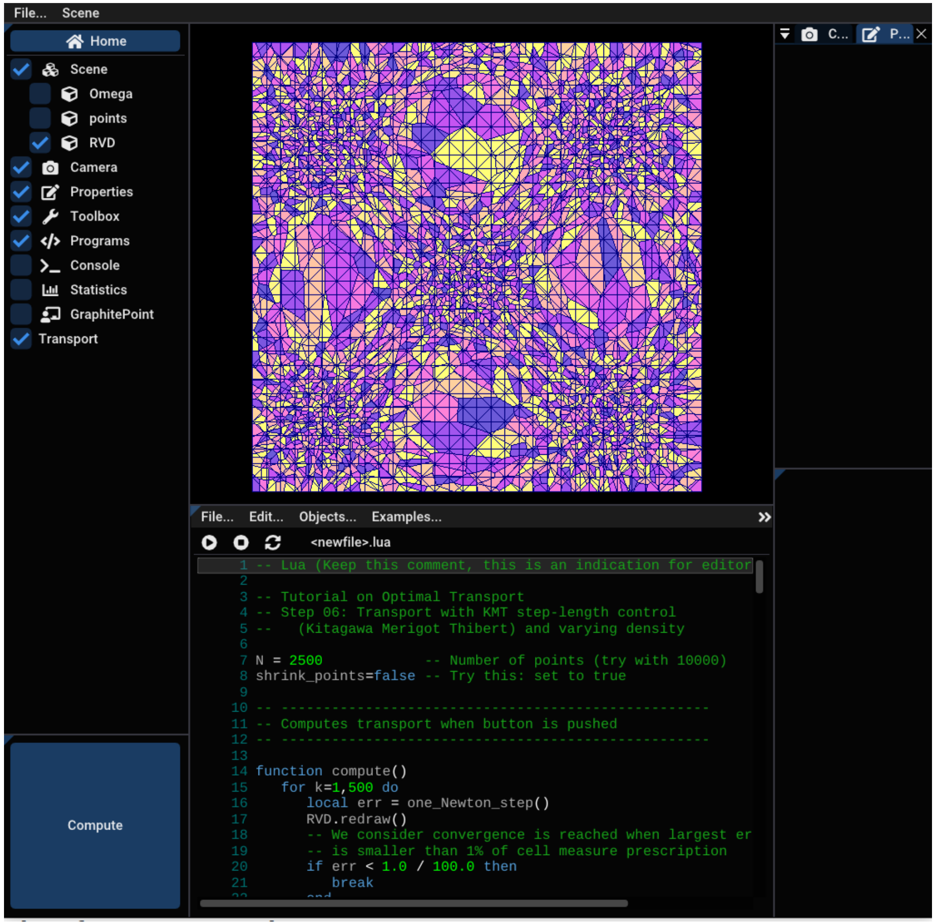
This corresponds to the Legendre-Fenchel transform
(relates Lagrangian with Hamiltonian, relates Entropy with Entalpy …)

3

Semi-Discrete Optimal Transport

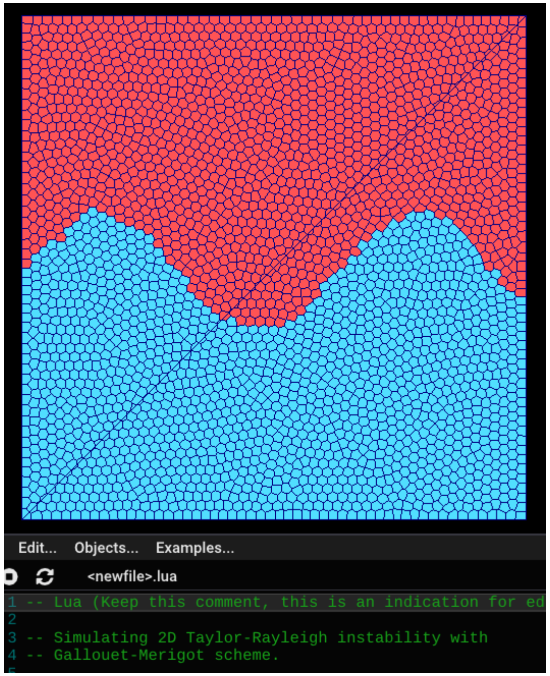
Part. 3 Optimal Transport – how to program ?

https://github.com/BrunoLevy/GraphiteThree/wiki/Transport



```
-- Lua (Keep this comment, this is an indication for editor

-- Tutorial on Optimal Transport
-- Step 06: Transport with KMT step-length control
--   (Kitagawa Merigot Thibert) and varying density

N = 2500             -- Number of points (try with 10000)
shrink_points=false -- Try this: set to true

-- ---------------------------------------------------
-- Computes transport when button is pushed
-- ---------------------------------------------------

function compute()
   for k=1,500 do
      local err = one_Newton_step()
      RVD.redraw()
      -- We consider convergence is reached when largest er
      -- is smaller than 1% of cell measure prescription
      if err < 1.0 / 100.0 then
         break
```

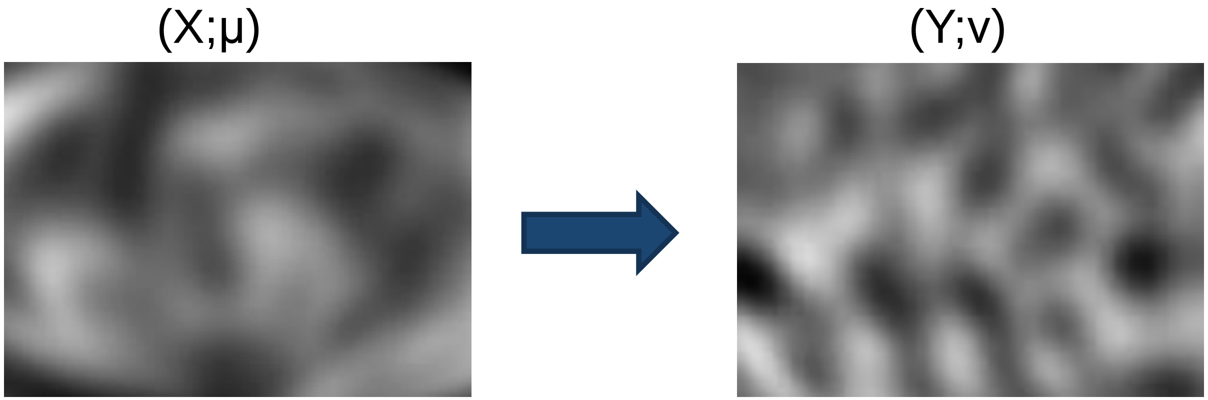
Source code
Windows/Mac/Linux
Windows binaries
Tutorials



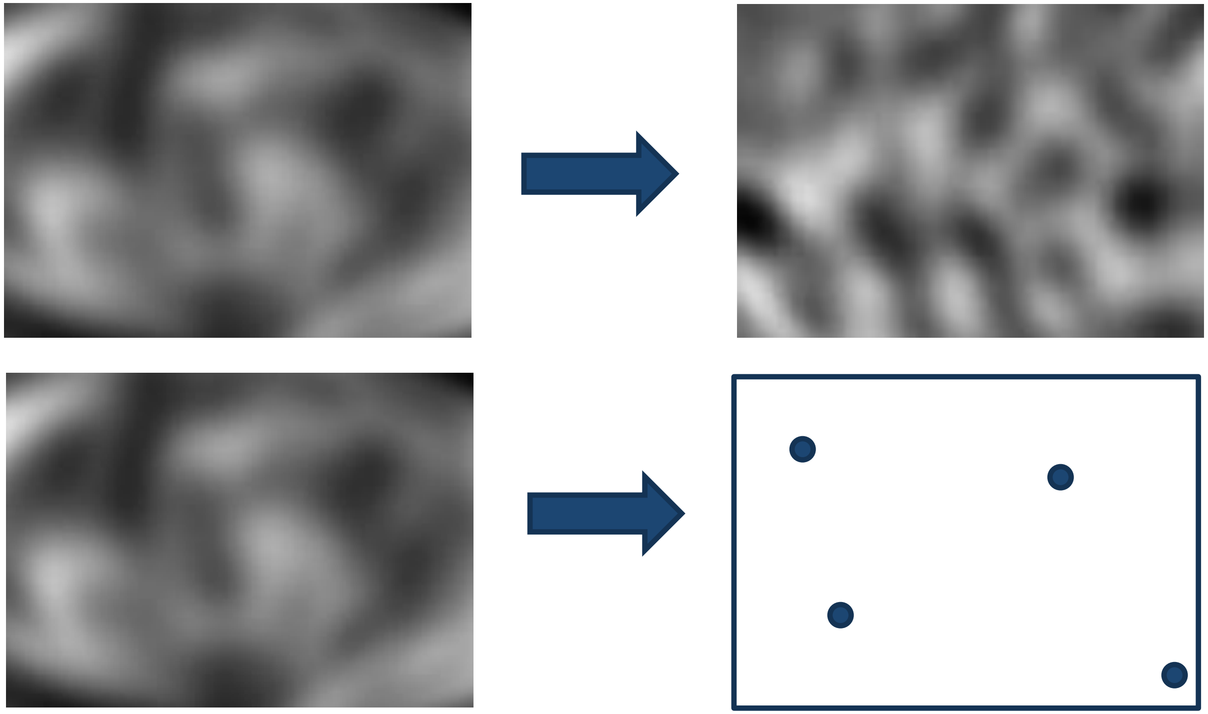
```
-- Lua (Keep this comment, this is an indication for ed

-- Simulating 2D Taylor-Rayleigh instability with
-- Gallouet-Merigot scheme.
```

Part. 3 Optimal Transport – how to program ?

Continuous



Part. 3 Optimal Transport – how to program ?



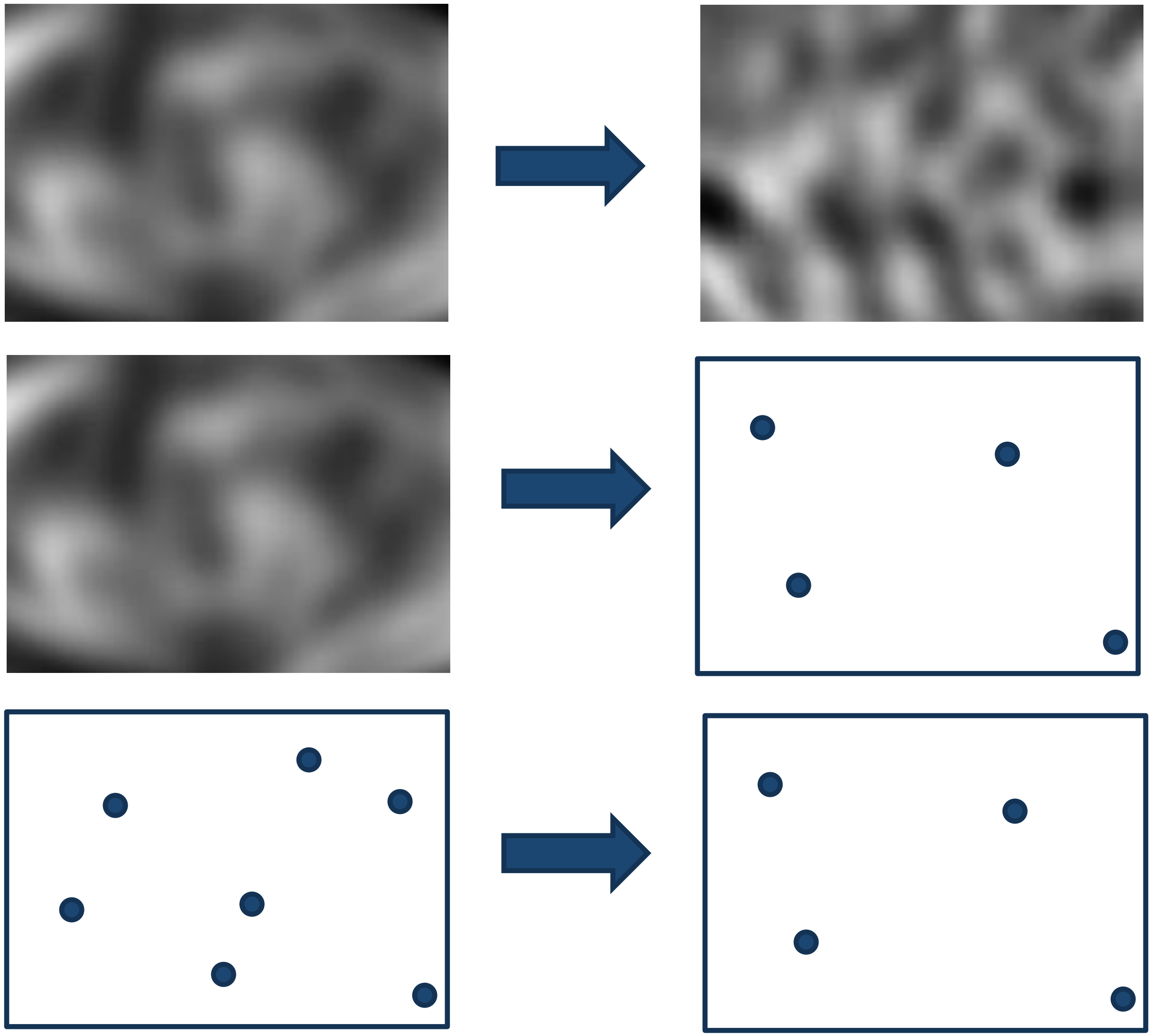
(X;μ)

(Y;v)

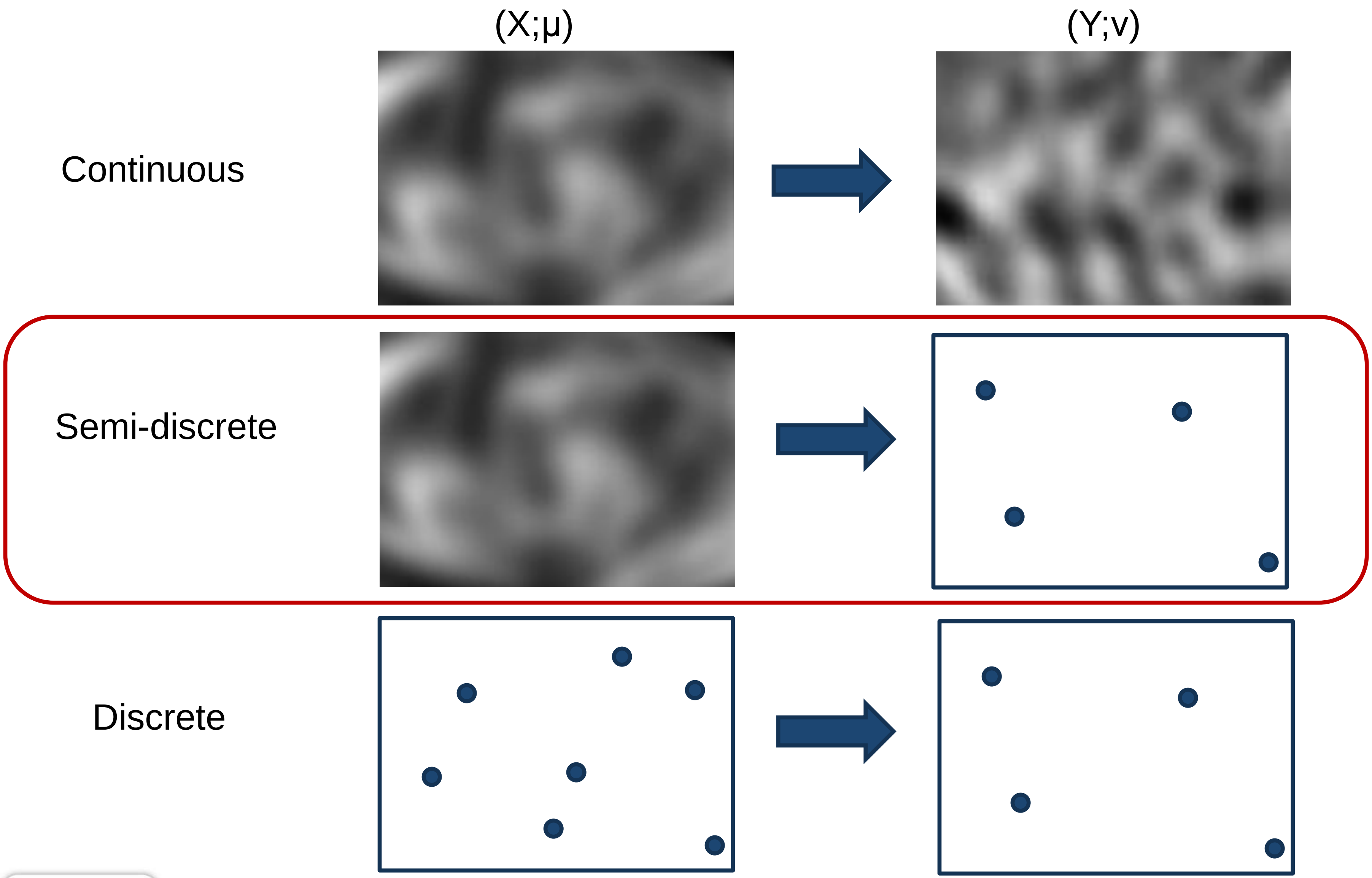
Continuous

Semi-discrete

Part. 3 Optimal Transport – how to program ?



Part. 3 Optimal Transport – how to program ?



(X;μ)

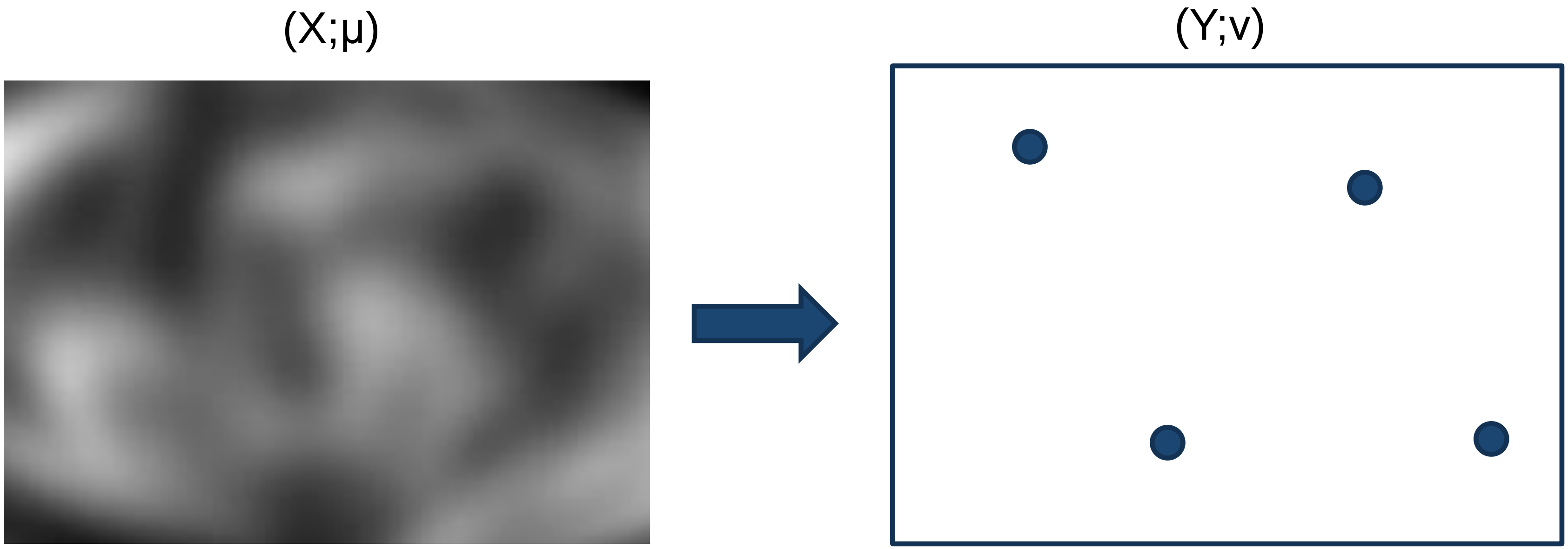
(Y;v)

Continuous

Semi-discrete

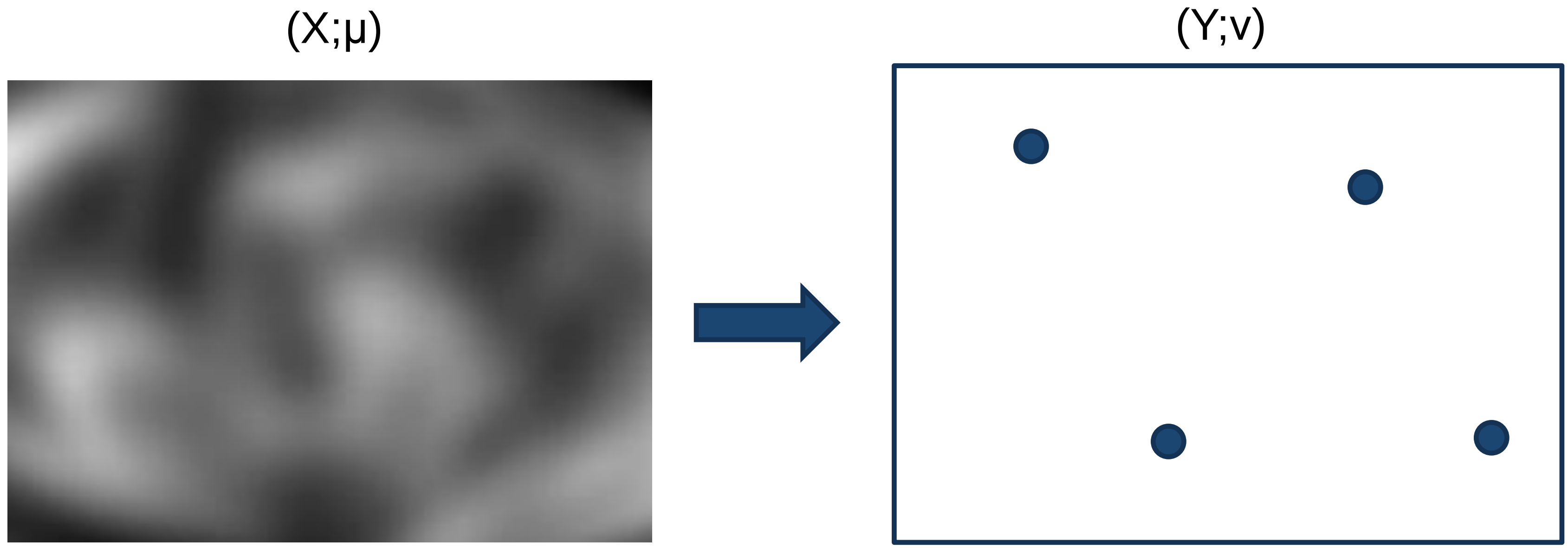
Discrete

Part. 3 Optimal Transport – semi-discrete



(DMK) $\mathrm{Sup}_{\psi \in \psi^c} \int_X \psi^c(x)d\mu + \int_Y \psi(y)dv$

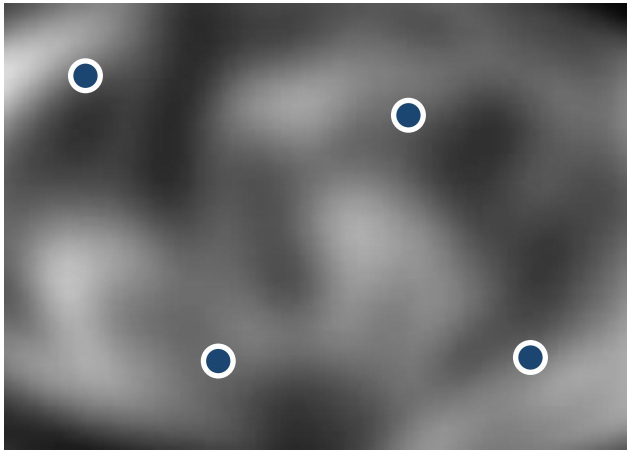
Part. 3 Optimal Transport – semi-discrete



(DMK) $$\underset{\psi \in \psi^c}{\text{Sup}} \int_X \psi^c(x)d\mu + \int_Y \psi(y)dv$$

$$\sum_j \psi(y_j)\, v_j$$

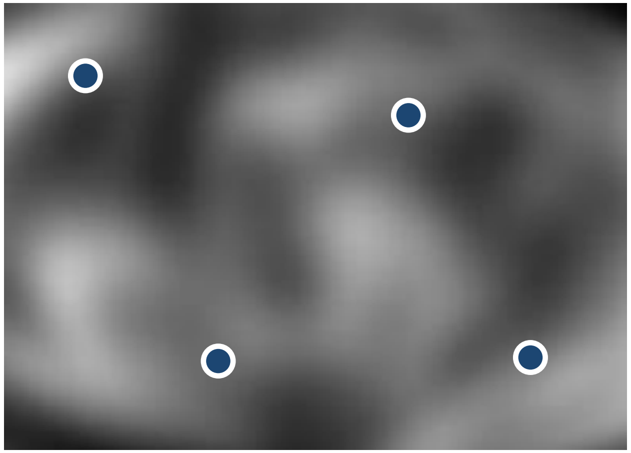
Part. 3 Optimal Transport – semi-discrete



(DMK) $$\sup_{\psi \in \psi^c} \int_X \psi^c(x)d\mu + \int_Y \psi(y)d\nu$$

$$\sum_j \psi(y_j)\, v_j$$

Part. 3 Optimal Transport – semi-discrete

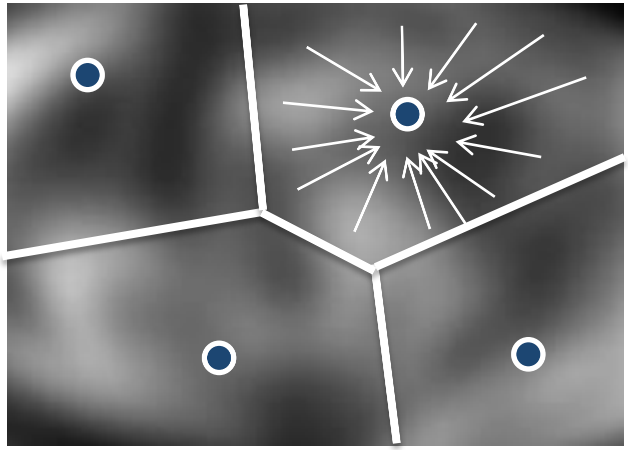


(DMK) $$\operatorname{Sup}_{\psi \in \psi^c} \int_X \psi^c(x) d\mu + \int_Y \psi(y) dv$$

$$\int_X \inf_{yj \in Y} [\, \| x - y_j \|^2 - \psi(y_j) \,] \, d\mu$$

$$\sum_j \psi(y_j) \, v_j$$

Part. 3 Optimal Transport – semi-discrete



(DMK) $$\sup_{\psi \in \psi^c} \int_X \psi^c(x)d\mu + \int_Y \psi(y)d\nu$$

$$\int_X \inf_{y_j \in Y} [\, \| x - y_j \|^2 - \psi(y_j) \,]\, d\mu$$

$$\sum_j \int_{\mathrm{Lag}_\psi(y_j)} \| x - y_j \|^2 - \psi(y_j)\, d\mu$$

$$\sum_j \psi(y_j)\, \nu_j$$

Part. 3 Optimal Transport – semi-discrete

(DMK) $$\sup_{\psi \in \boldsymbol{\psi}^c} \quad G(\psi) = \sum_j \int_{\text{Lag }\psi(yj)} \| x - y_j \|^2 - \psi(y_j)\, d\mu \; + \; \sum_j \psi(y_j)\, v_j$$

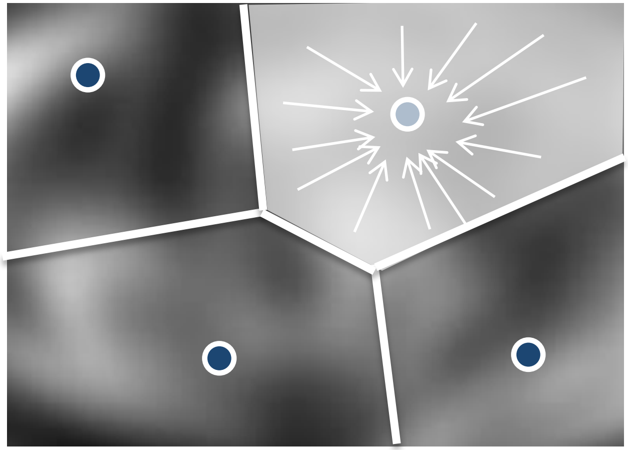
Where: $\text{Lag }\psi(yj) = \left\{ x \;|\; \| x - y_j \|^2 - \psi(y_j) < \| x - y_j \|^2 - \psi(y_{j'}) \right\}$ for all $j' \neq j$

Part. 3 Optimal Transport – semi-discrete

(DMK) $$\sup_{\psi \in \psi^c} G(\psi) = \sum_j \int_{\mathrm{Lag}\ \psi(yj)} \| x - y_j \|^2 - \psi(y_j)\, d\mu \ + \ \sum_j \psi(y_j)\, v_j$$

Where: $\mathrm{Lag}\ \psi(yj) = \{ x \mid \| x - y_j \|^2 - \psi(y_j) < \| x - y_{j'} \|^2 - \psi(y_{j'}) \}$ for all $j' \neq j$

Laguerre diagram of the y_j's
(with the L_2 cost $\| x - y \|^2$ used here, Power diagram)



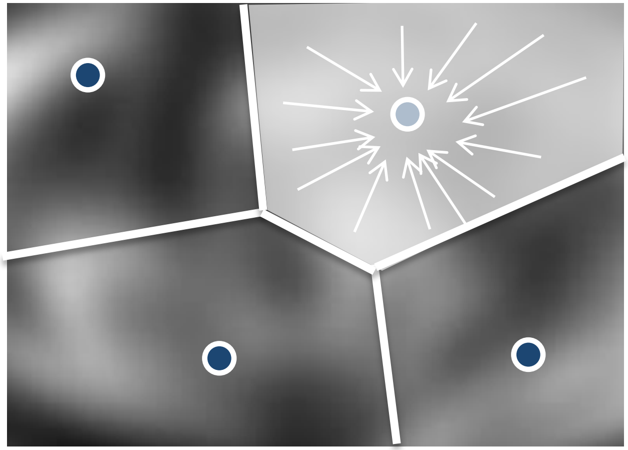
Part. 3 Optimal Transport – semi-discrete

(DMK) $$\sup_{\psi \in \boldsymbol{\psi}^c} G(\psi) = \sum_j \int_{\mathrm{Lag}\ \psi(yj)} \| x - y_j \|^2 - \psi(y_j)\, d\mu \ + \ \sum_j \psi(y_j)\, v_j$$

Where: $$\mathrm{Lag}\ \psi(yj) = \{ x \mid \| x - y_j \|^2 - \psi(y_j) < \| x - y_{j'} \|^2 - \psi(y_{j'}) \} \text{ for all } j' \neq j$$

Laguerre diagram of the y_j's
(with the L_2 cost $\| x - y \|^2$ used here, Power diagram)

Weight of y_j in the power diagram



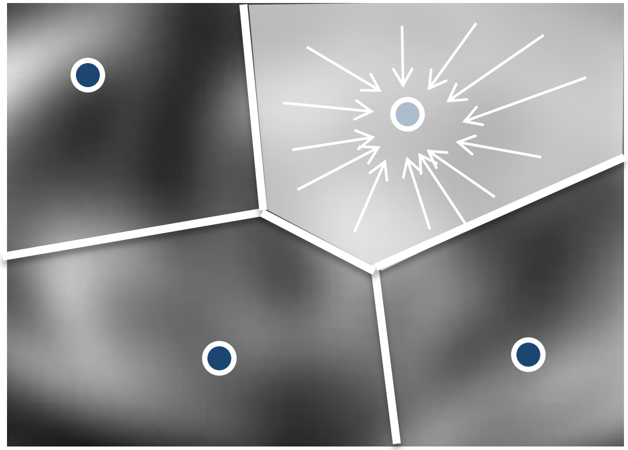
Part. 3 Optimal Transport – semi-discrete

(DMK) $$\sup_{\psi \in \boldsymbol{\psi}^c} \quad G(\psi) = \sum_j \int_{\mathrm{Lag}\ \psi(yj)} \| x - y_j \|^2 - \psi(y_j)\, d\mu \ + \ \sum_j \psi(y_j)\, v_j$$

Where: $\mathrm{Lag}\ \psi(yj) = \{ x \mid \| x - y_j \|^2 - \psi(y_j) < \| x - y_j \|^2 - \psi(y_{j'}) \}$ for all $j' \neq j$

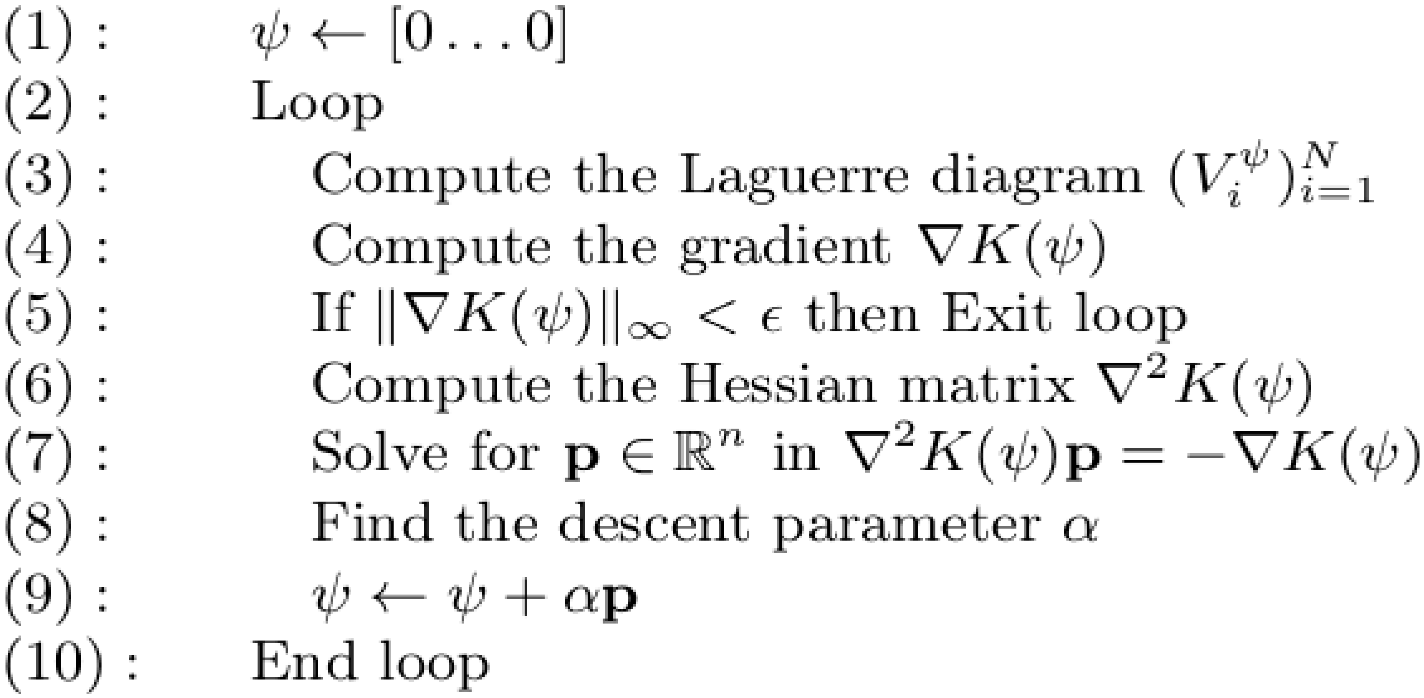
Laguerre diagram of the y_j's
(with the L_2 cost $\| x - y \|^2$ used here, Power diagram)

Weight of y_j in the power diagram



ψ is determined by the
weight vector $[\psi(y_1)\ \psi(y_2)\ \dots\ \psi(y_m)]$

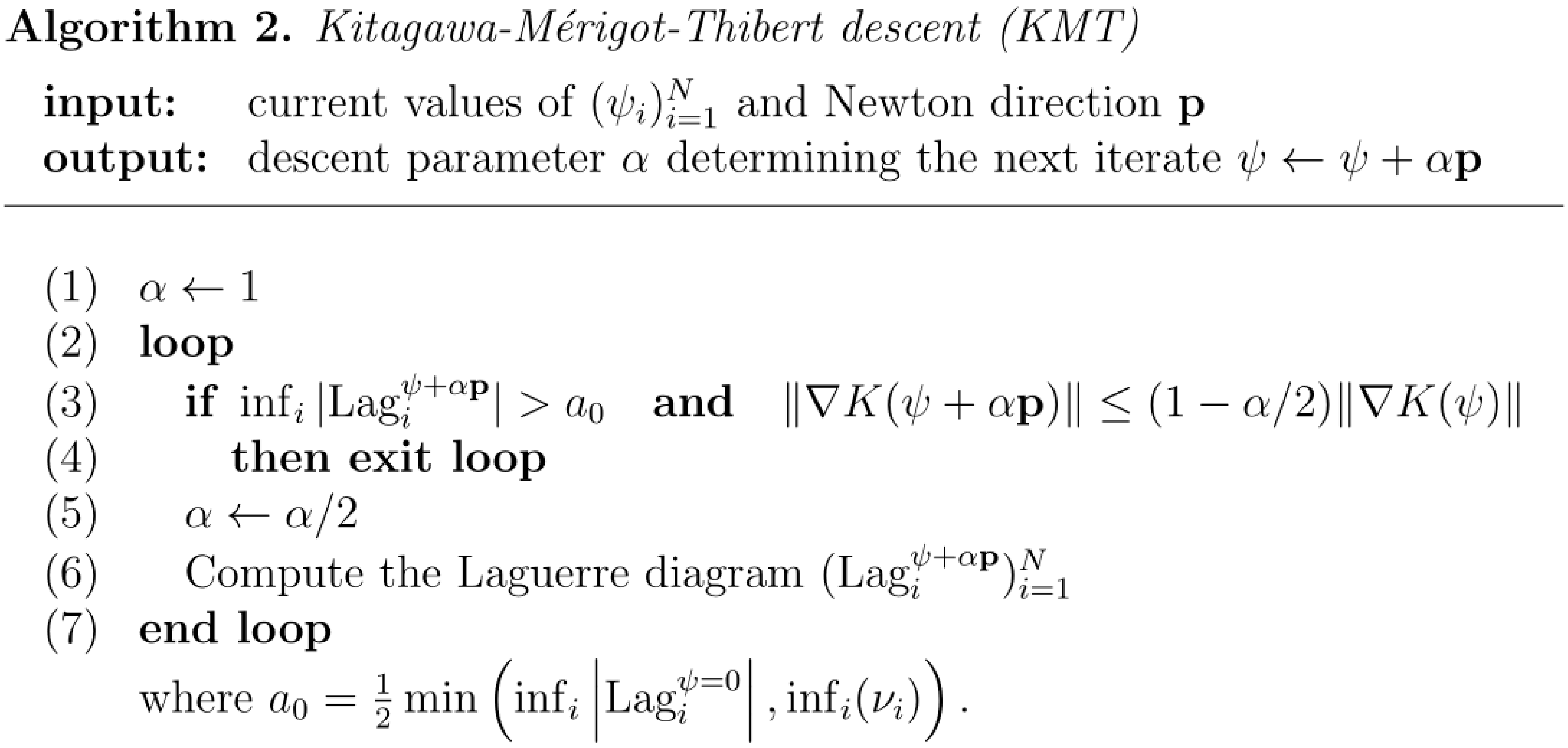
Part. 3 Optimal Transport – semi-discrete



```
$\psi \leftarrow [0 \dots 0]$
Loop
    Compute the Laguerre diagram $(V_i^\psi)_{i=1}^N$
    Compute the gradient $\nabla K(\psi)$
    If $\|\nabla K(\psi)\|_\infty < \epsilon$ then Exit loop
    Compute the Hessian matrix $\nabla^2 K(\psi)$
    Solve for $\mathbf{p} \in \mathbb{R}^n$ in $\nabla^2 K(\psi)\mathbf{p} = -\nabla K(\psi)$
    Find the descent parameter $\alpha$
    $\psi \leftarrow \psi + \alpha \mathbf{p}$
End loop
```

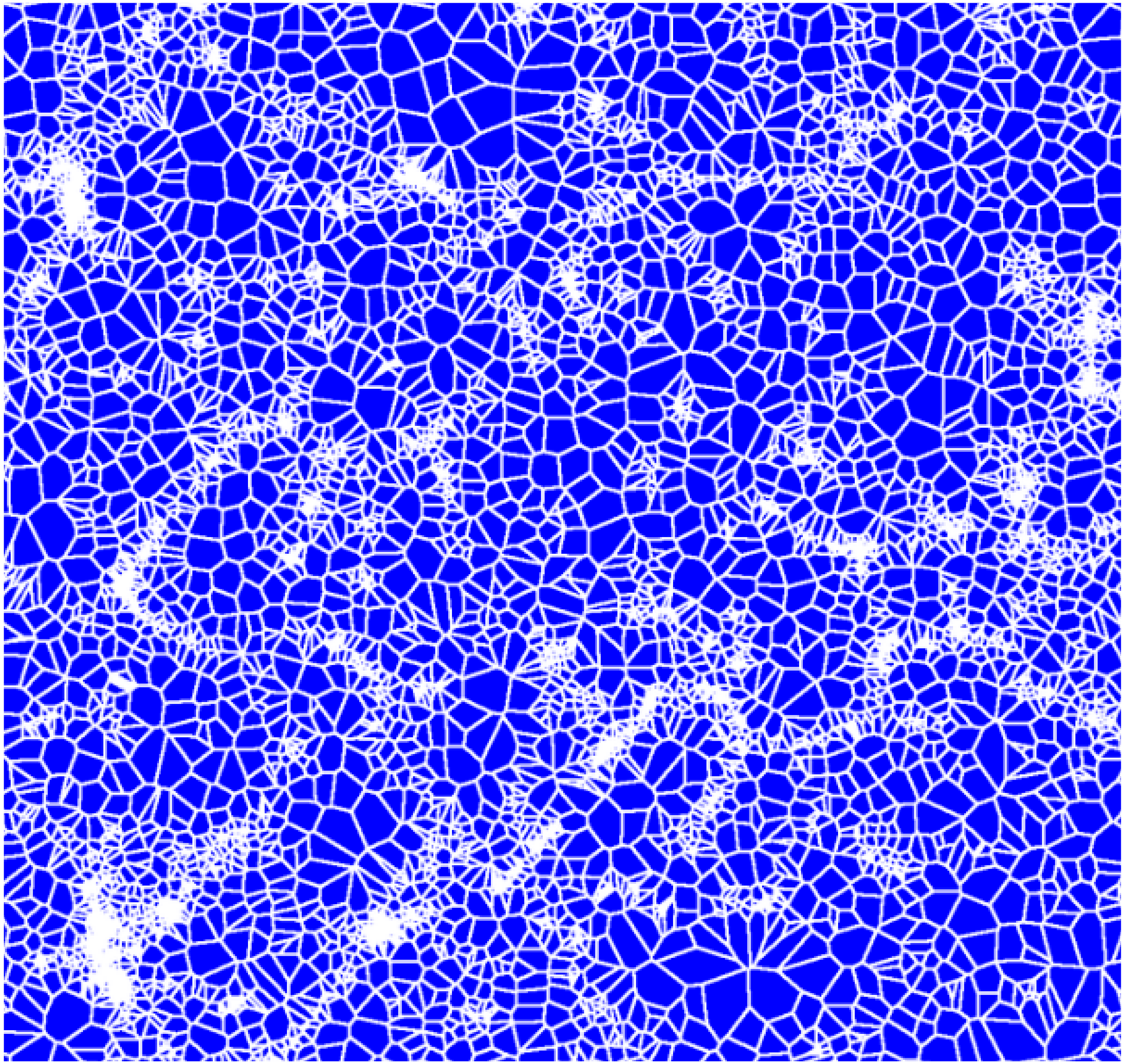
[Kitagawa Merigot Thibert 2019, JEMS]
[L 2015, M2AN]
[L 2021, JCP]
[Nikhaktar, Seth, L, Mohayaee 2022, PRL]
[von Hausseger, L, Mohayaee 2021, PRL]
[L, Ray, Merigot, Leclerc, JCP (pend. rev.)]

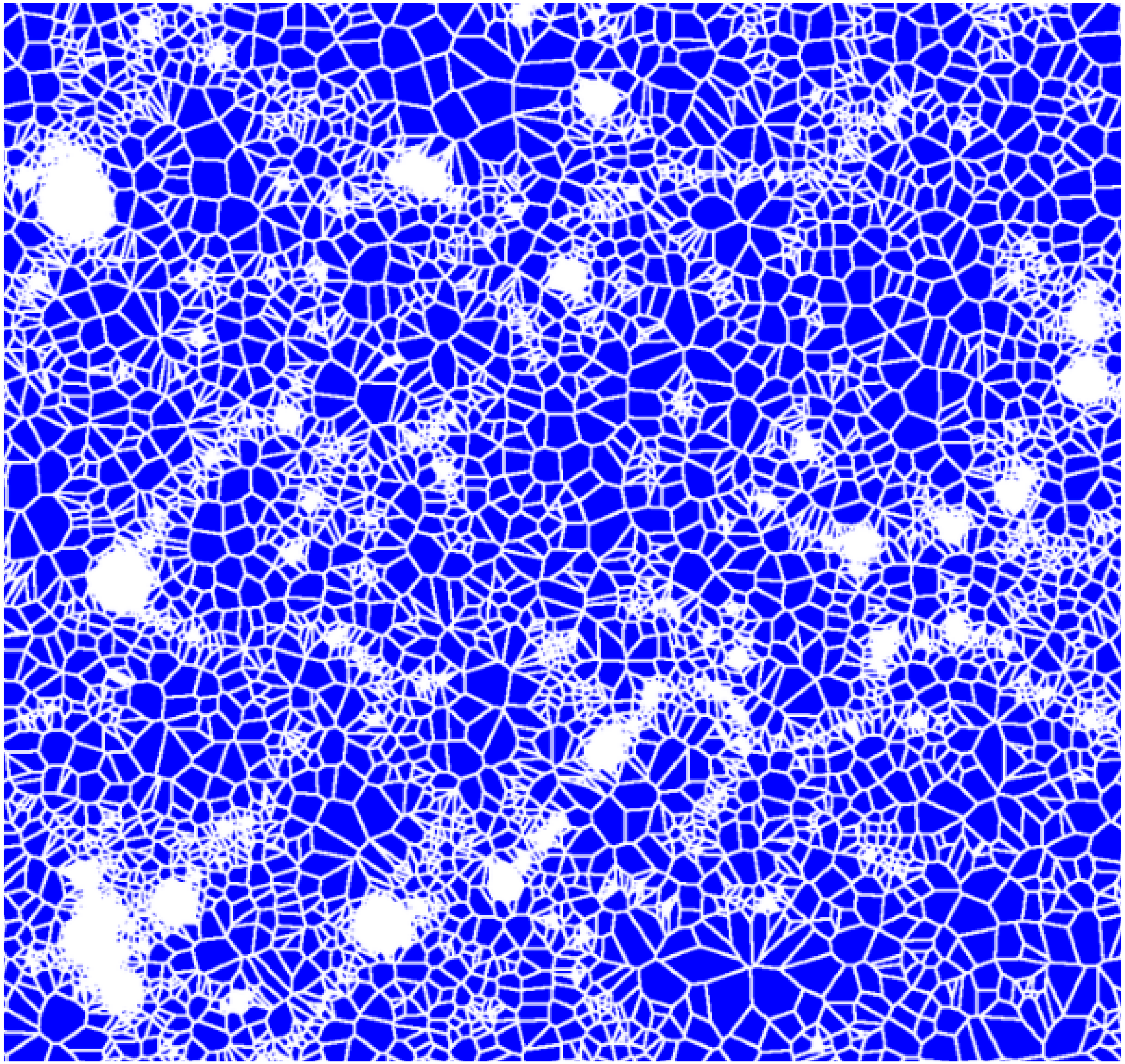
Part. 3 Optimal Transport – semi-discrete

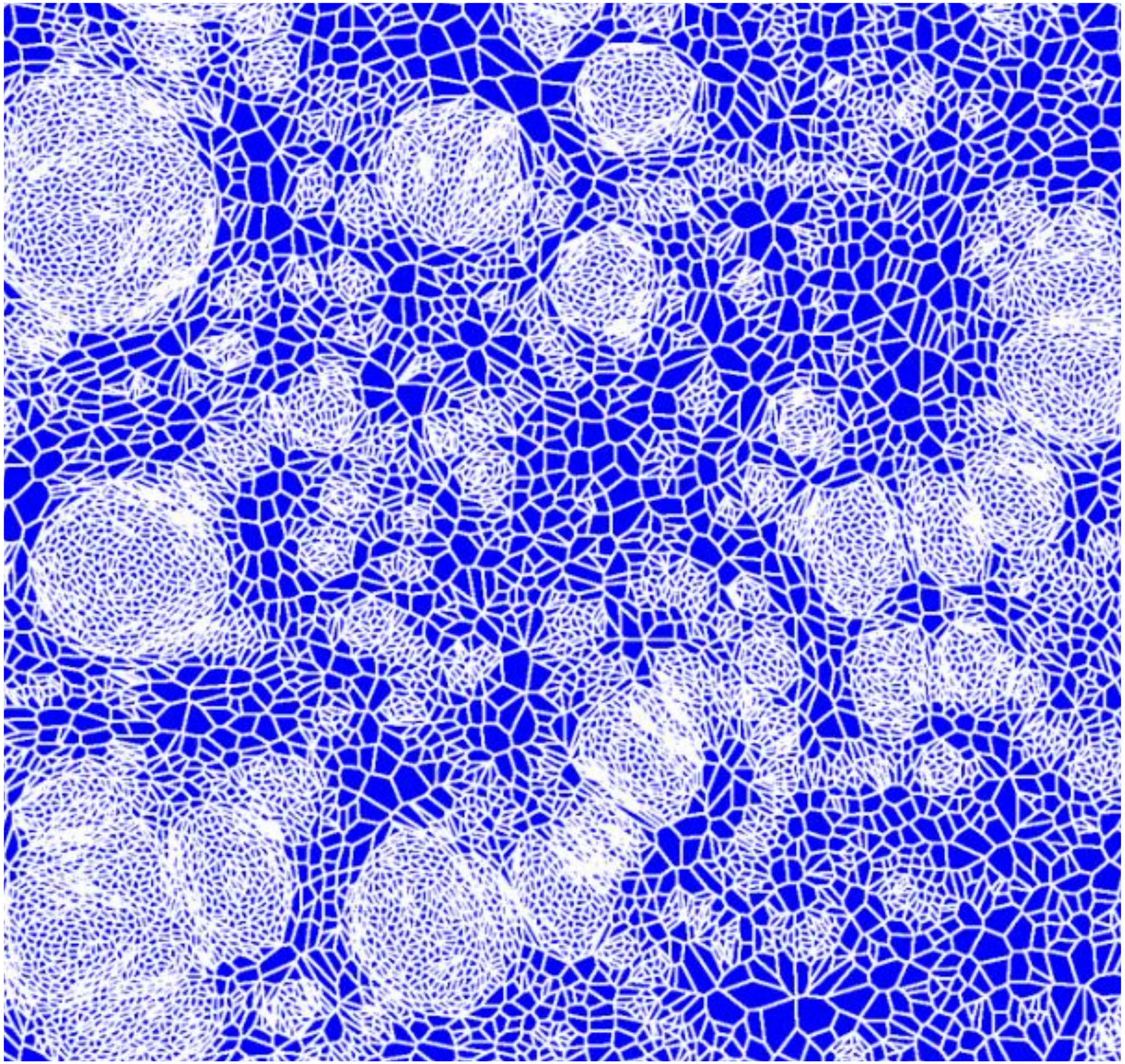


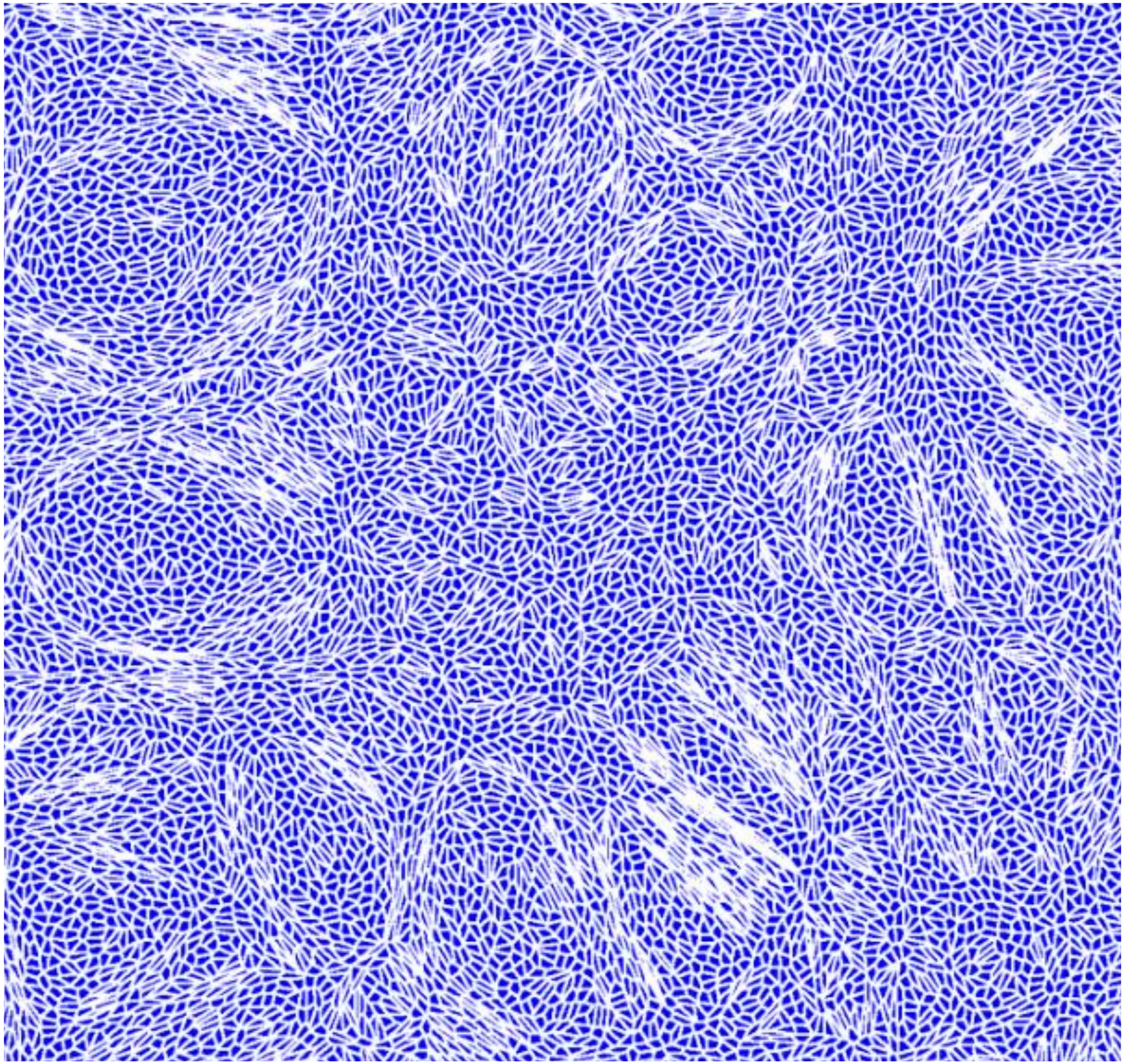
Algorithm 2. *Kitagawa-Mérigot-Thibert descent (KMT)*

```
input:   current values of $(\psi_i)_{i=1}^N$ and Newton direction $\mathbf{p}$
output:  descent parameter $\alpha$ determining the next iterate $\psi \leftarrow \psi + \alpha\mathbf{p}$

$\alpha \leftarrow 1$
loop
    if $\inf_i |\mathrm{Lag}_i^{\psi+\alpha\mathbf{p}}| > a_0$ and $\|\nabla K(\psi + \alpha\mathbf{p})\| \leq (1 - \alpha/2)\|\nabla K(\psi)\|$
        then exit loop
    $\alpha \leftarrow \alpha/2$
    Compute the Laguerre diagram $(\mathrm{Lag}_i^{\psi+\alpha\mathbf{p}})_{i=1}^N$
end loop
where $a_0 = \frac{1}{2}\min\left(\inf_i \left|\mathrm{Lag}_i^{\psi=0}\right|, \inf_i(\nu_i)\right)$.
```



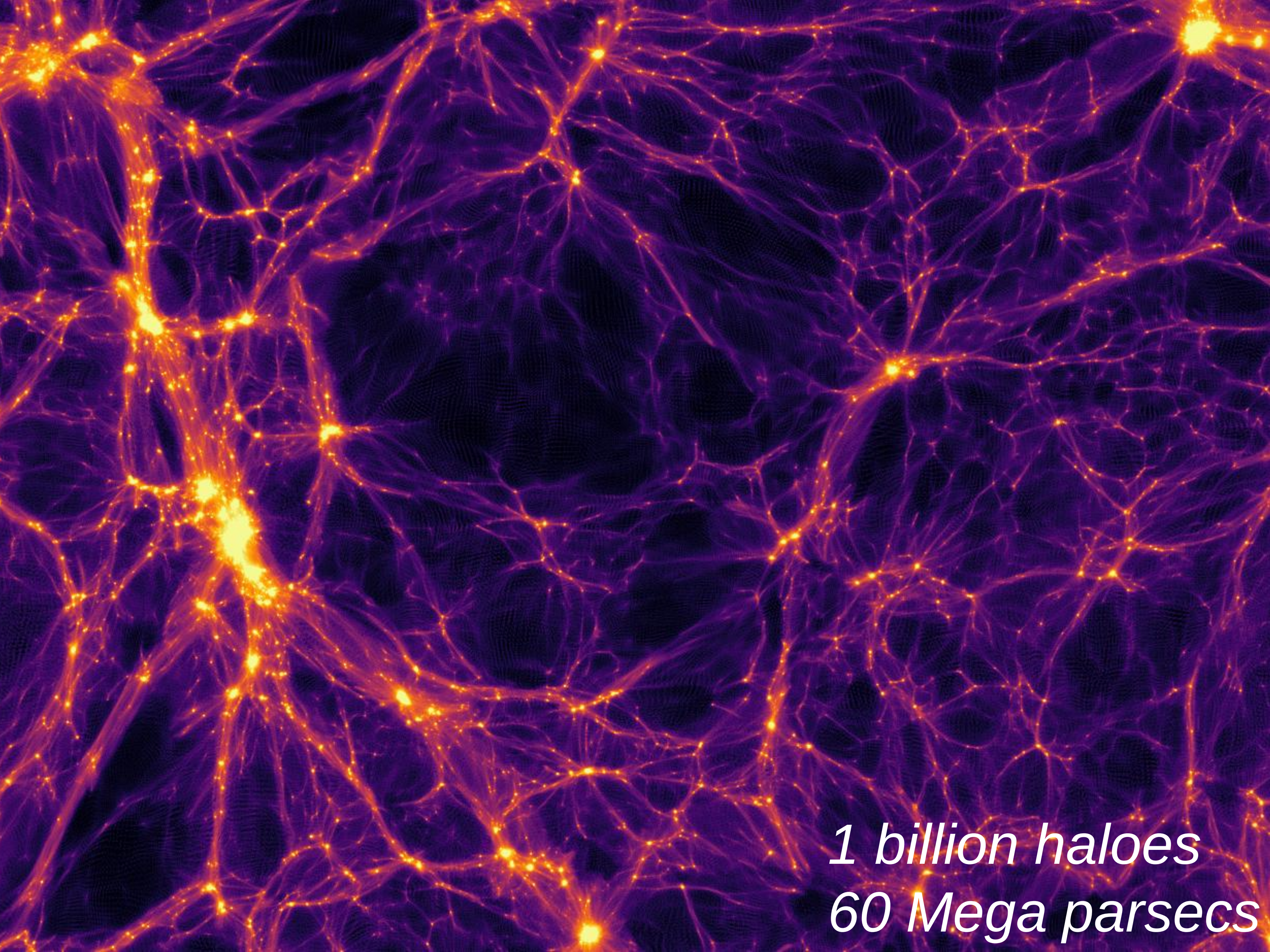






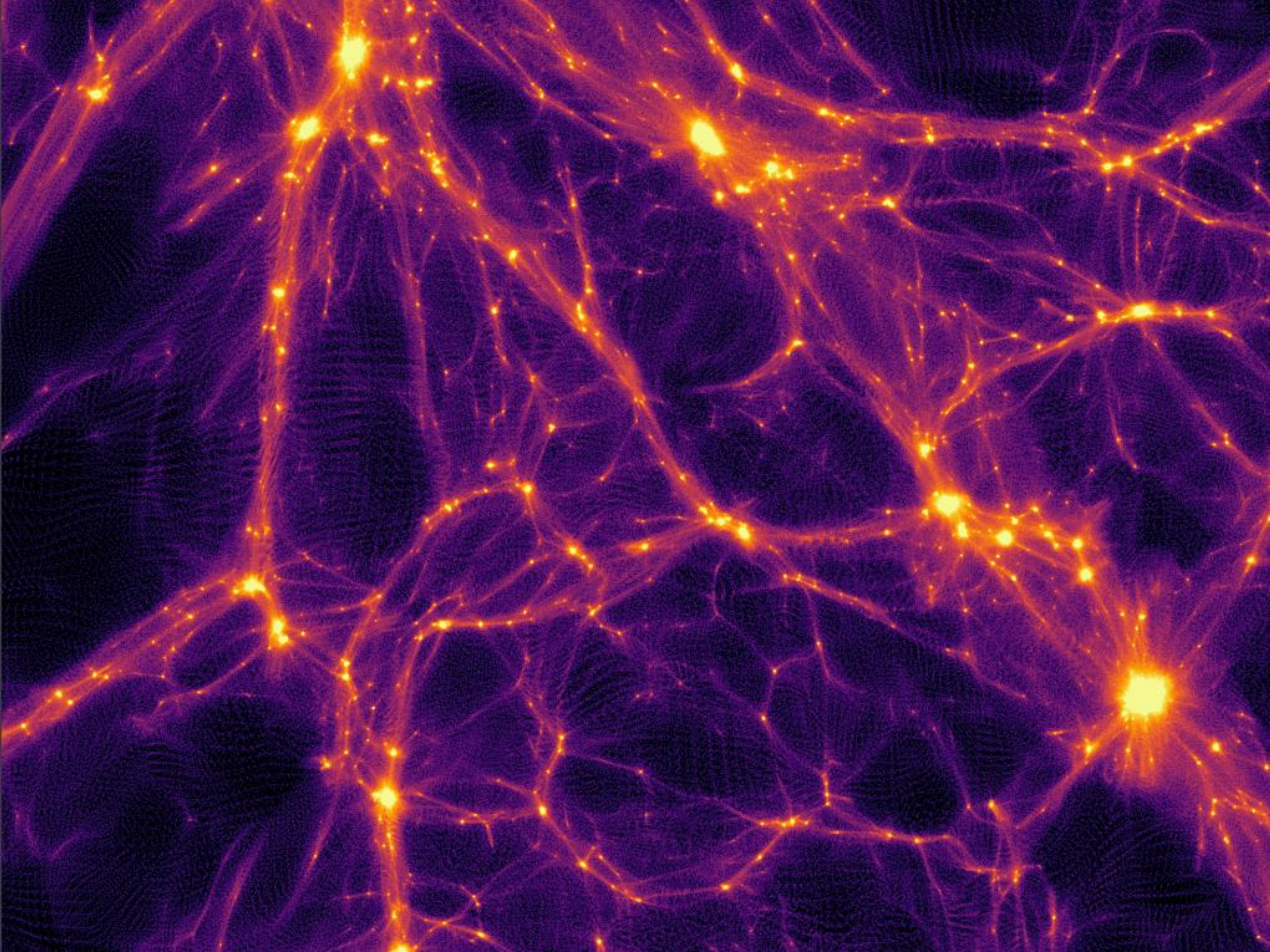
4

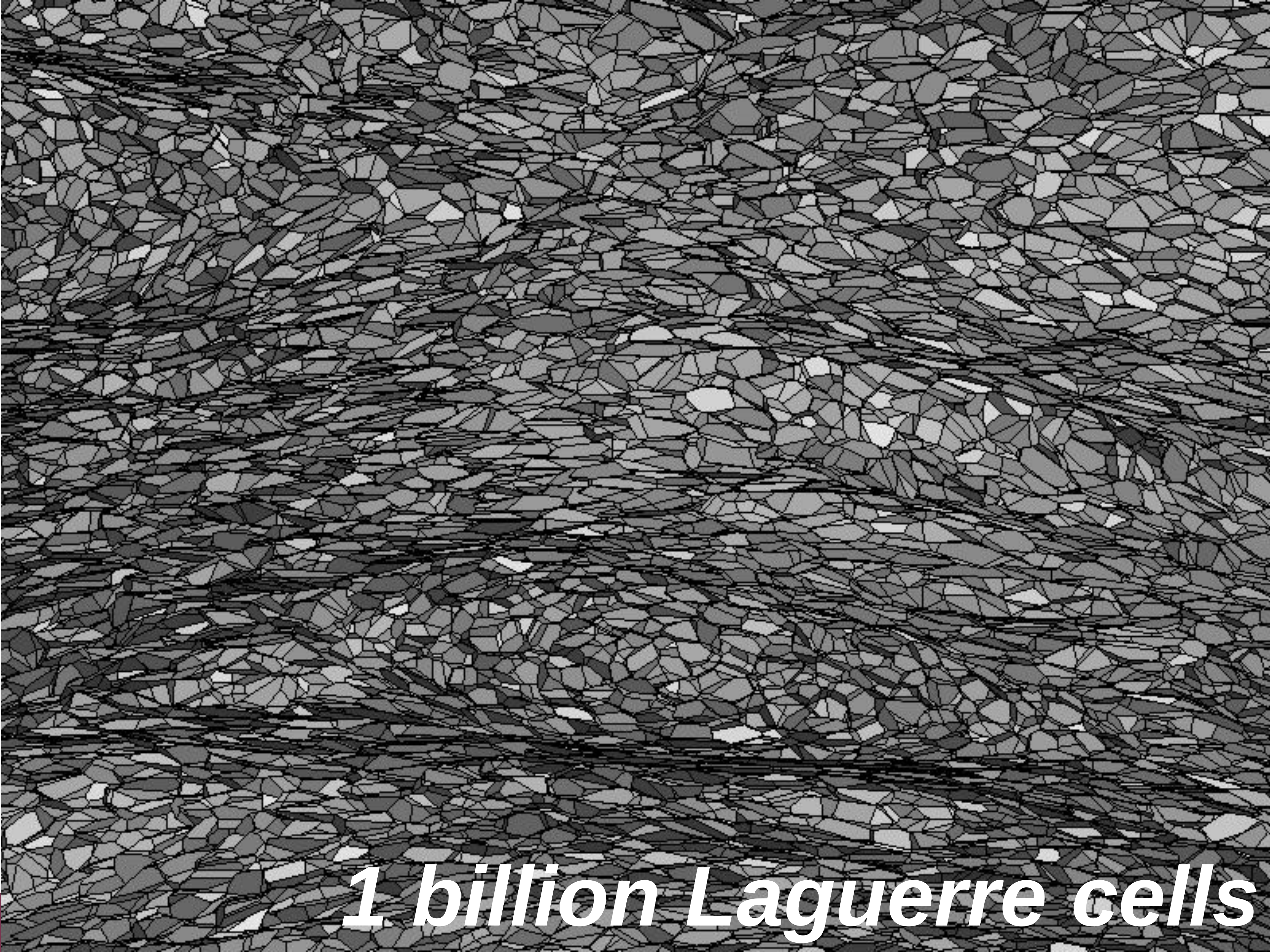
Scaling-up !



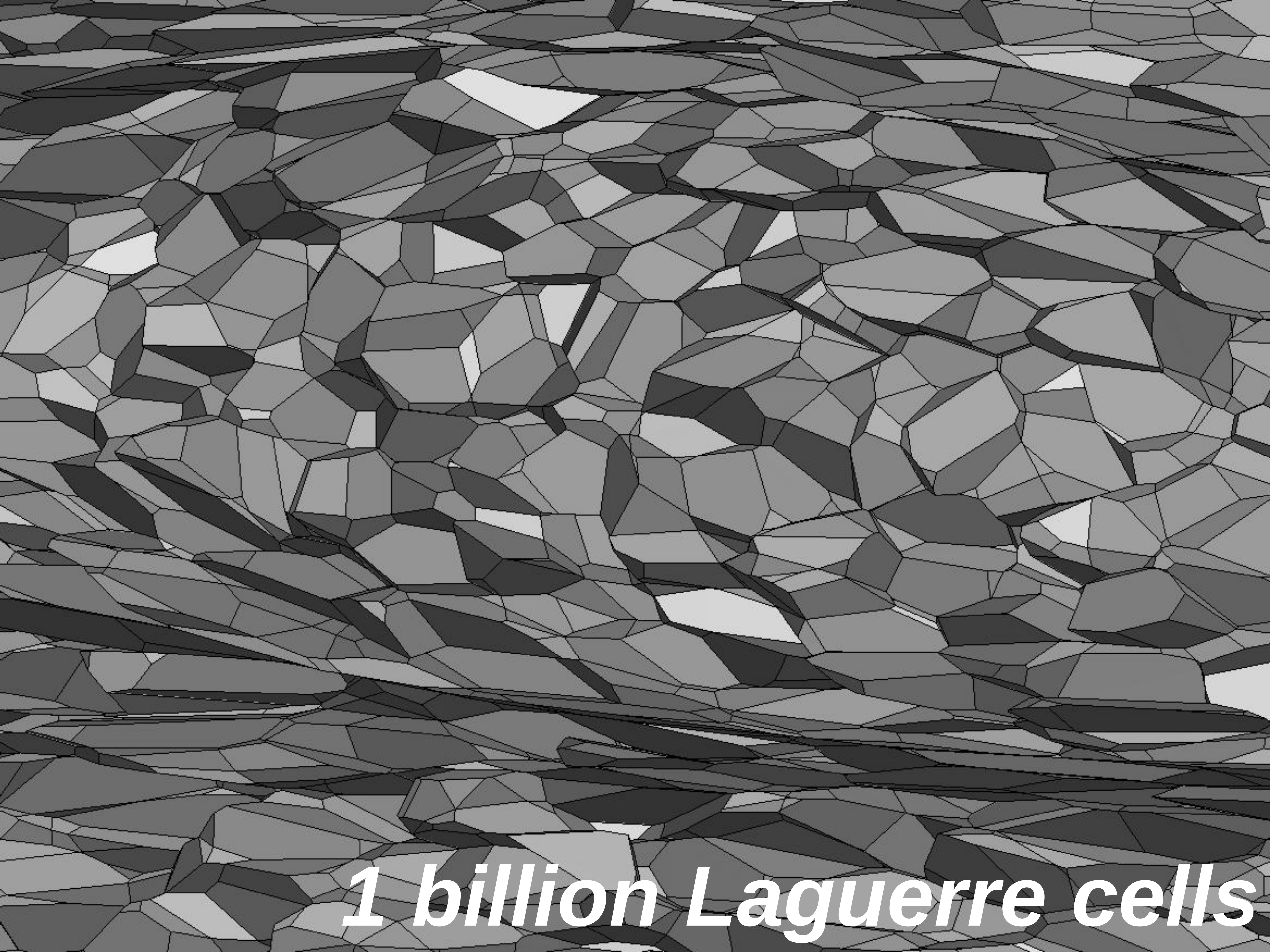
1 billion haloes

60 Mega parsecs





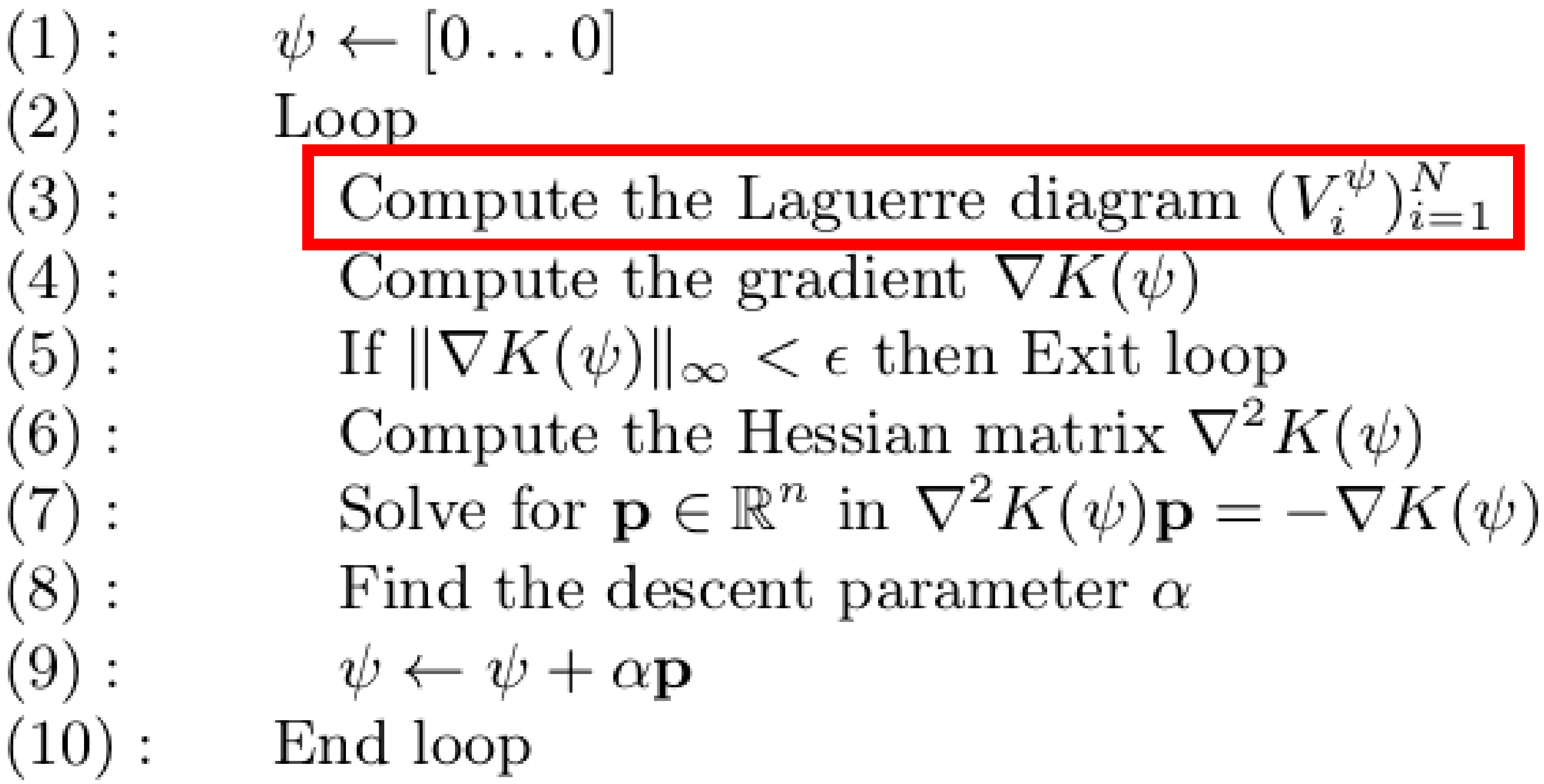
1 billion Laguerre cells



1 billion Laguerre cells

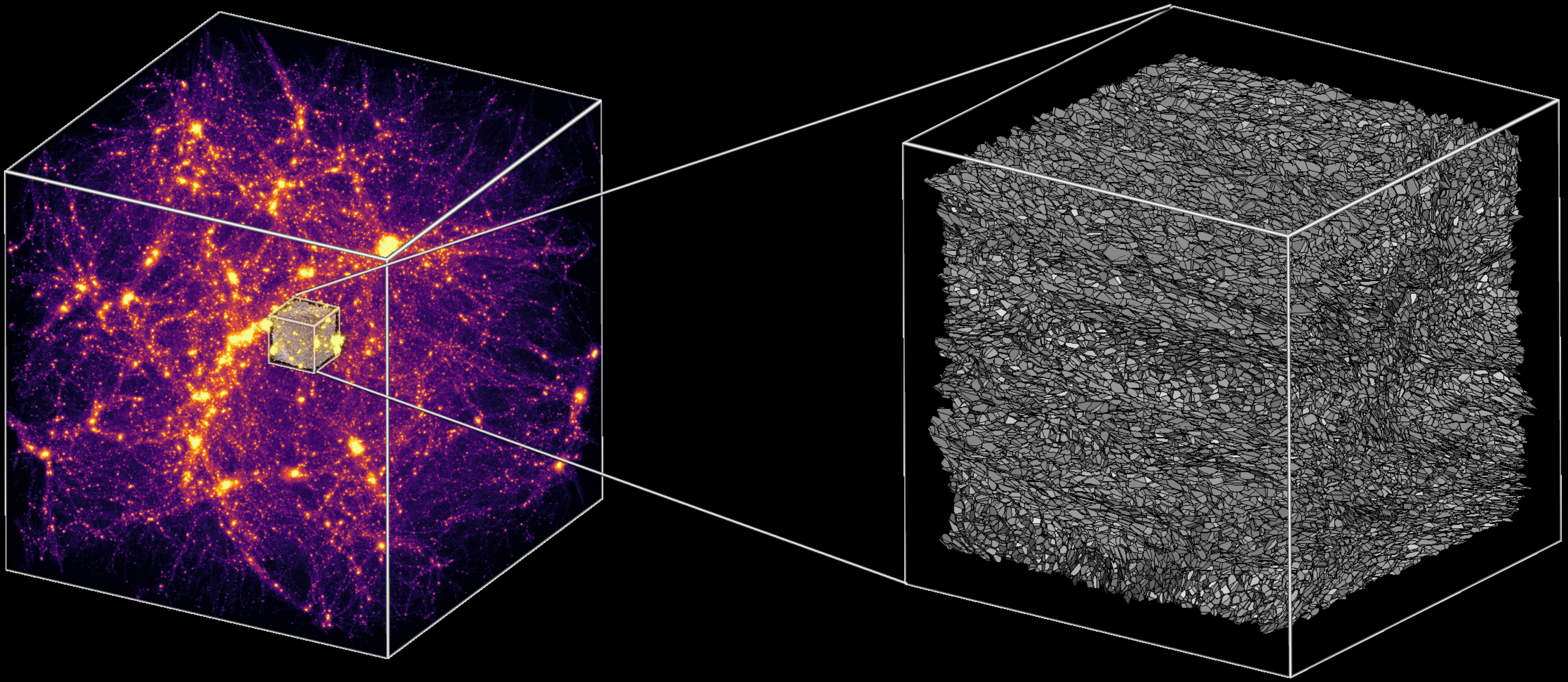
Part. 4 Scaling-up

1. Lion’s share I: geometry



```
$\psi \leftarrow [0 \ldots 0]$
Loop
    Compute the Laguerre diagram $(V_i^{\psi})_{i=1}^{N}$
    Compute the gradient $\nabla K(\psi)$
    If $\|\nabla K(\psi)\|_{\infty} < \epsilon$ then Exit loop
    Compute the Hessian matrix $\nabla^2 K(\psi)$
    Solve for $\mathbf{p} \in \mathbb{R}^n$ in $\nabla^2 K(\psi)\mathbf{p} = -\nabla K(\psi)$
    Find the descent parameter $\alpha$
    $\psi \leftarrow \psi + \alpha \mathbf{p}$
End loop
```

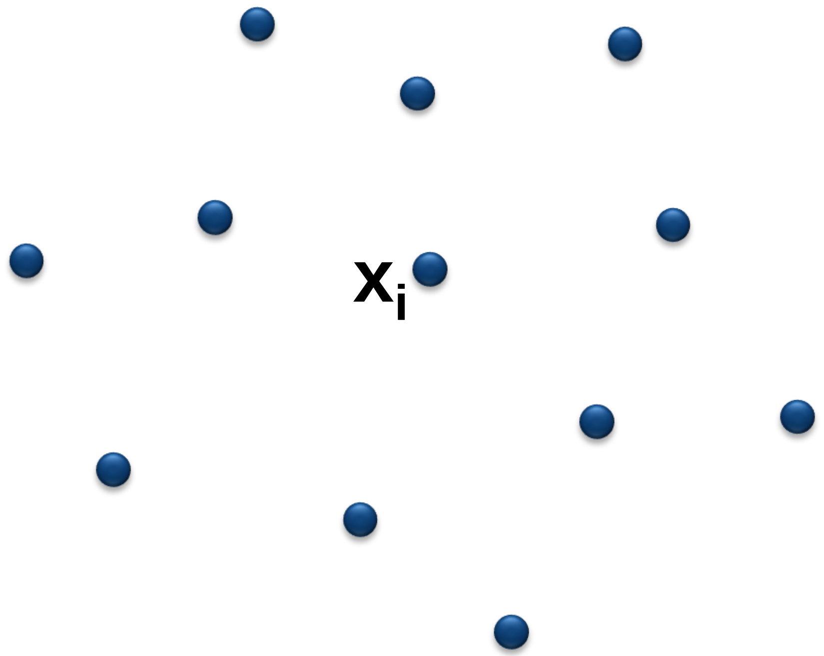
Part. 4 Scaling-up



Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

"Meshless Voronoi diagrams"

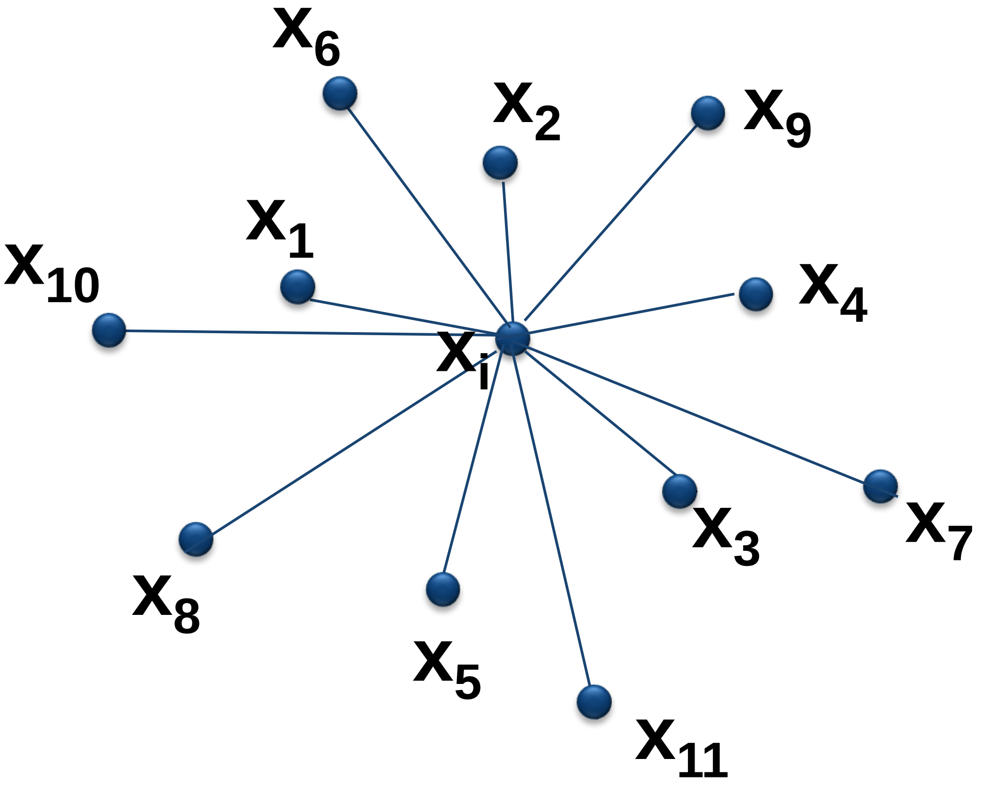


[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Neighbors in increasing distance from $\mathbf{x}_i$

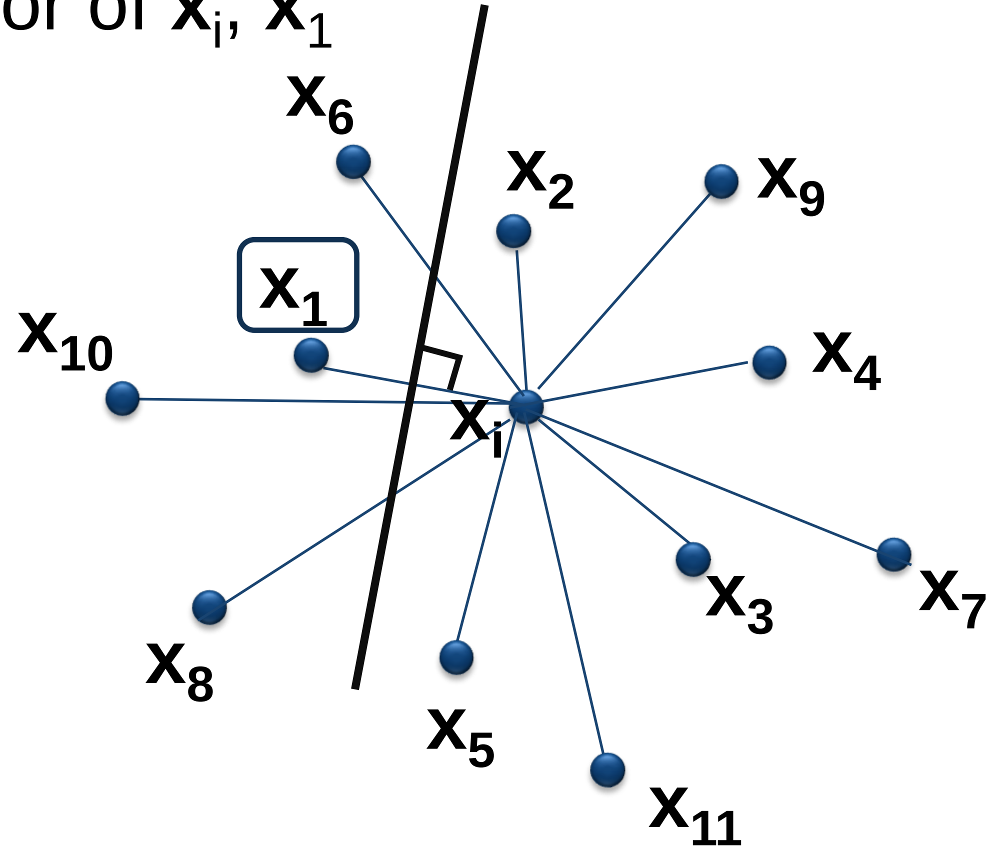


[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Bisector of $\mathbf{x}_i$, $\mathbf{x}_1$



[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

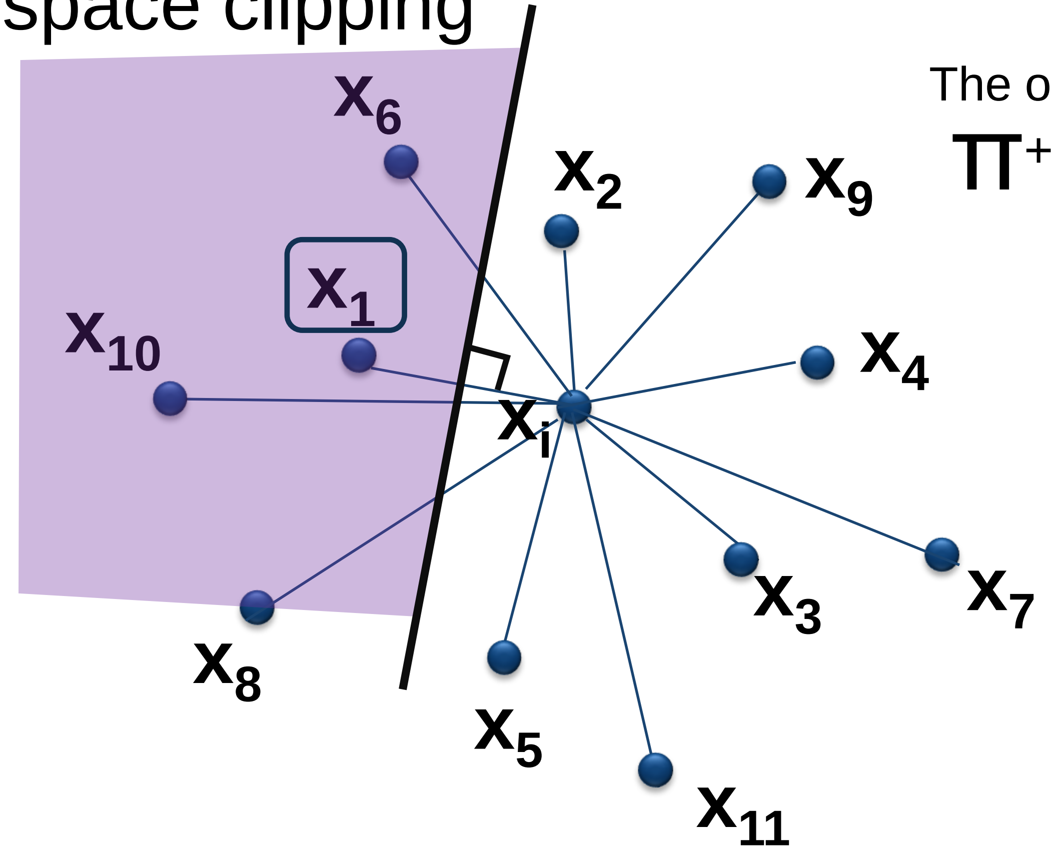
Half-space clipping

This side:

$\Pi^{-}(i,1)$

The other side:

$\Pi^{+}(i,1)$



[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

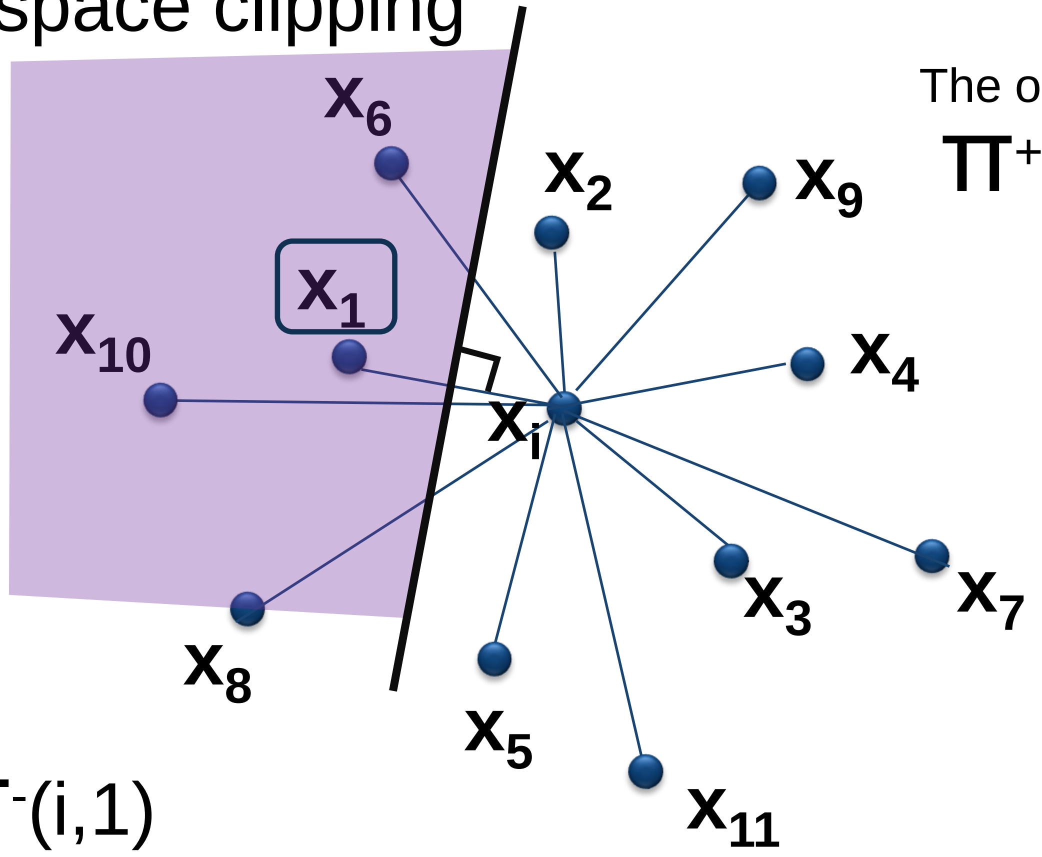
Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Half-space clipping

This side:
$\Pi^{-}(i,1)$

The other side:
$\Pi^{+}(i,1)$



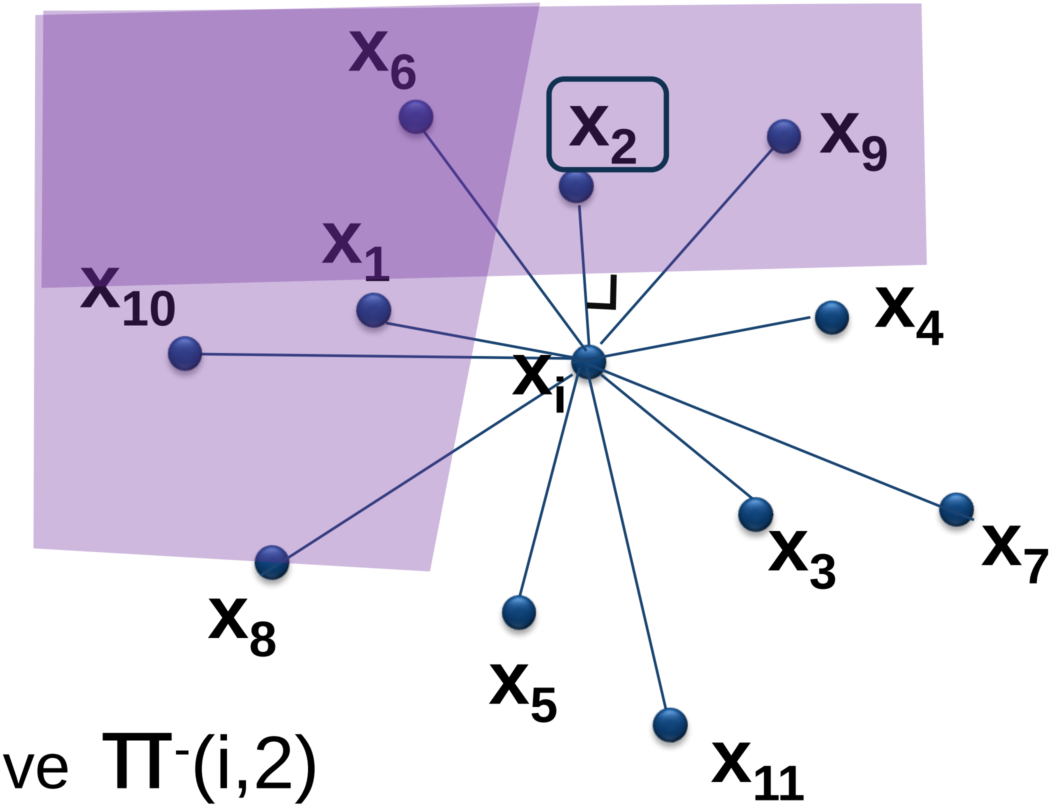
Remove $\Pi^{-}(i,1)$

[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Half-space clipping

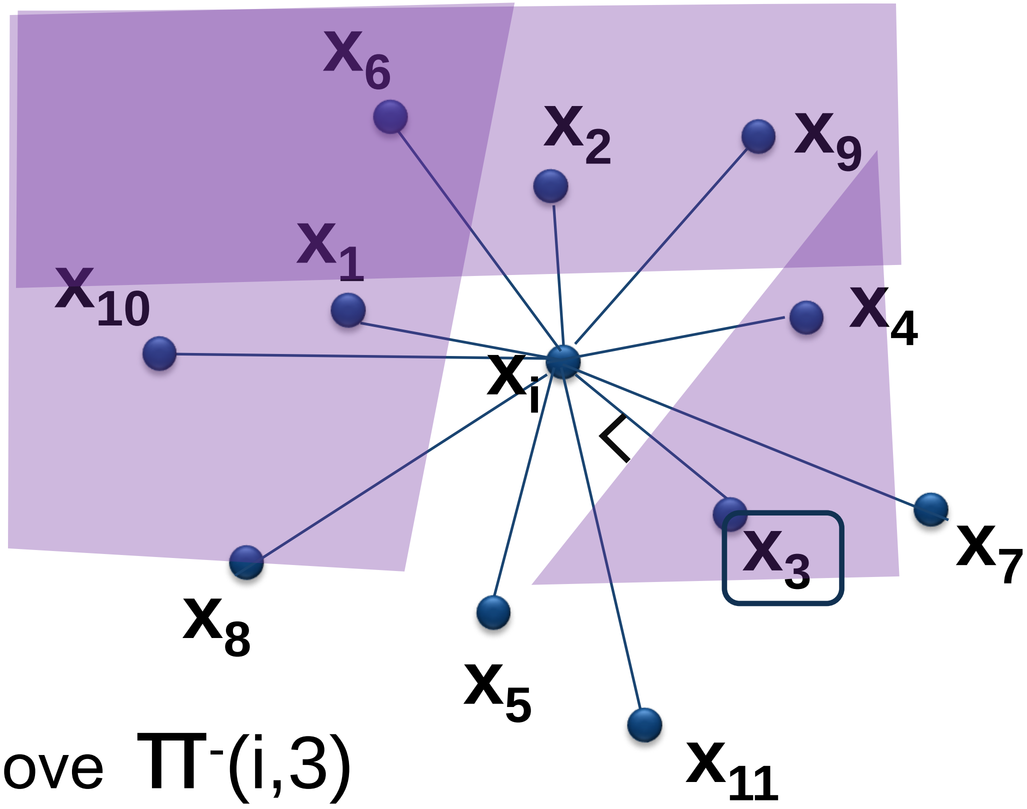


Then remove $\Pi^-(i,2)$

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Half-space clipping



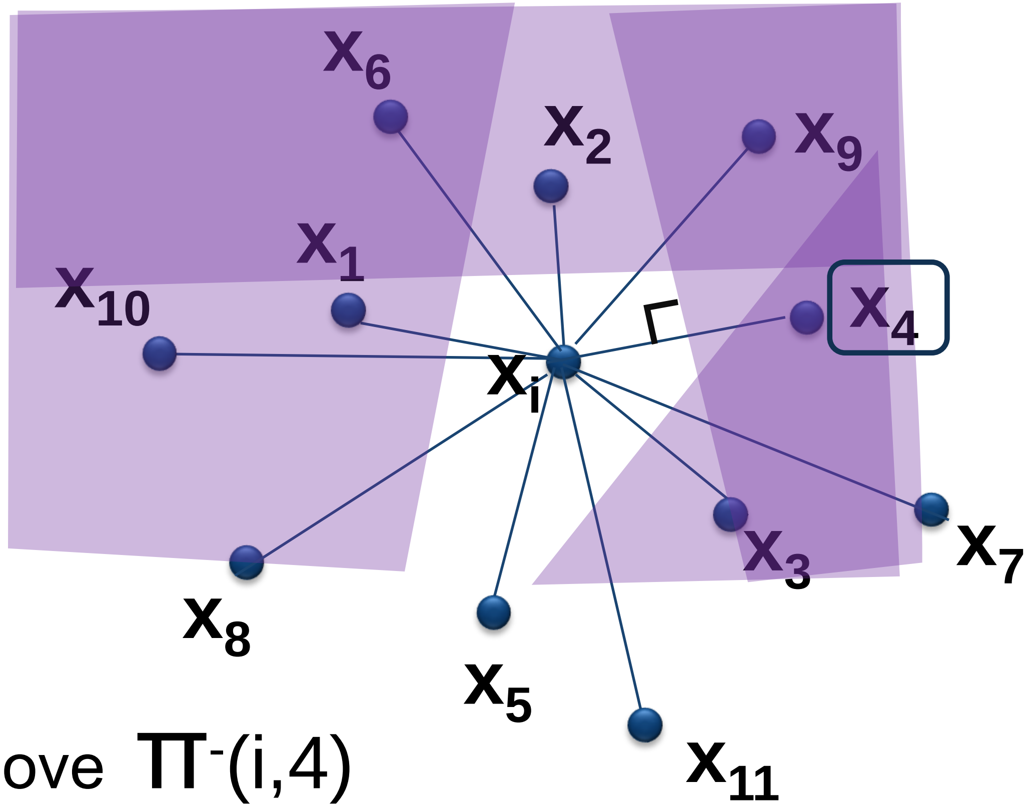
… then remove $\Pi^{-}(i,3)$

[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Half-space clipping



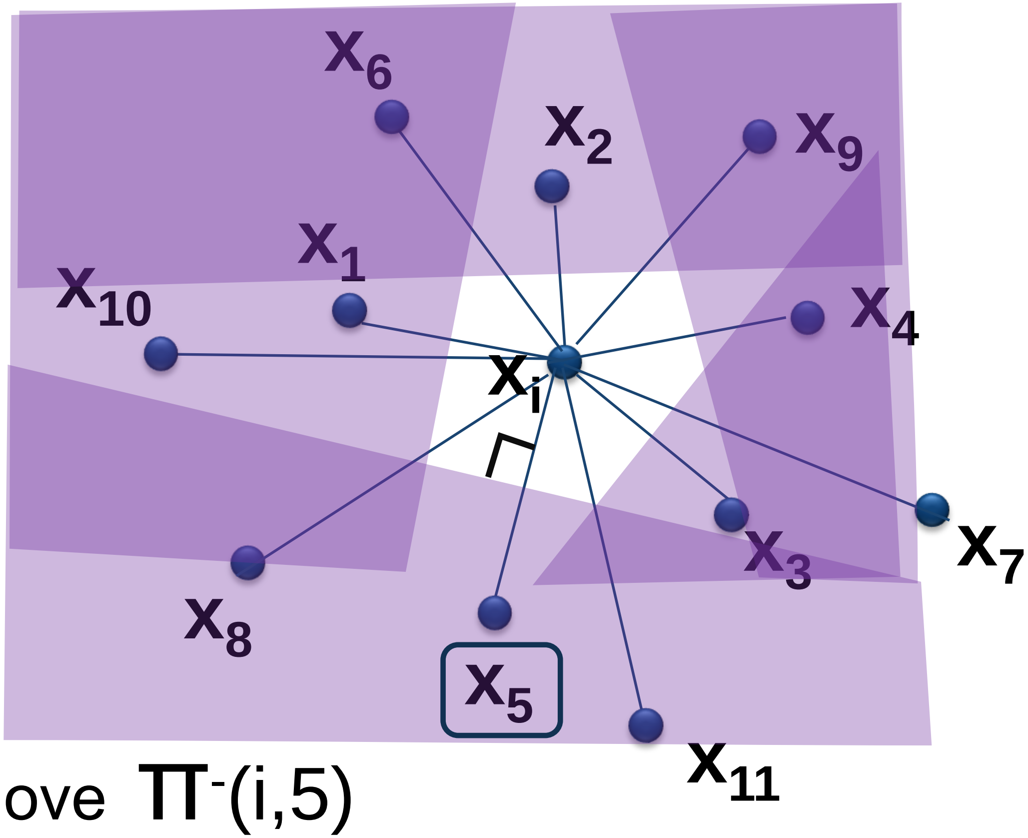
… then remove $\Pi^-(i,4)$

[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

Half-space clipping



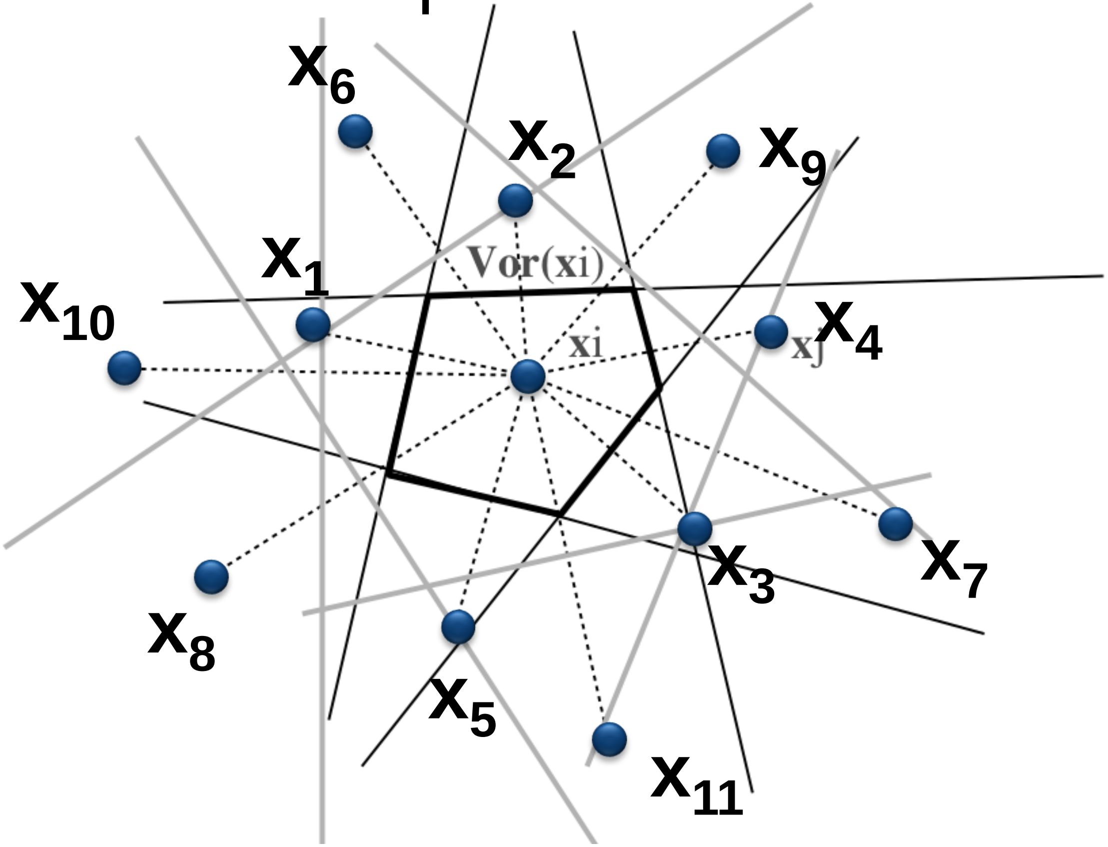
… then remove $\Pi^-(i,5)$

[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

When should I stop ?

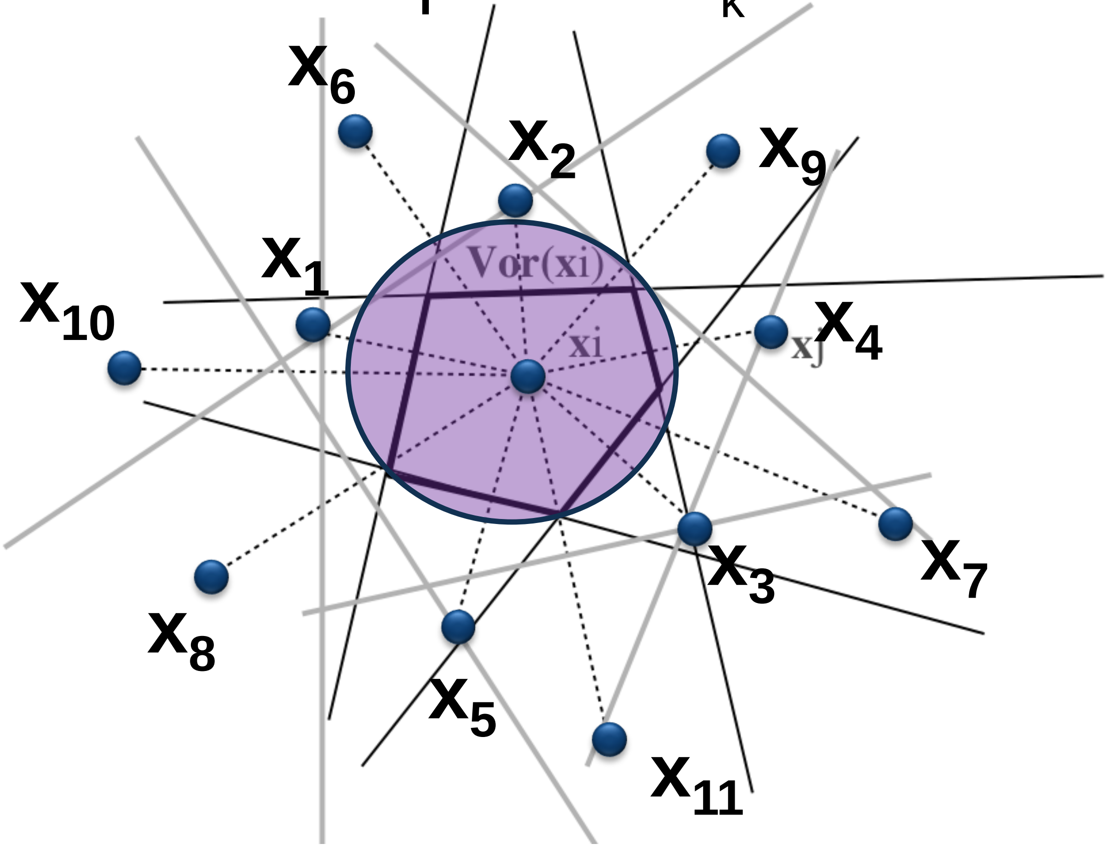


[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

When should I stop ? R_k

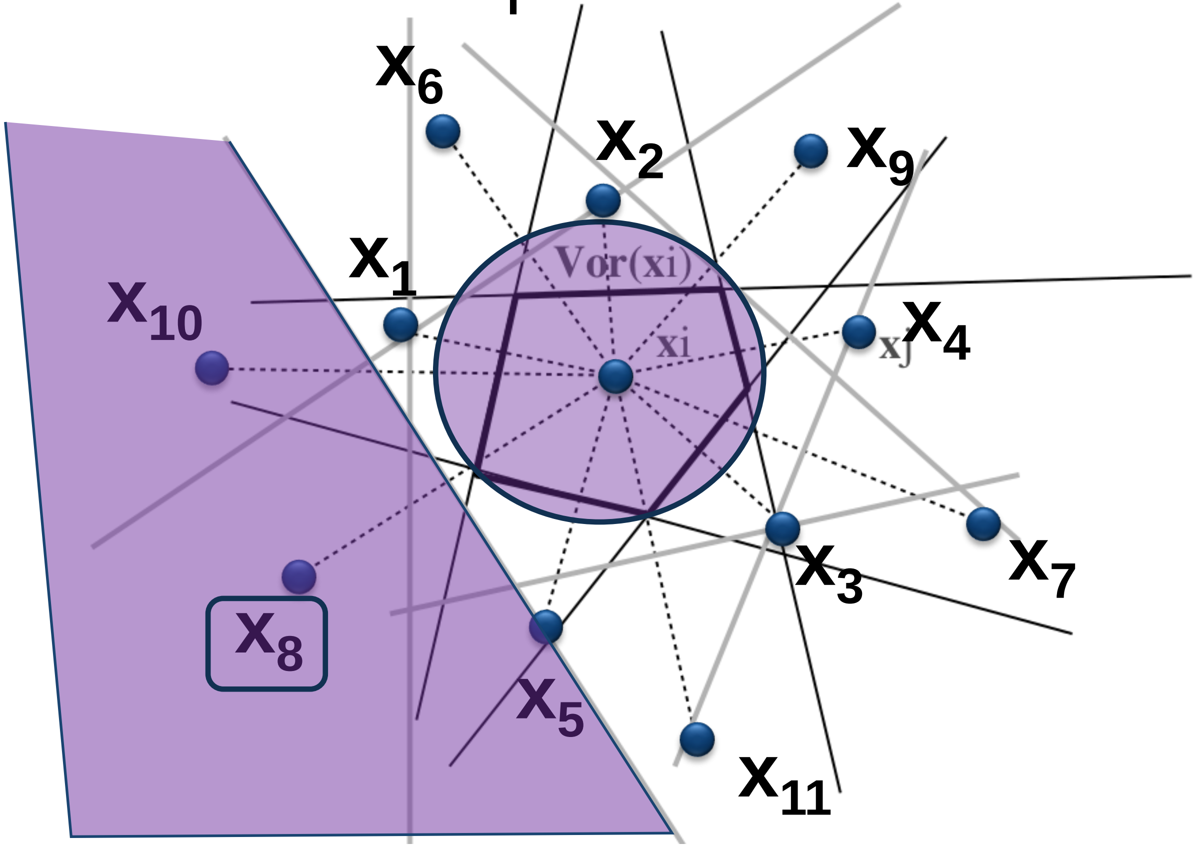


[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

When should I stop ?

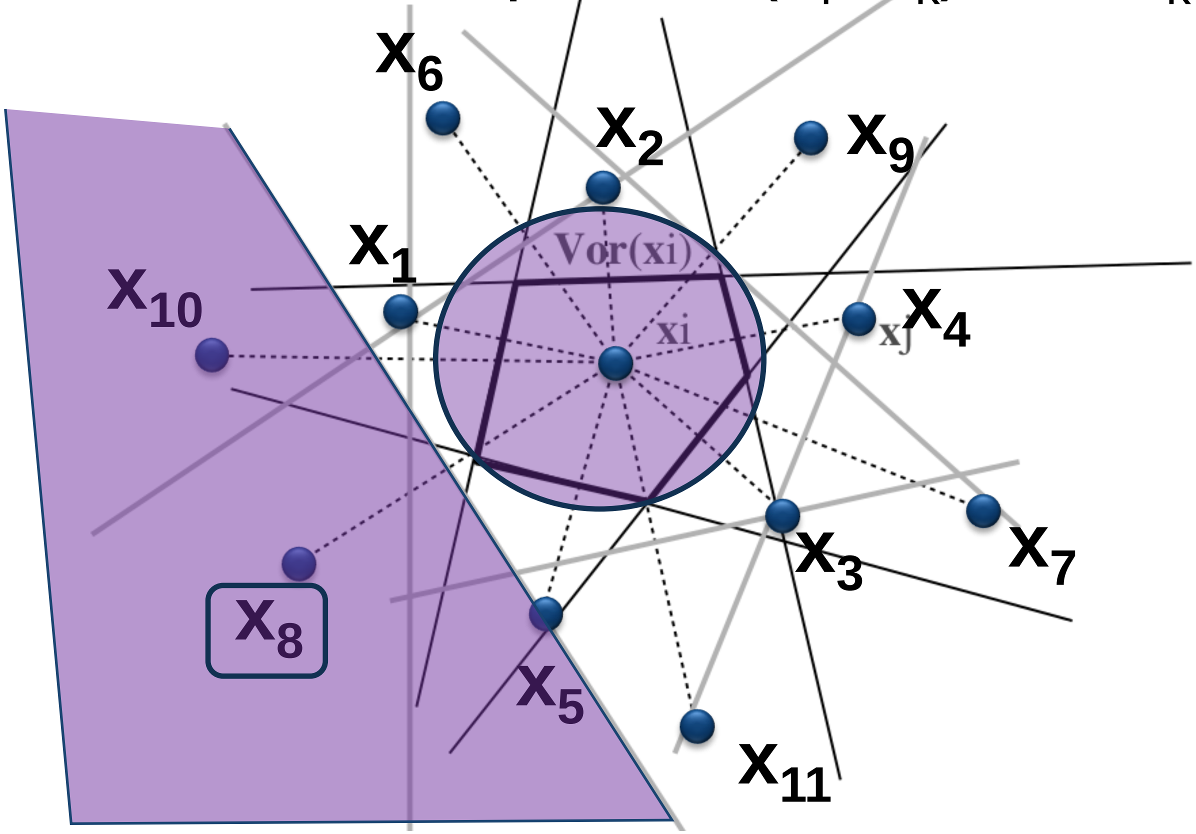


[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

When should I stop ? $d(\mathbf{x}_i, \mathbf{x}_k) > 2\ R_k$



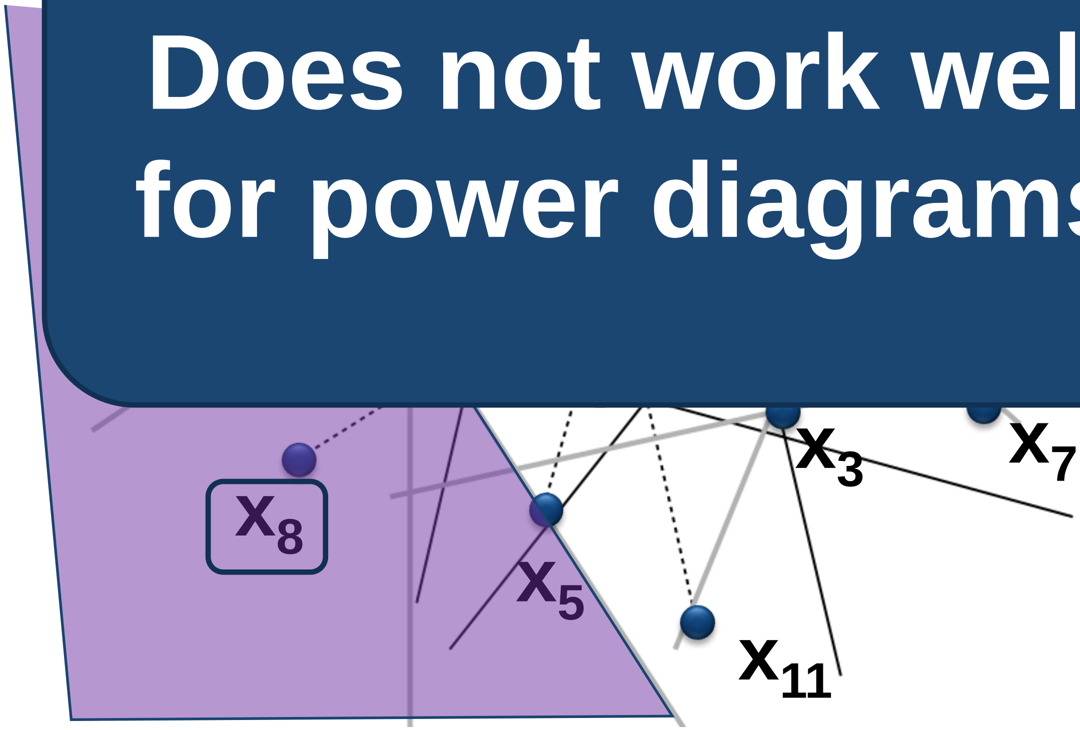
[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

Part. 4 Scaling-up

Voronoi cells as iterative convex clipping

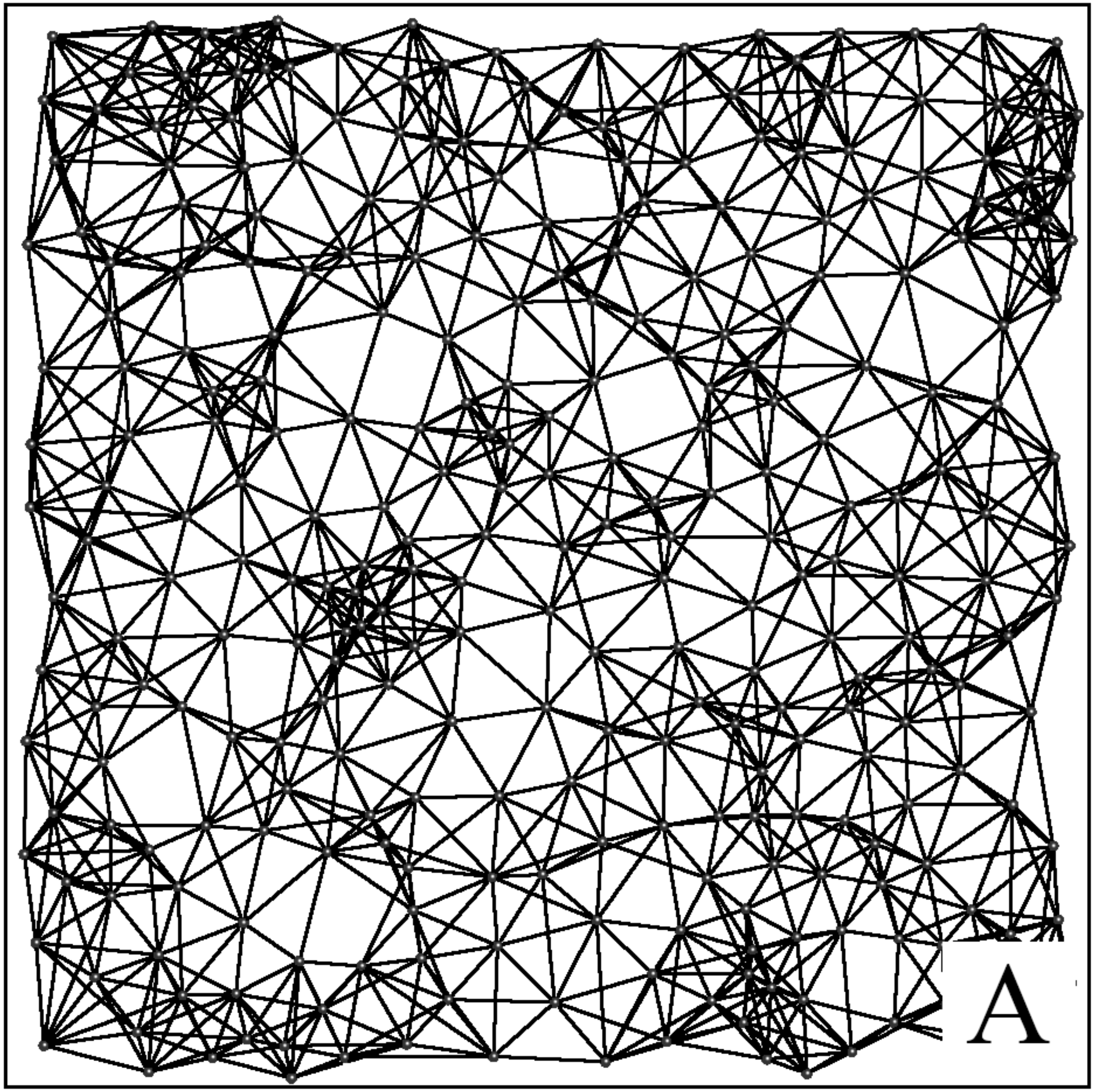
When should I stop ? $d(\mathbf{x}, \mathbf{x}) > 2 R_k$

Does not work well for power diagrams

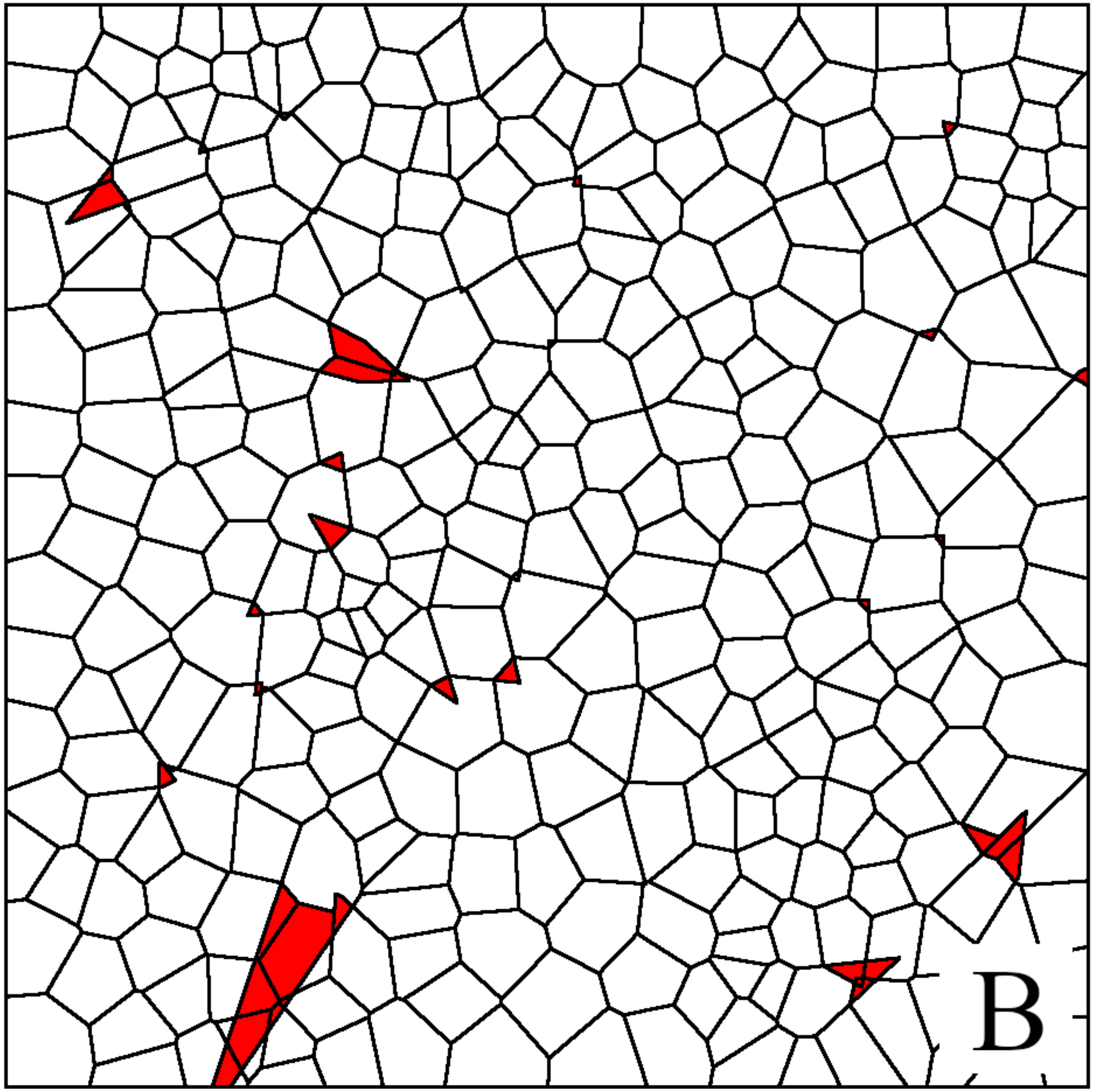


[Bonneel & **L**], [Ray, Sokolov, Lefebvre & **L**]

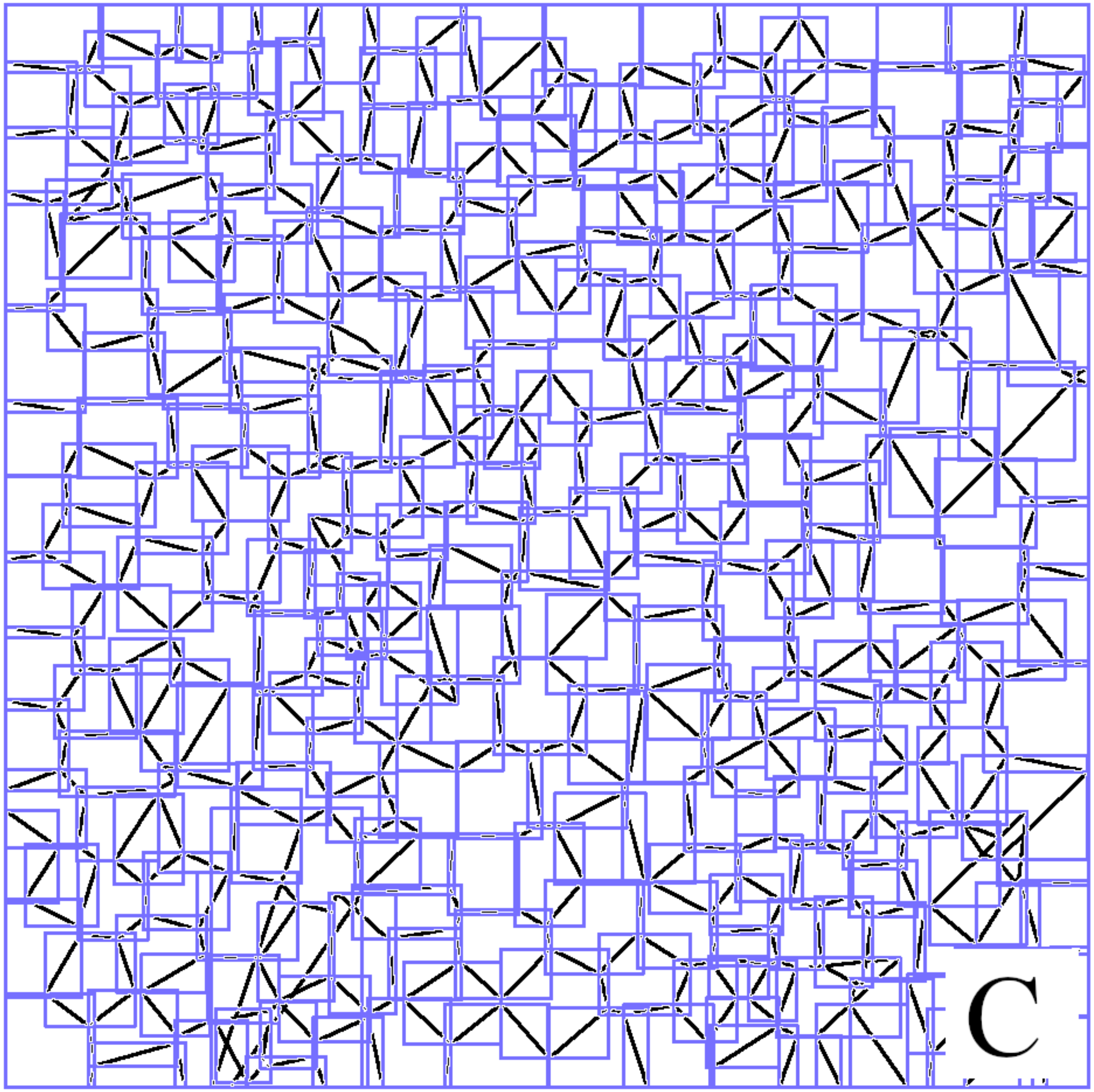
Part. 4 Scaling-up – Parallel Voronoi Diagram



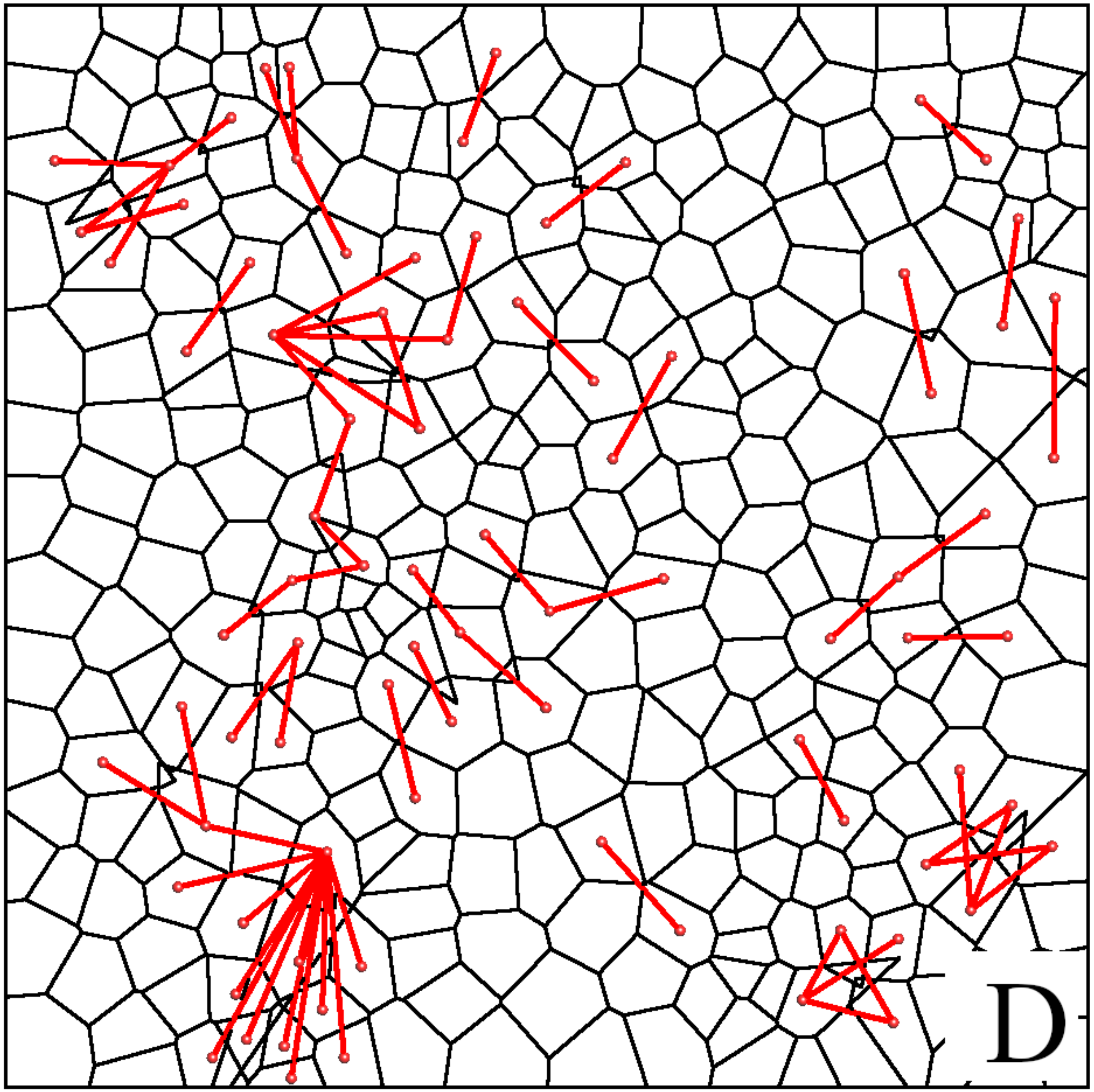
Part. 4 Scaling-up – Parallel Voronoi Diagram



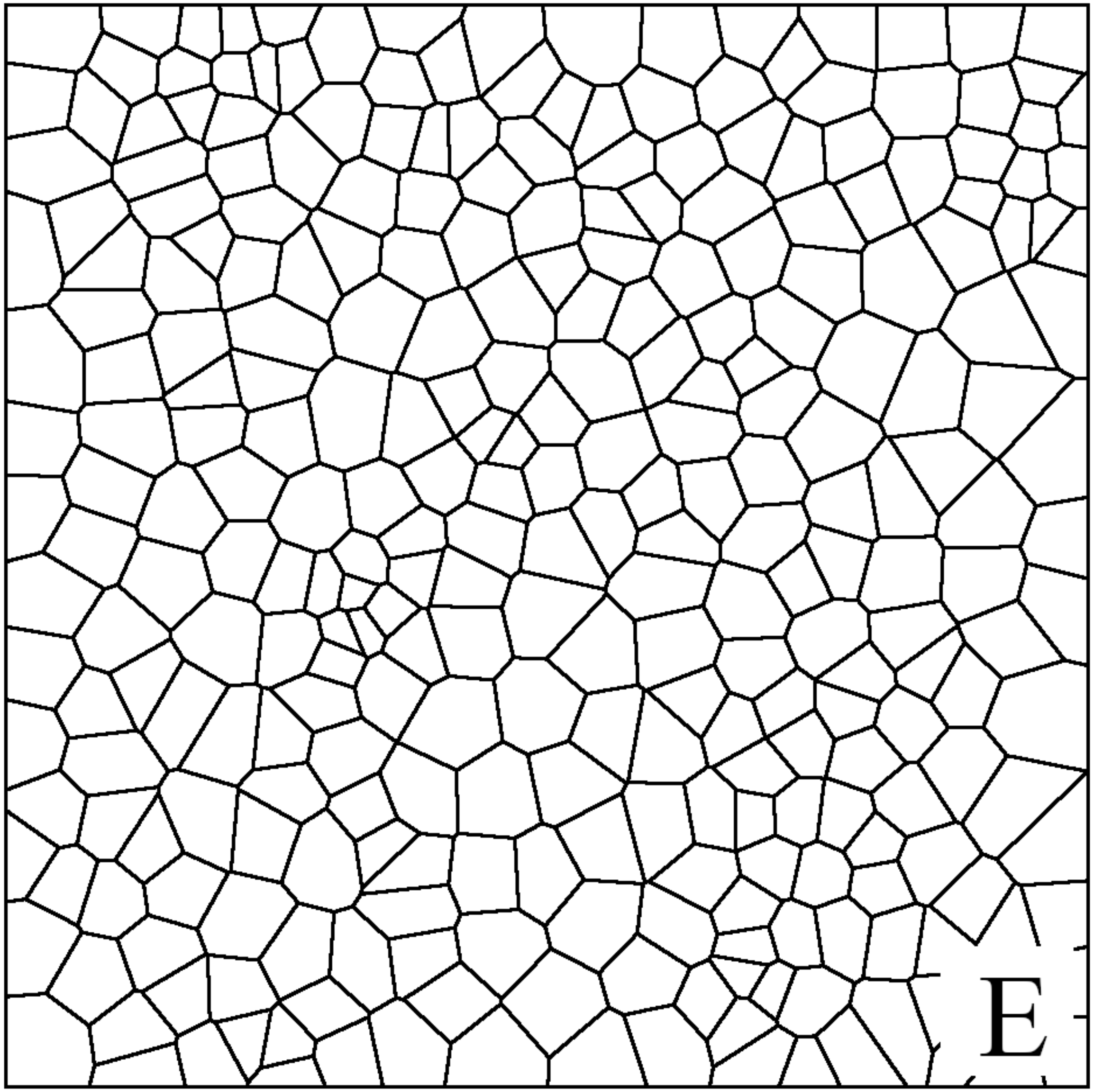
Part. 4 Scaling-up – Parallel Voronoi Diagram



Part. 4 Scaling-up – Parallel Voronoi Diagram

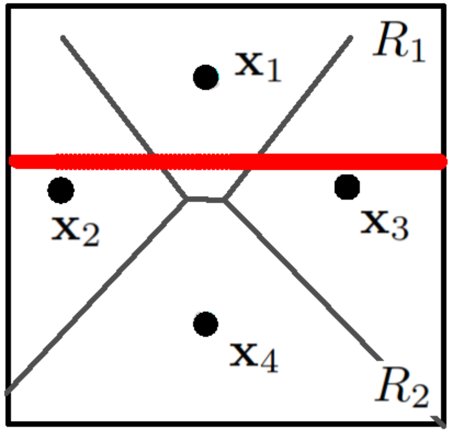


Part. 4 Scaling-up – Parallel Voronoi Diagram



Part. 4 Scaling-up – Distributed Voronoi Diagram

$\mathbf{X}_1 = \{\mathbf{x}_1\}$

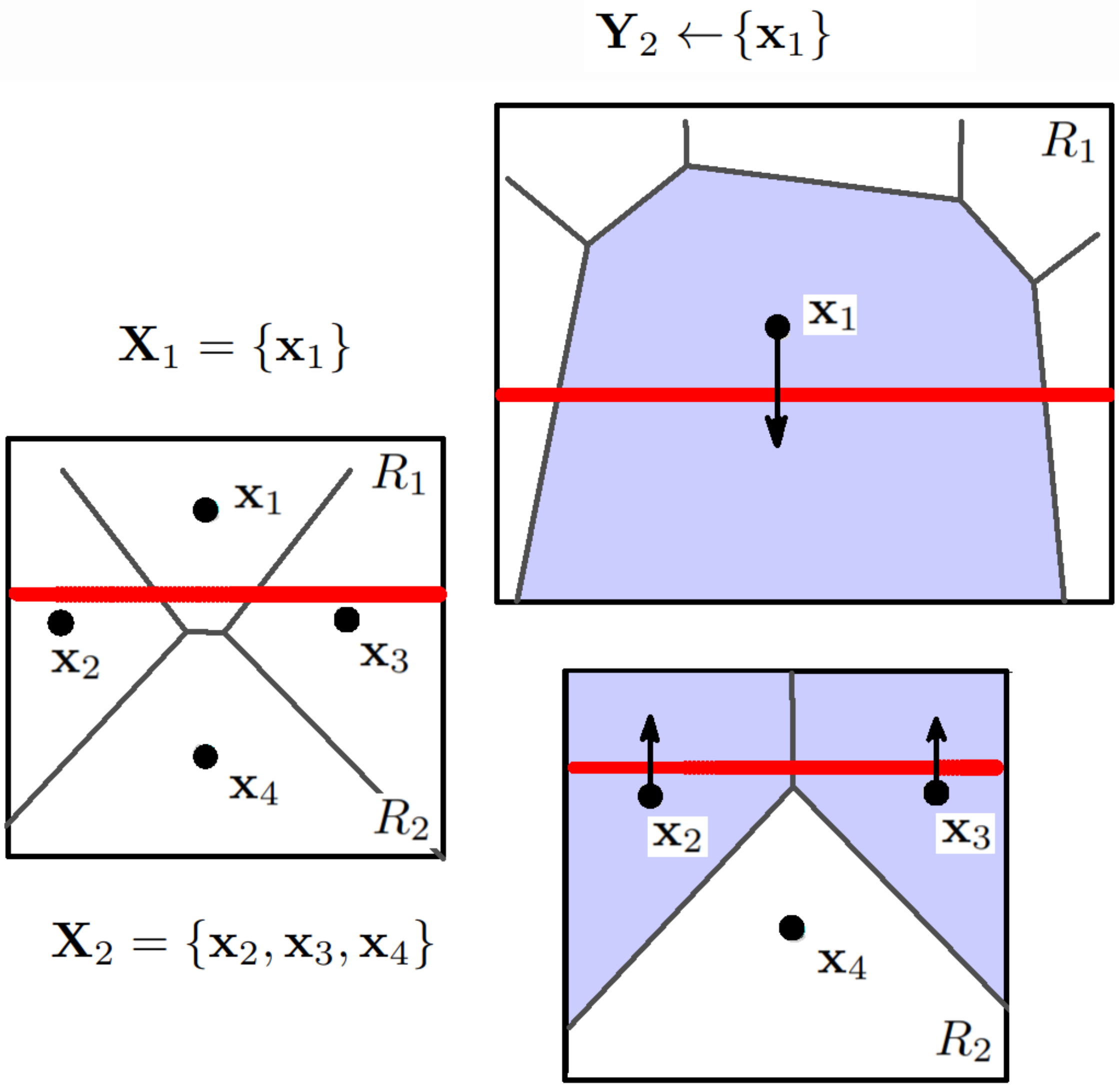


$\mathbf{X}_2 = \{\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$

Computer #1

Computer #2

Part. 4 Scaling-up – Distributed Voronoi Diagram

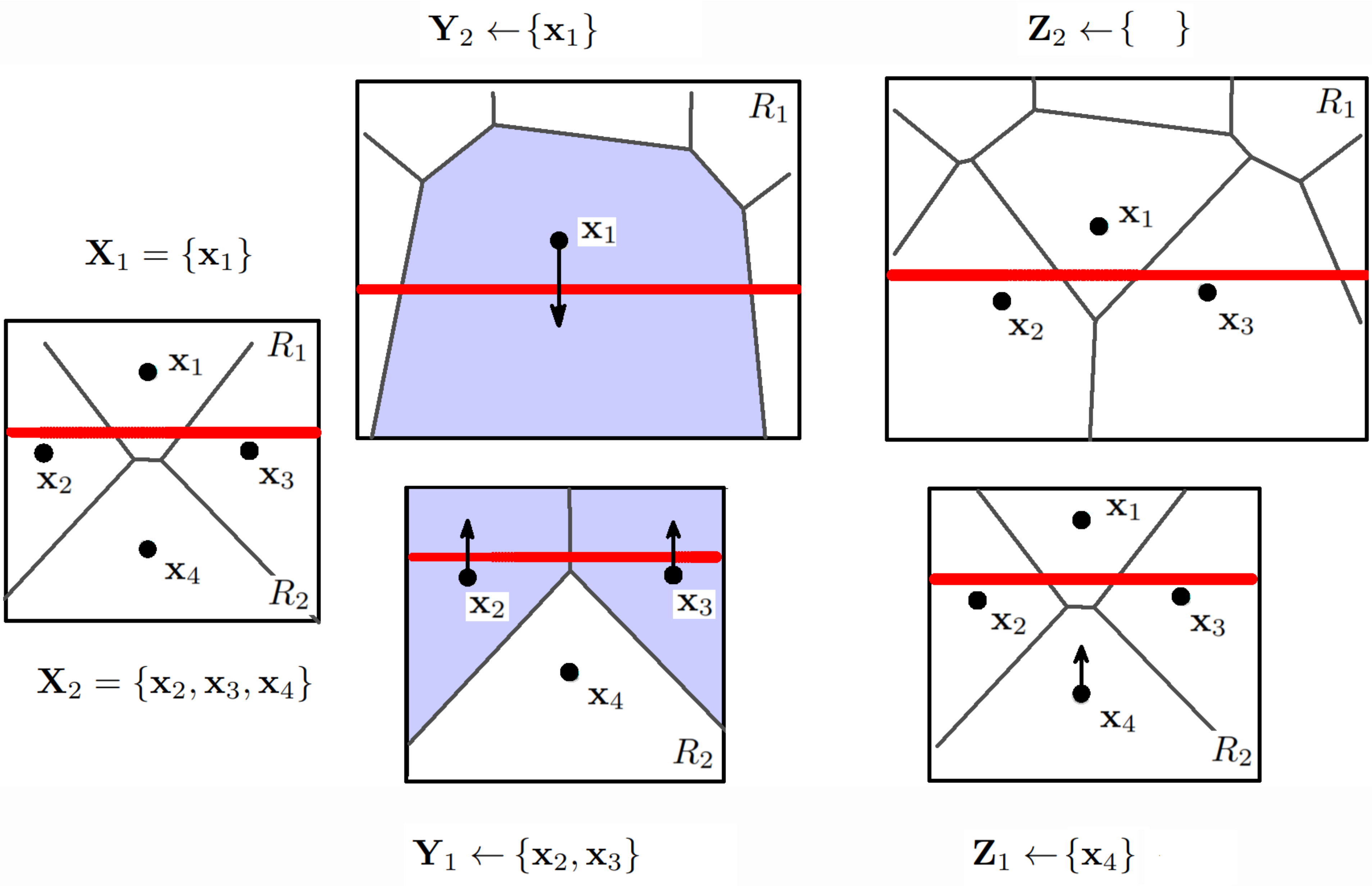


$$\mathbf{Y}_2 \leftarrow \{\mathbf{x}_1\}$$

$$\mathbf{X}_1 = \{\mathbf{x}_1\}$$

$$\mathbf{X}_2 = \{\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$$

Part. 4 Scaling-up – Distributed Voronoi Diagram



$\mathbf{Y}_2 \leftarrow \{\mathbf{x}_1\}$

$\mathbf{Z}_2 \leftarrow \{\quad\}$

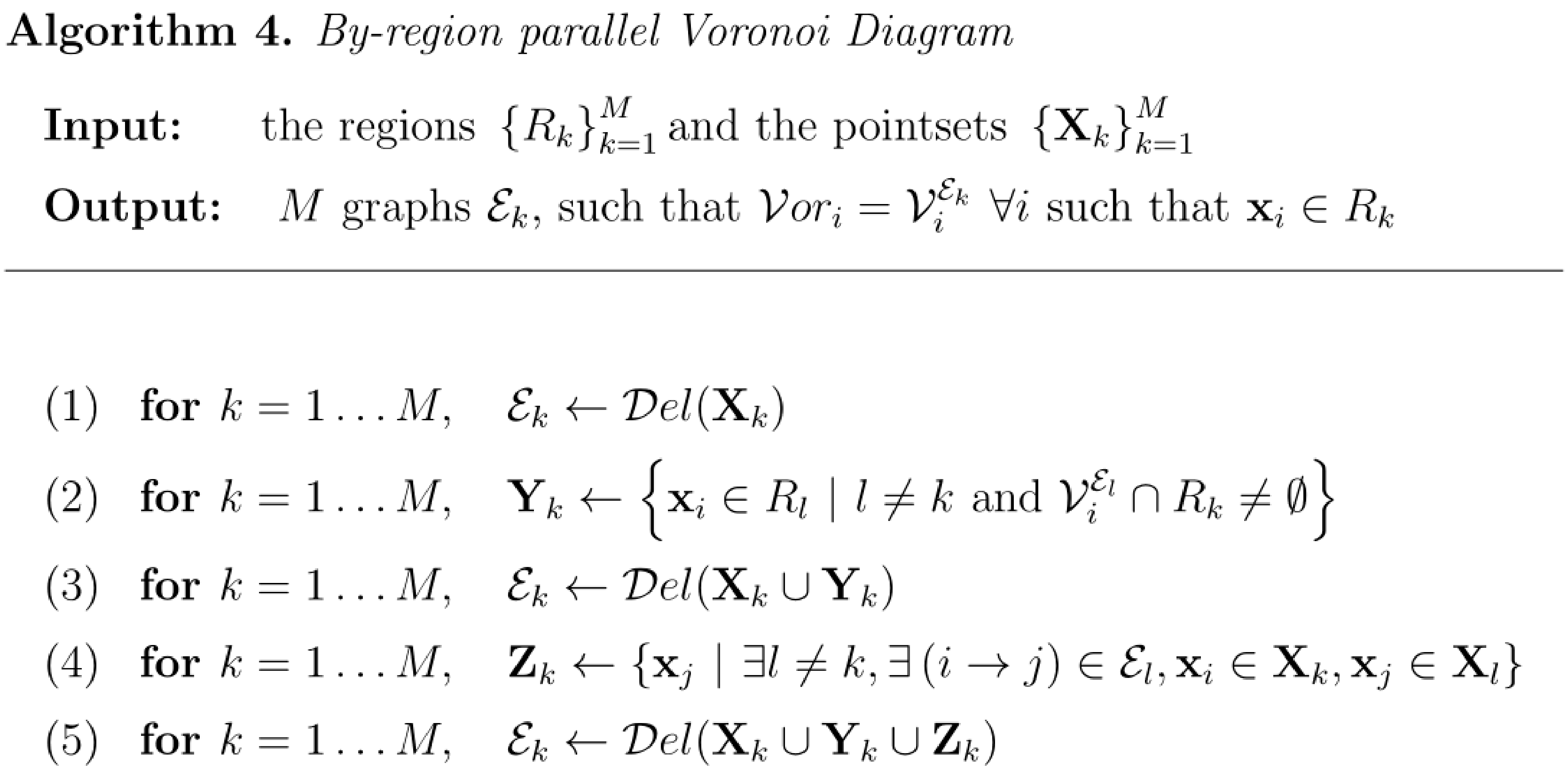
$\mathbf{X}_1 = \{\mathbf{x}_1\}$

$\mathbf{X}_2 = \{\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$

$\mathbf{Y}_1 \leftarrow \{\mathbf{x}_2, \mathbf{x}_3\}$

$\mathbf{Z}_1 \leftarrow \{\mathbf{x}_4\}$

Part. 4 Scaling-up – Distributed Voronoi Diagram



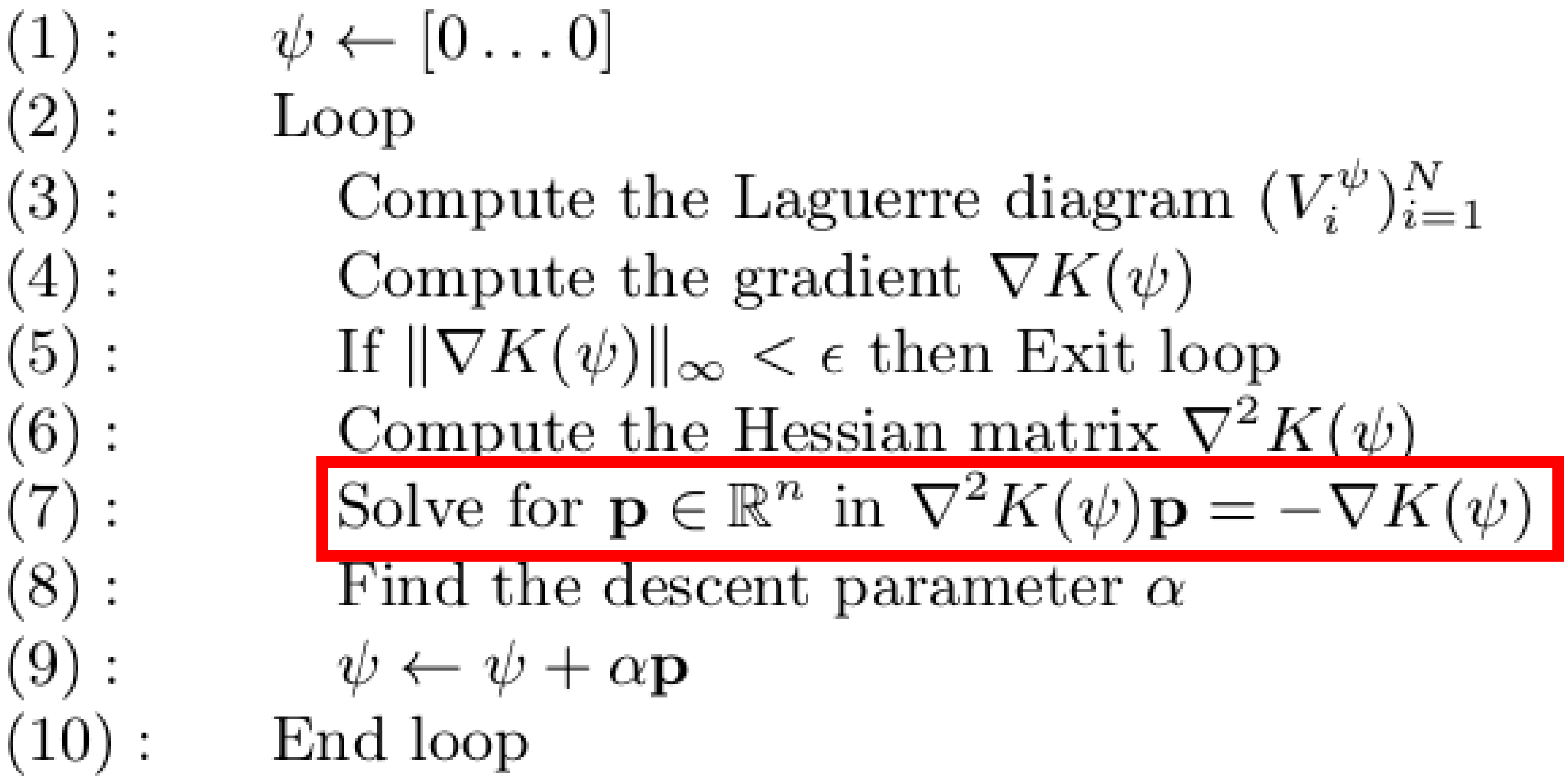
Algorithm 4. *By-region parallel Voronoi Diagram*

Input: the regions $\{R_k\}_{k=1}^{M}$ and the pointsets $\{\mathbf{X}_k\}_{k=1}^{M}$

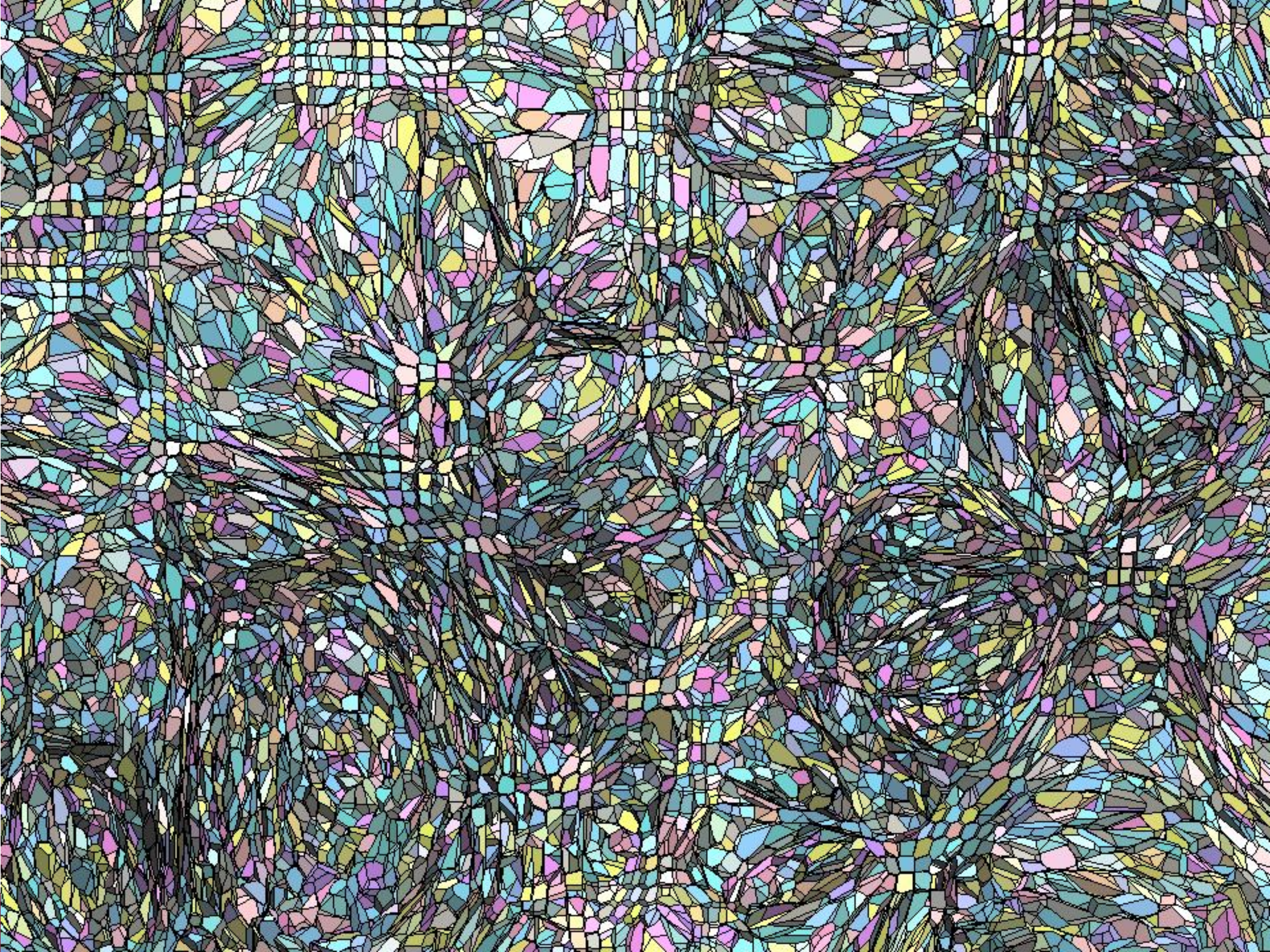
Output: M graphs $\mathcal{E}_k$, such that $\mathcal{V}or_i = \mathcal{V}_i^{\mathcal{E}_k}$ $\forall i$ such that $\mathbf{x}_i \in R_k$

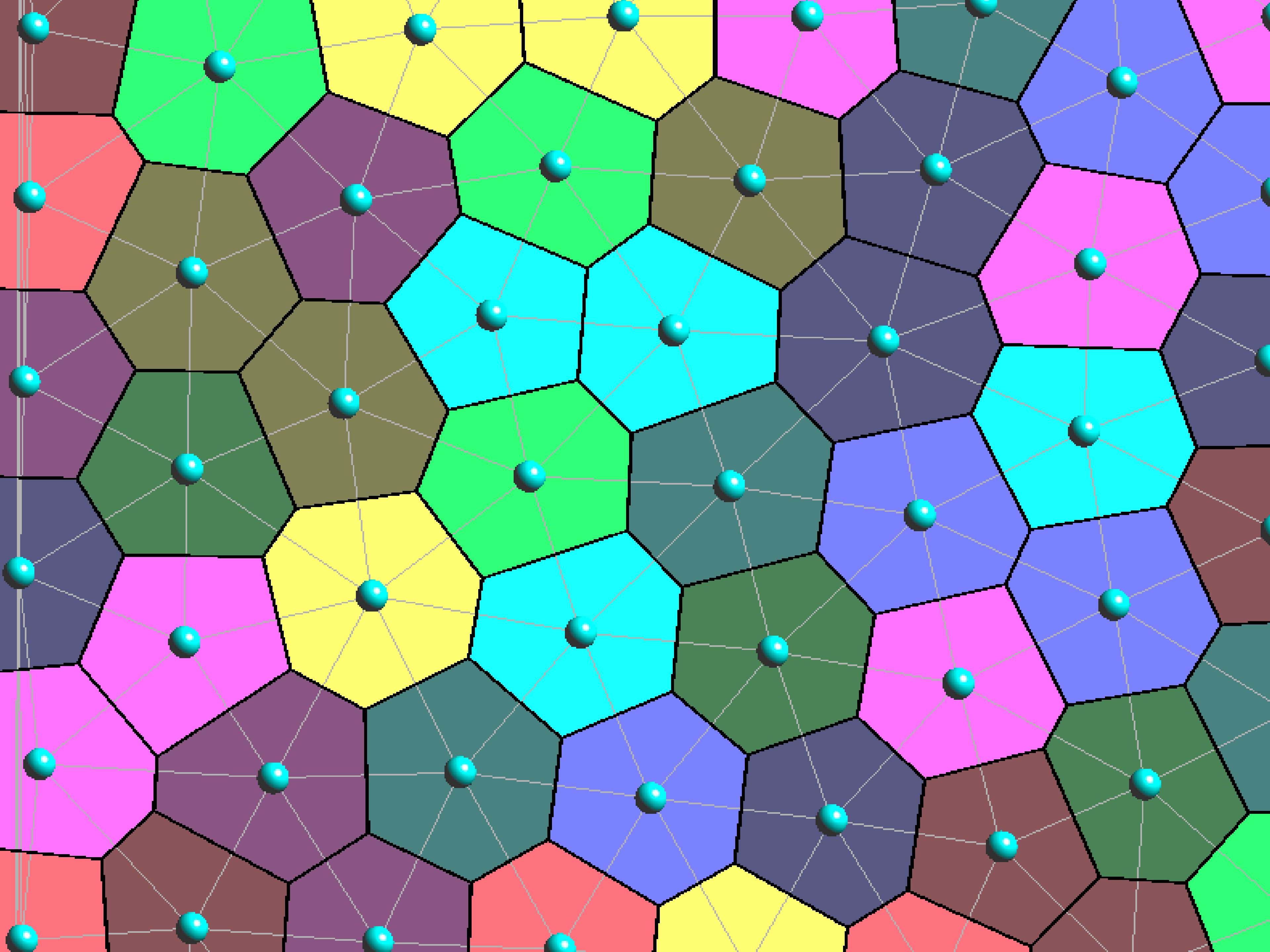
```
(1)  for $k = 1 \ldots M$,   $\mathcal{E}_k \leftarrow \mathcal{D}el(\mathbf{X}_k)$
(2)  for $k = 1 \ldots M$,   $\mathbf{Y}_k \leftarrow \left\{\mathbf{x}_i \in R_l \mid l \neq k \text{ and } \mathcal{V}_i^{\mathcal{E}_l} \cap R_k \neq \emptyset\right\}$
(3)  for $k = 1 \ldots M$,   $\mathcal{E}_k \leftarrow \mathcal{D}el(\mathbf{X}_k \cup \mathbf{Y}_k)$
(4)  for $k = 1 \ldots M$,   $\mathbf{Z}_k \leftarrow \{\mathbf{x}_j \mid \exists l \neq k, \exists (i \rightarrow j) \in \mathcal{E}_l, \mathbf{x}_i \in \mathbf{X}_k, \mathbf{x}_j \in \mathbf{X}_l\}$
(5)  for $k = 1 \ldots M$,   $\mathcal{E}_k \leftarrow \mathcal{D}el(\mathbf{X}_k \cup \mathbf{Y}_k \cup \mathbf{Z}_k)$
```

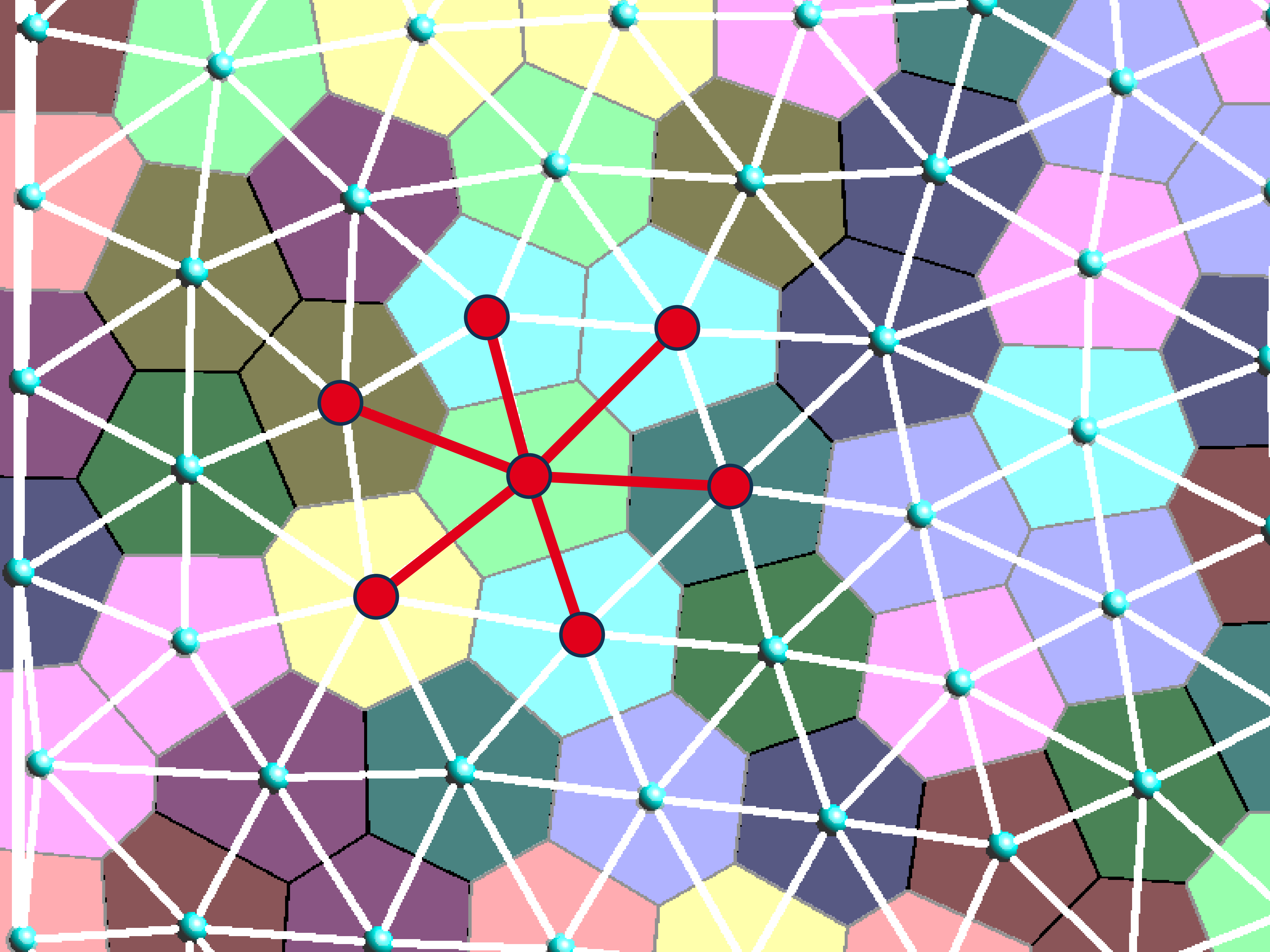
2. Lion's share II: linsolve



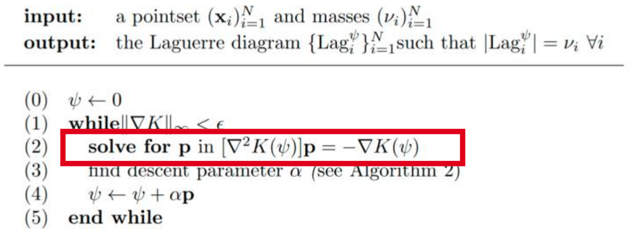
```
$\psi \leftarrow [0 \ldots 0]$
Loop
    Compute the Laguerre diagram $(V_i^\psi)_{i=1}^N$
    Compute the gradient $\nabla K(\psi)$
    If $\|\nabla K(\psi)\|_\infty < \epsilon$ then Exit loop
    Compute the Hessian matrix $\nabla^2 K(\psi)$
    Solve for $\mathbf{p} \in \mathbb{R}^n$ in $\nabla^2 K(\psi)\mathbf{p} = -\nabla K(\psi)$
    Find the descent parameter $\alpha$
    $\psi \leftarrow \psi + \alpha \mathbf{p}$
End loop
```







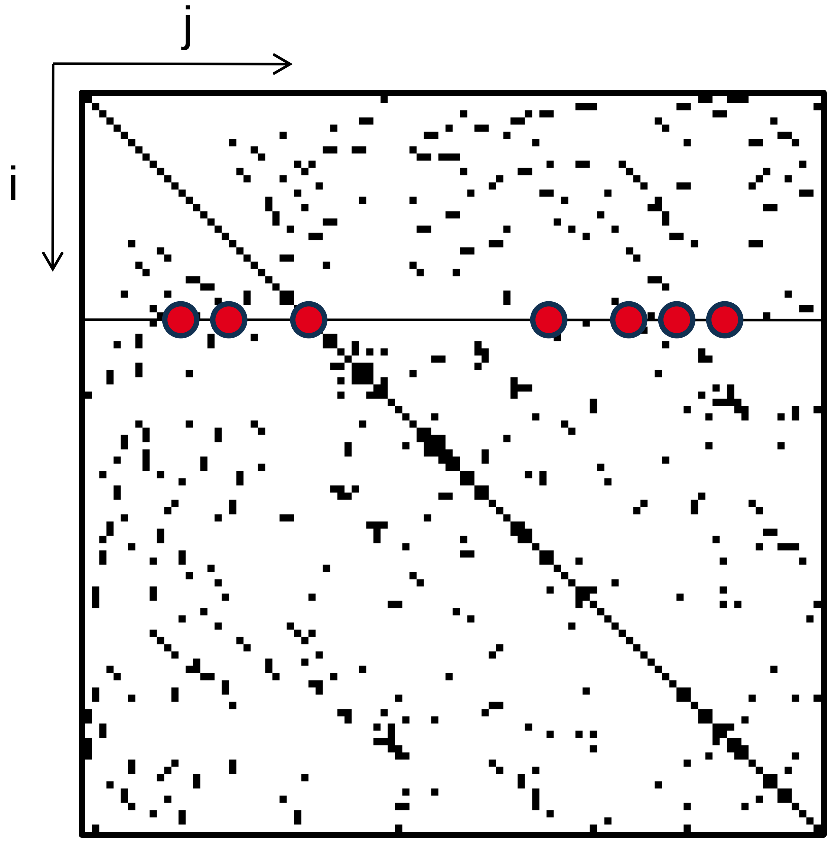
solve for $\mathbf{p}$ in $[\nabla^2 K(\psi)]\mathbf{p} = -\nabla K(\psi)$

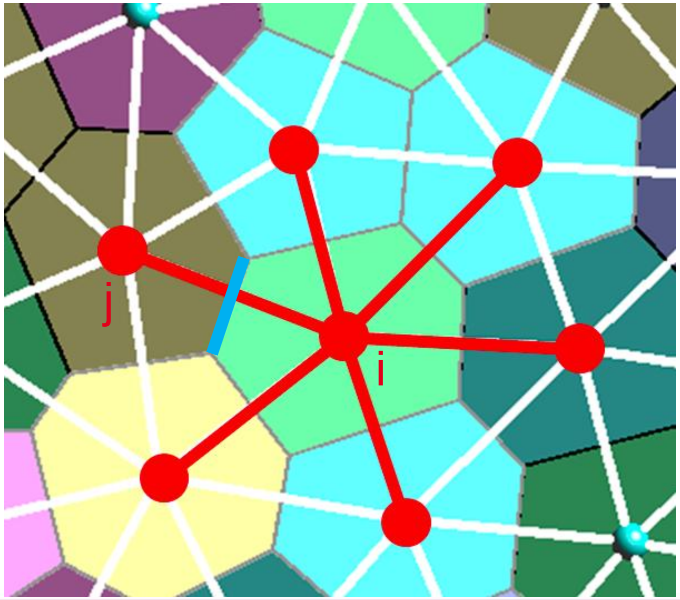


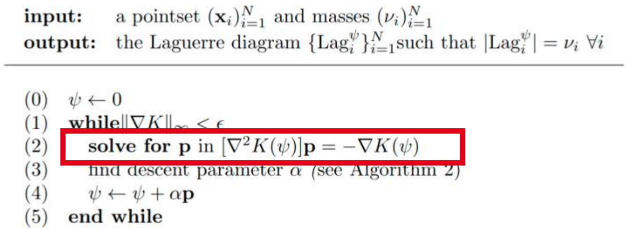
input: a pointset $(\mathbf{x}_i)_{i=1}^N$ and masses $(\nu_i)_{i=1}^N$

output: the Laguerre diagram $\{\text{Lag}_i^\psi\}_{i=1}^N$such that $|\text{Lag}_i^\psi| = \nu_i \ \forall i$

```
$\psi \leftarrow 0$
while $\|\nabla K\|_\infty < \epsilon$
    solve for p in $[\nabla^2 K(\psi)]\mathbf{p} = -\nabla K(\psi)$
    find descent parameter $\alpha$ (see Algorithm 2)
    $\psi \leftarrow \psi + \alpha\mathbf{p}$
end while
```







input: a pointset $(\mathbf{x}_i)_{i=1}^N$ and masses $(\nu_i)_{i=1}^N$
output: the Laguerre diagram $\{\text{Lag}_i^\psi\}_{i=1}^N$ such that $|\text{Lag}_i^\psi| = \nu_i \ \forall i$

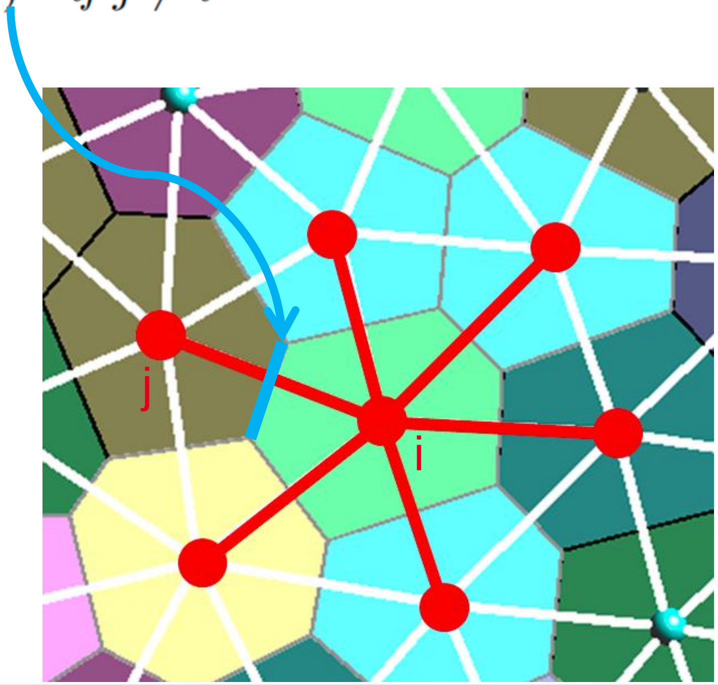
```
$\psi \leftarrow 0$
while $\|\nabla K\|_\infty < \epsilon$
    solve for $\mathbf{p}$ in $[\nabla^2 K(\psi)]\mathbf{p} = -\nabla K(\psi)$
    find descent parameter $\alpha$ (see Algorithm 2)
    $\psi \leftarrow \psi + \alpha\mathbf{p}$
end while
```

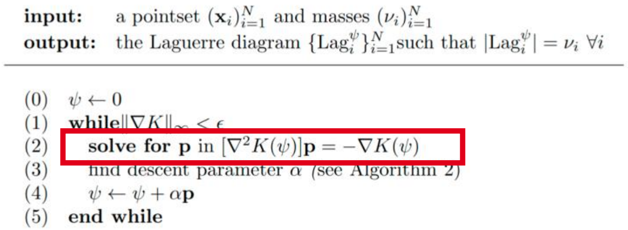
solve for p in $[\nabla^2 K(\psi)]\mathbf{p} = -\nabla K(\psi)$

Matrix of the system: the classical P1 Laplacian

$$\frac{\partial^2 K}{\partial \psi_i \partial \psi_j}(\psi) = \frac{1}{2} \frac{1}{\|\mathbf{x}_j - \mathbf{x}_j\|} \int_{\text{Lag}_{i,j}^\psi} \mu(x) d\text{vol}^{d-1}(x) \quad \textit{if } j \neq i$$

$$\frac{\partial^2 K}{\partial \psi_i^2}(\psi) = -\sum_{j \neq i} \frac{\partial^2 K}{\partial \psi_i \partial \psi_j}(\psi)$$





input: a pointset $(\mathbf{x}_i)_{i=1}^N$ and masses $(\nu_i)_{i=1}^N$
output: the Laguerre diagram $\{\mathrm{Lag}_i^\psi\}_{i=1}^N$such that $|\mathrm{Lag}_i^\psi| = \nu_i \ \forall i$

```
$\psi \leftarrow 0$
while$\|\nabla K\|_\infty < \epsilon$
    solve for $\mathbf{p}$ in $[\nabla^2 K(\psi)]\mathbf{p} = -\nabla K(\psi)$
    find descent parameter $\alpha$ (see Algorithm 2)
    $\psi \leftarrow \psi + \alpha\mathbf{p}$
end while
```

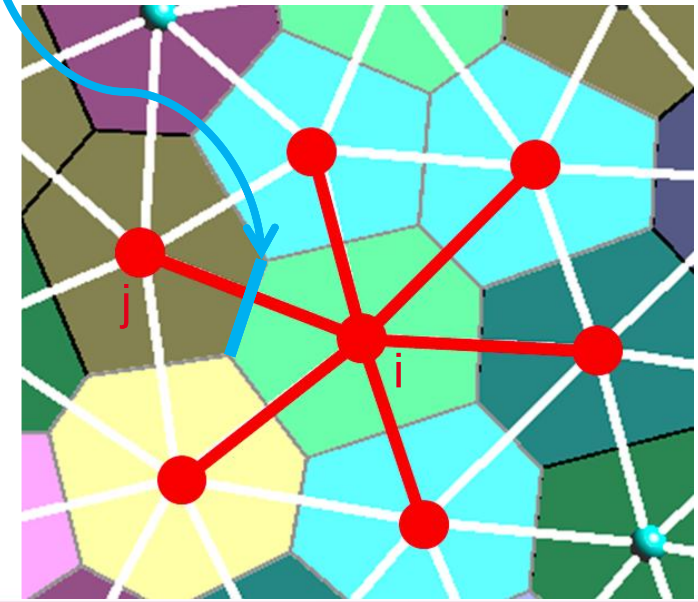
solve for p in $[\nabla^2 K(\psi)]\mathbf{p} = -\nabla K(\psi)$

Matrix of the system: the classical P1 Laplacian

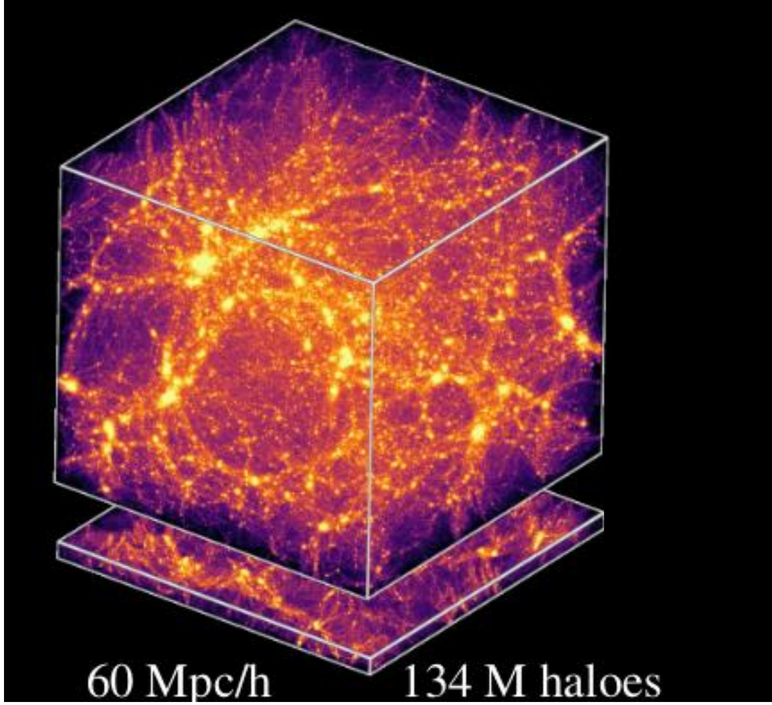
$$\frac{\partial^2 K}{\partial\psi_i \partial\psi_j}(\psi) = \frac{1}{2}\frac{1}{\|\mathbf{x}_j - \mathbf{x}_j\|}\int_{\mathrm{Lag}_{i,j}^\psi} \mu(x)d\mathrm{vol}^{d-1}(x) \quad \textit{if } j \neq i$$

$$\frac{\partial^2 K}{\partial\psi_i^2}(\psi) = -\sum_{j\neq i}\frac{\partial^2 K}{\partial\psi_i \partial\psi_j}(\psi)$$

In 3D: 16 NNZs per row in average
N = 100 million points
Matrix: 25.6 GBytes



On the testbench …
… scaling up !!



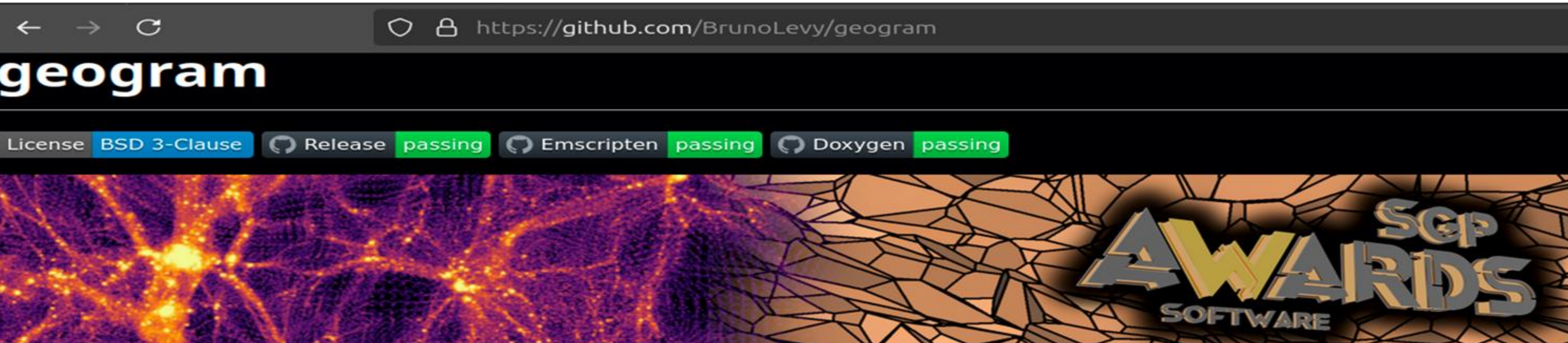
130 M haloes … we need to **upgrade !!!**

- **Hardware side**: 4x Nvidia A100 Grid'5000

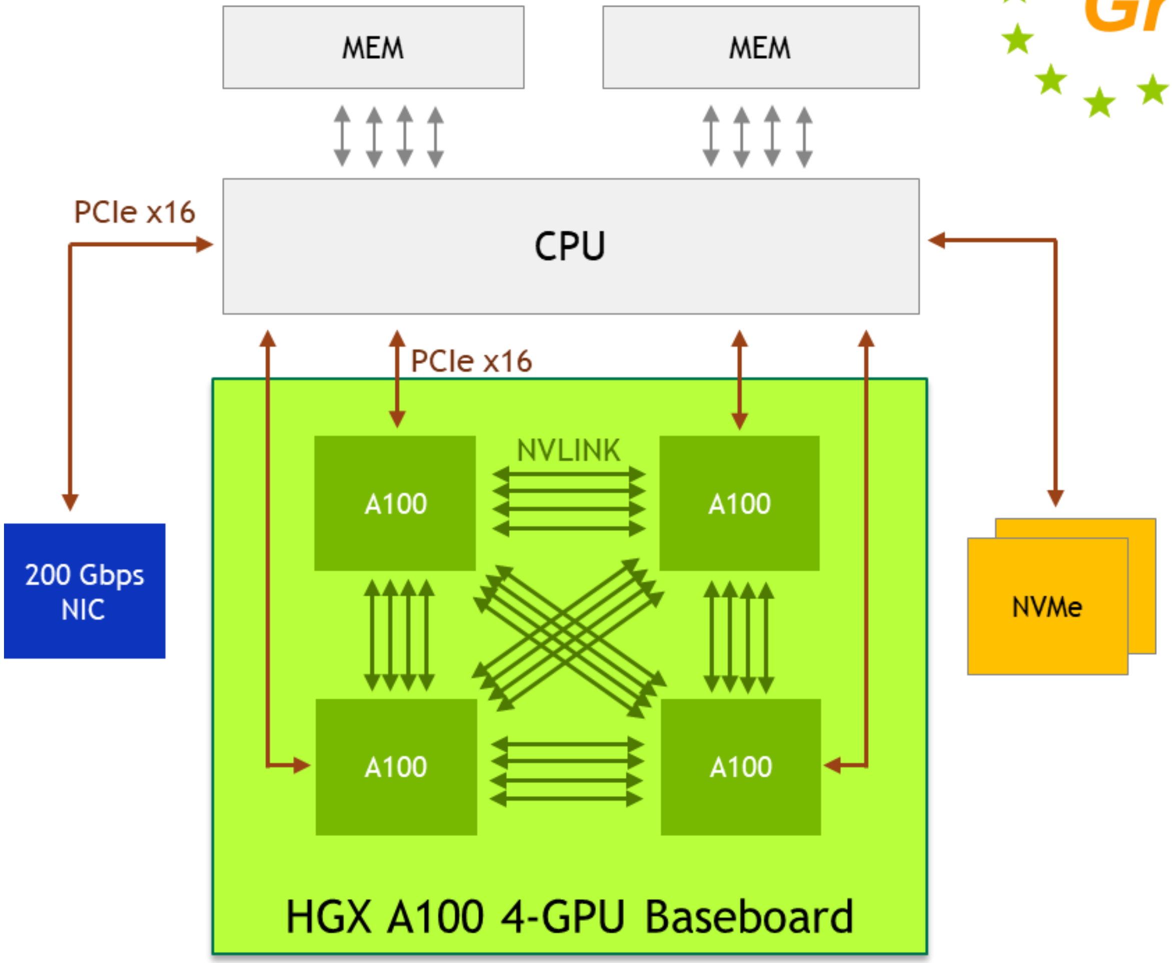
- **Algorithmic side:**
  algebraic multigrid preconditioner

- **Sofware side:** AMGCL [Demidov] +
  custom backend for multi-GPU (OpenNL/geogram), Object-oriented C
  - BLAS abstraction layer
  - Sparse Matrix abstraction layer
  - Matrix assembly helper

https://github.com/BrunoLevy/geogram



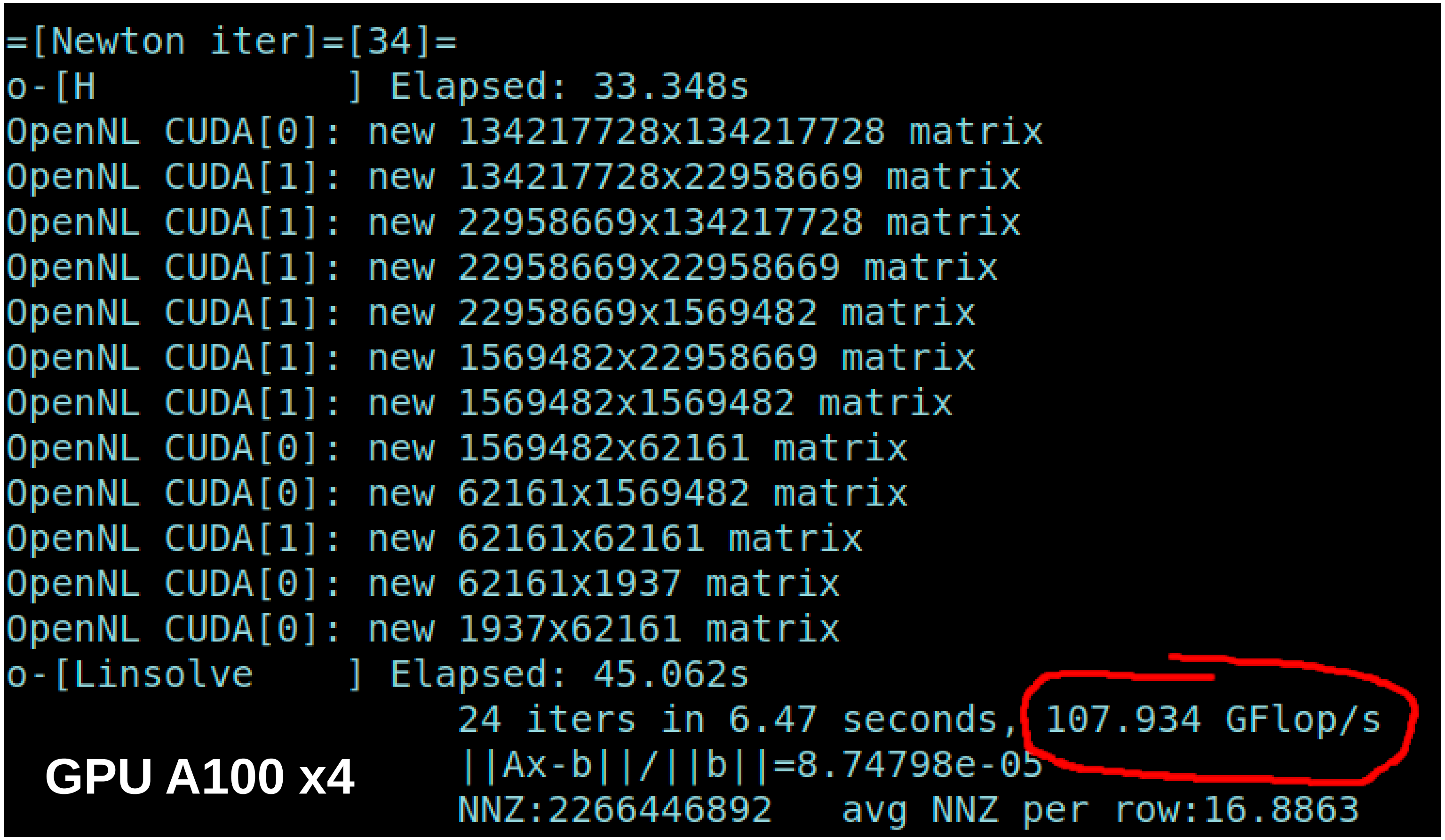
On the testbench …



Unified memory can do the work for you …

On the testbench …

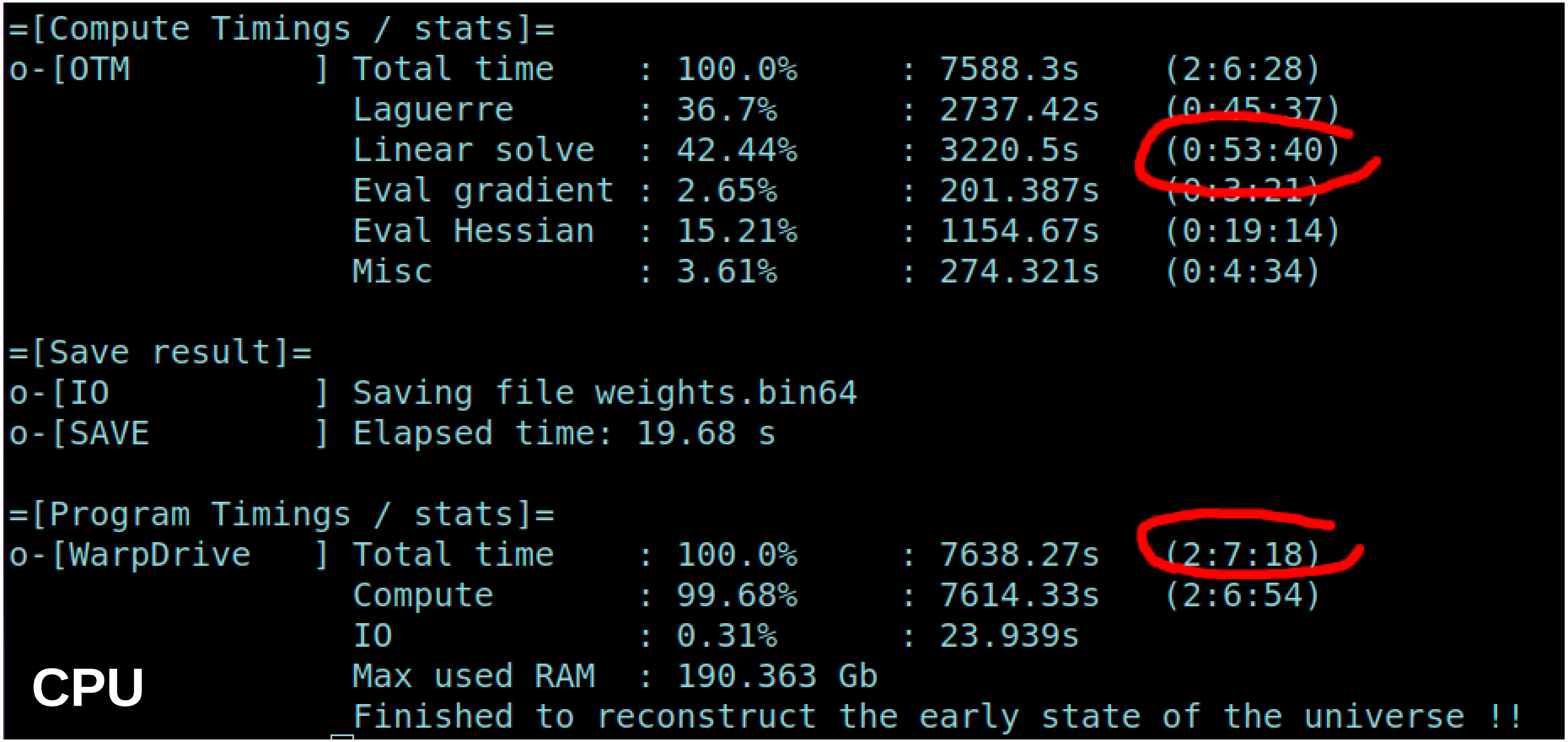
Unified memory can do the work for you …
… but it is (in general) faster to transfer memory explicitly



```
=[Newton iter]=[34]=
o-[H           ] Elapsed: 33.348s
OpenNL CUDA[0]: new 134217728x134217728 matrix
OpenNL CUDA[1]: new 134217728x22958669 matrix
OpenNL CUDA[1]: new 22958669x134217728 matrix
OpenNL CUDA[1]: new 22958669x22958669 matrix
OpenNL CUDA[1]: new 22958669x1569482 matrix
OpenNL CUDA[1]: new 1569482x22958669 matrix
OpenNL CUDA[1]: new 1569482x1569482 matrix
OpenNL CUDA[0]: new 1569482x62161 matrix
OpenNL CUDA[0]: new 62161x1569482 matrix
OpenNL CUDA[1]: new 62161x62161 matrix
OpenNL CUDA[0]: new 62161x1937 matrix
OpenNL CUDA[0]: new 1937x62161 matrix
o-[Linsolve    ] Elapsed: 45.062s
                    24 iters in 6.47 seconds, 107.934 GFlop/s
                    ||Ax-b||/||b||=8.74798e-05
                    NNZ:2266446892   avg NNZ per row:16.8863
```

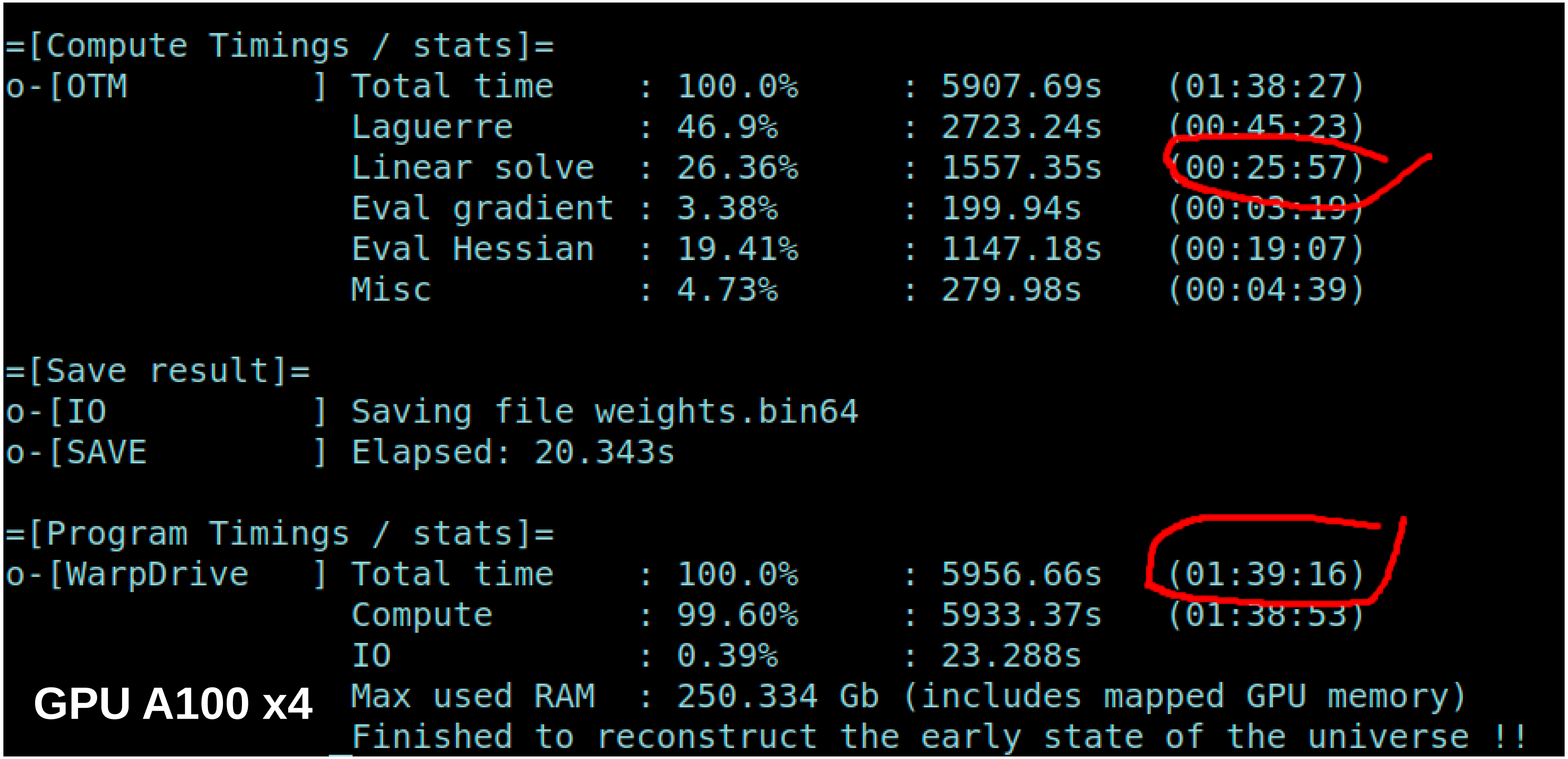
GPU A100 x4

On the testbench …



```
=[Compute Timings / stats]=
o-[OTM          ] Total time     : 100.0%      : 7588.3s    (2:6:28)
                  Laguerre       : 36.7%       : 2737.42s   (0:45:37)
                  Linear solve   : 42.44%      : 3220.5s    (0:53:40)
                  Eval gradient  : 2.65%       : 201.387s   (0:3:21)
                  Eval Hessian   : 15.21%      : 1154.67s   (0:19:14)
                  Misc           : 3.61%       : 274.321s   (0:4:34)

=[Save result]=
o-[IO           ] Saving file weights.bin64
o-[SAVE         ] Elapsed time: 19.68 s

=[Program Timings / stats]=
o-[WarpDrive    ] Total time     : 100.0%      : 7638.27s   (2:7:18)
                  Compute        : 99.68%      : 7614.33s   (2:6:54)
                  IO             : 0.31%       : 23.939s
                  Max used RAM   : 190.363 Gb
                  Finished to reconstruct the early state of the universe !!
```

On the testbench …



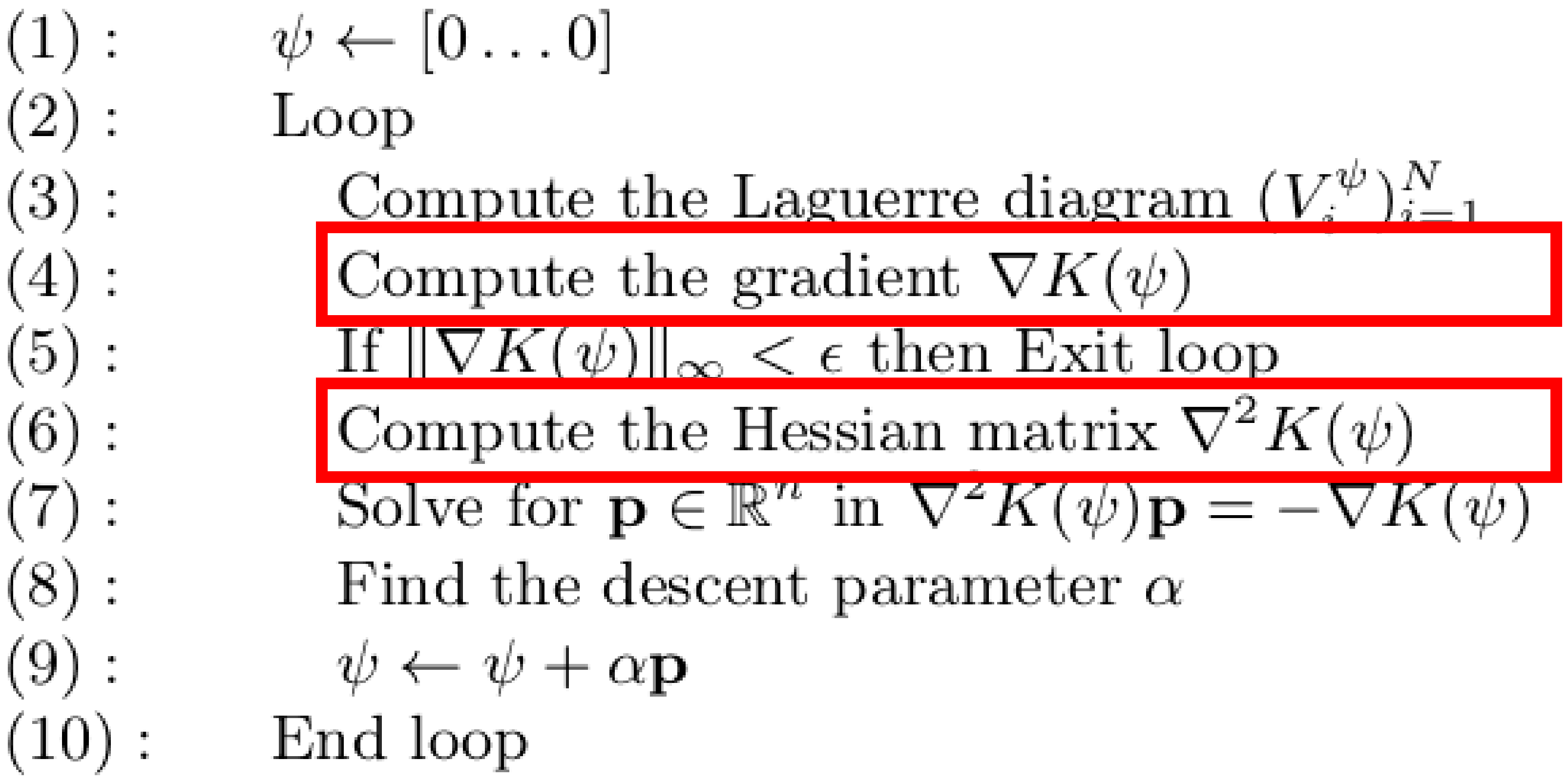
```
=[Compute Timings / stats]=
o-[OTM            ] Total time     : 100.0%      : 5907.69s    (01:38:27)
                    Laguerre       : 46.9%       : 2723.24s    (00:45:23)
                    Linear solve   : 26.36%      : 1557.35s    (00:25:57)
                    Eval gradient  : 3.38%       : 199.94s     (00:03:19)
                    Eval Hessian   : 19.41%      : 1147.18s    (00:19:07)
                    Misc           : 4.73%       : 279.98s     (00:04:39)

=[Save result]=
o-[IO             ] Saving file weights.bin64
o-[SAVE           ] Elapsed: 20.343s

=[Program Timings / stats]=
o-[WarpDrive      ] Total time     : 100.0%      : 5956.66s    (01:39:16)
                    Compute        : 99.60%      : 5933.37s    (01:38:53)
                    IO             : 0.39%       : 23.288s
                    Max used RAM   : 250.334 Gb (includes mapped GPU memory)
                    Finished to reconstruct the early state of the universe !!
```

GPU A100 x4

linear solve takes 25 min (instead of 53 min on CPU, multithreaded)

Part. 4 Scaling-up

3. Matrix assembly



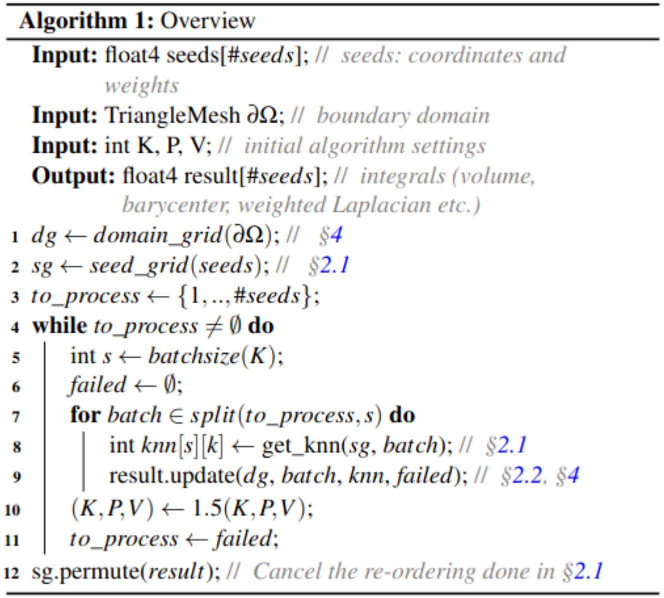
```
$\psi \leftarrow [0 \dots 0]$
Loop
    Compute the Laguerre diagram $(V_i^\psi)_{i=1}^N$
    Compute the gradient $\nabla K(\psi)$
    If $\|\nabla K(\psi)\|_\infty < \epsilon$ then Exit loop
    Compute the Hessian matrix $\nabla^2 K(\psi)$
    Solve for $\mathbf{p} \in \mathbb{R}^n$ in $\nabla^2 K(\psi)\mathbf{p} = -\nabla K(\psi)$
    Find the descent parameter $\alpha$
    $\psi \leftarrow \psi + \alpha \mathbf{p}$
End loop
```

Part. 4 Scaling-up

Coming next: **construction of preconditioner** on GPU too.

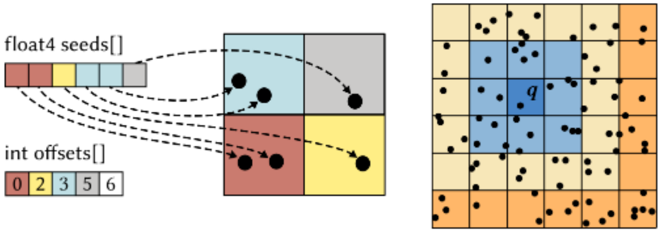
Laguerre diagram on GPU ?

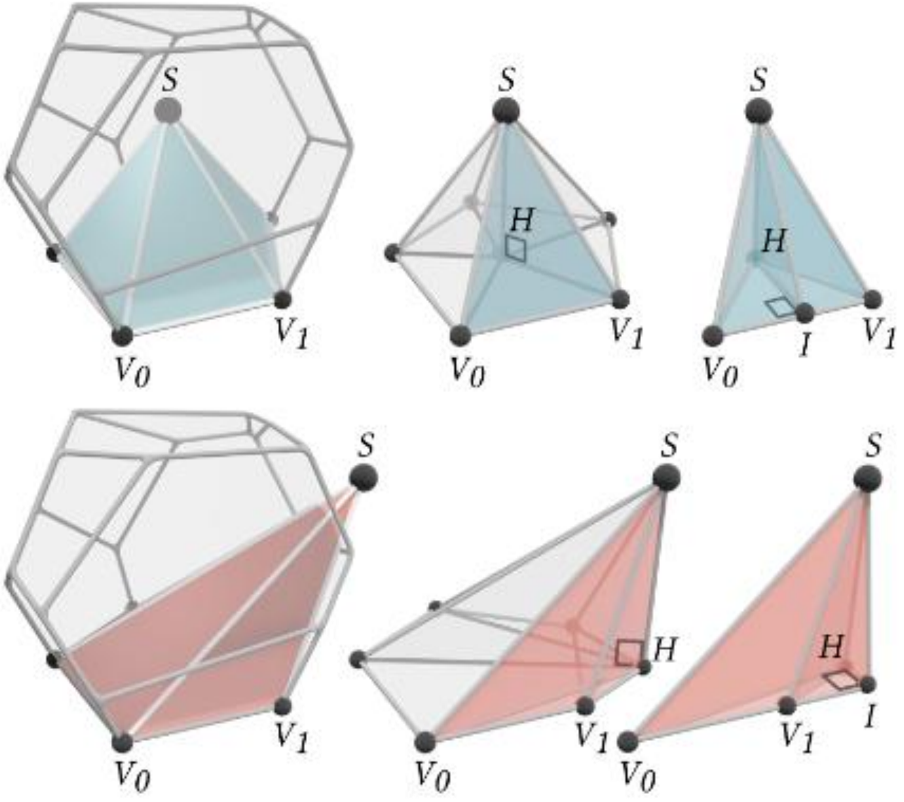
possible but harder… [Ray, Basselin, Alonso, Sokolov, **L**, Lefebvre]



Algorithm 1: Overview

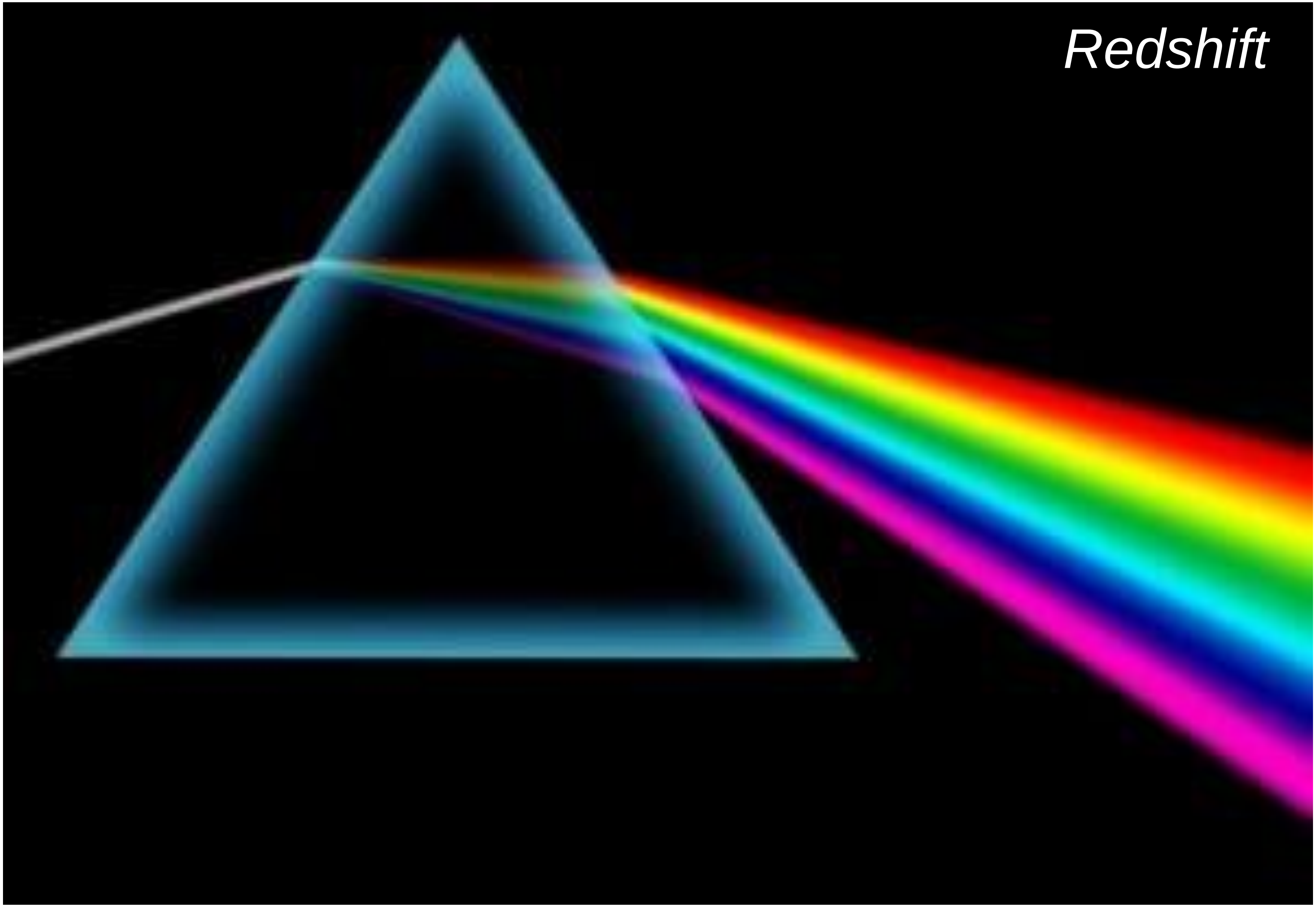
```
Input: float4 seeds[#seeds]; // seeds: coordinates and weights
Input: TriangleMesh ∂Ω; // boundary domain
Input: int K, P, V; // initial algorithm settings
Output: float4 result[#seeds]; // integrals (volume, barycenter, weighted Laplacian etc.)
dg ← domain_grid(∂Ω); // §4
sg ← seed_grid(seeds); // §2.1
to_process ← {1, .., #seeds};
while to_process ≠ ∅ do
    int s ← batchsize(K);
    failed ← ∅;
    for batch ∈ split(to_process, s) do
        int knn[s][k] ← get_knn(sg, batch); // §2.1
        result.update(dg, batch, knn, failed); // §2.2, §4
    (K, P, V) ← 1.5(K, P, V);
    to_process ← failed;
sg.permute(result); // Cancel the re-ordering done in §2.1
```





5

Red-shift distortion

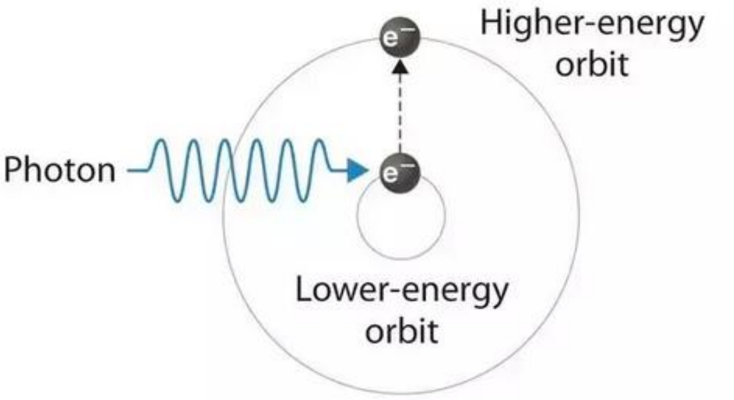


Redshift

Redshift

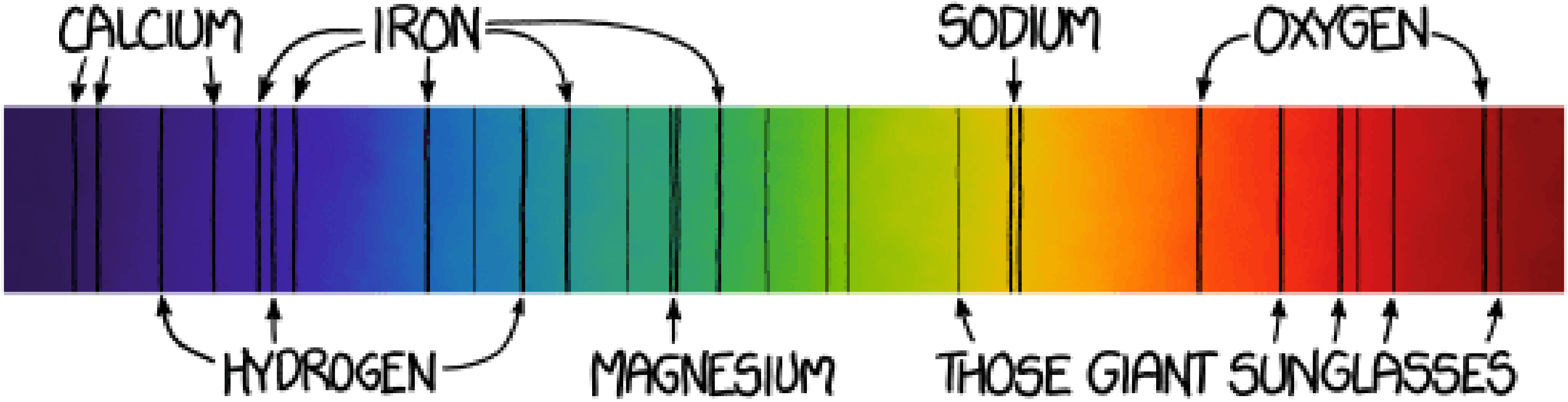
Joseph von Franhofer 1814

Redshift

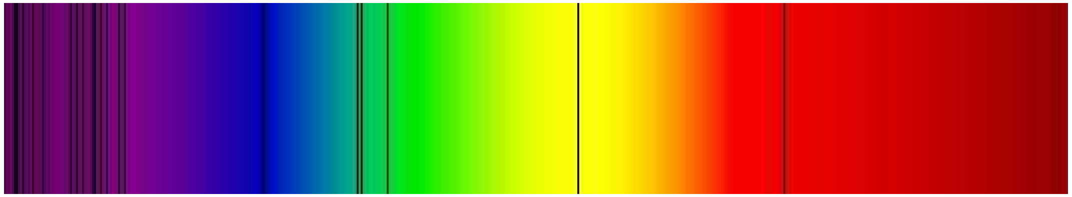


Joseph von Franhofer 1814

Redshift

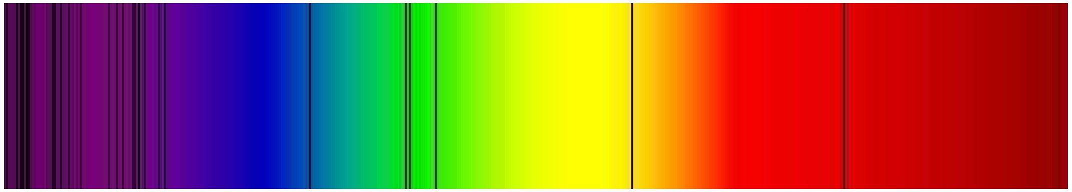

CALCIUM
IRON
SODIUM
OXYGEN
HYDROGEN
MAGNESIUM
THOSE GIANT SUNGLASSES

Redshift



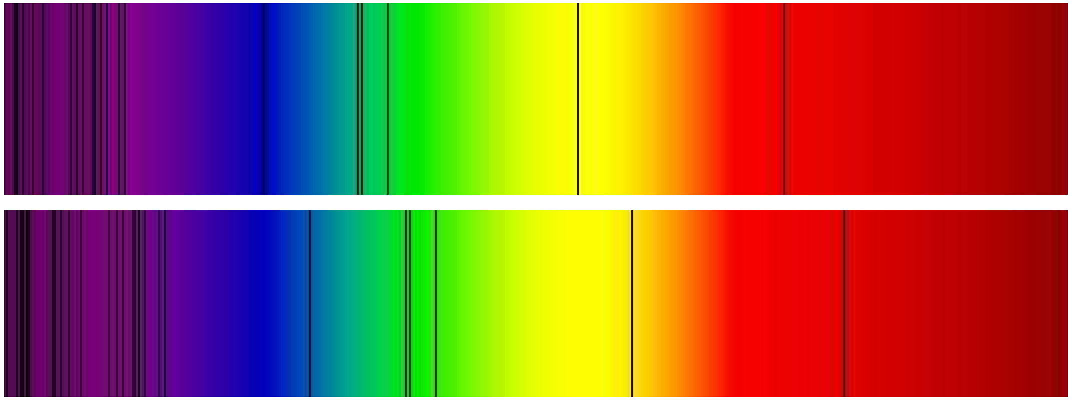
The sun

Redshift



A distant star

Redshift

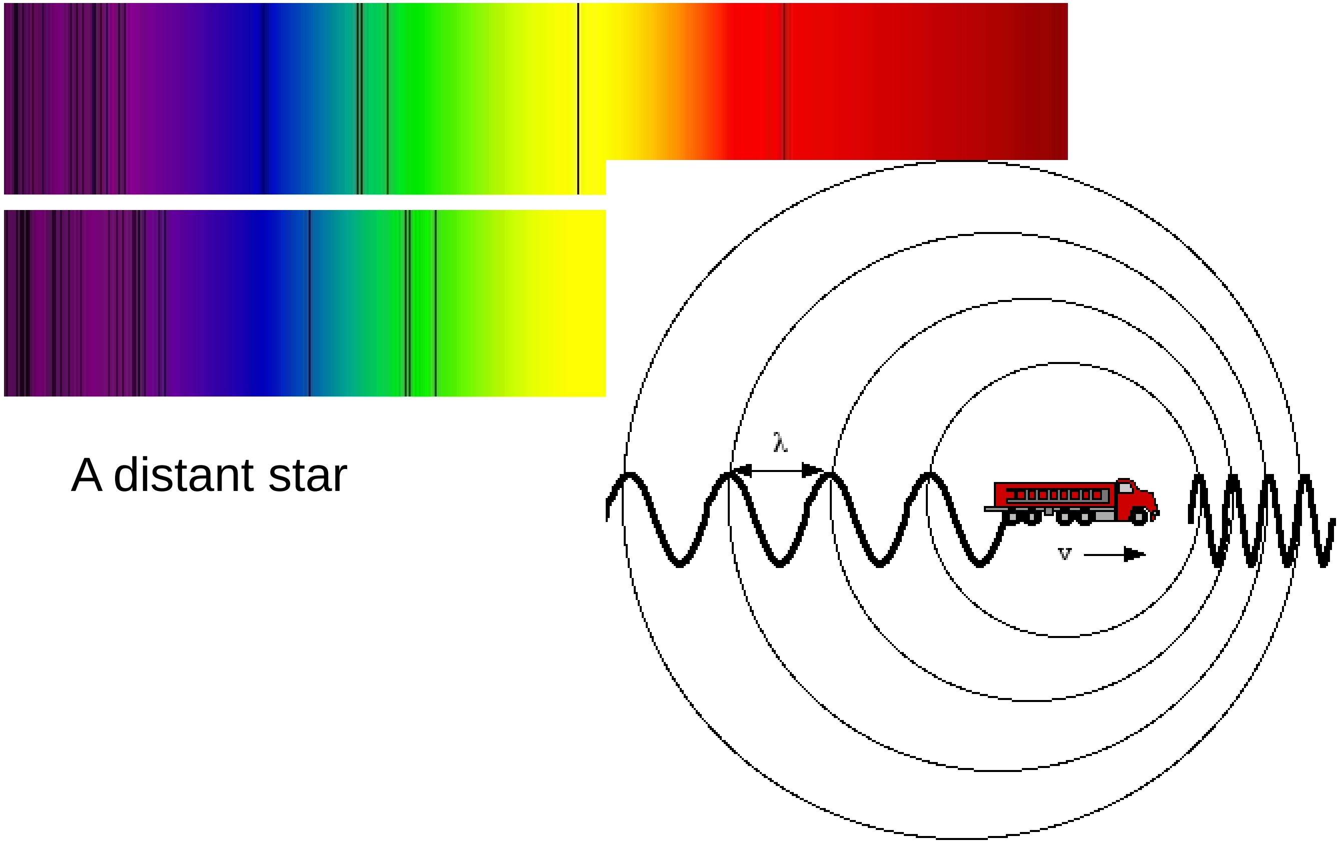


The sun

A distant star

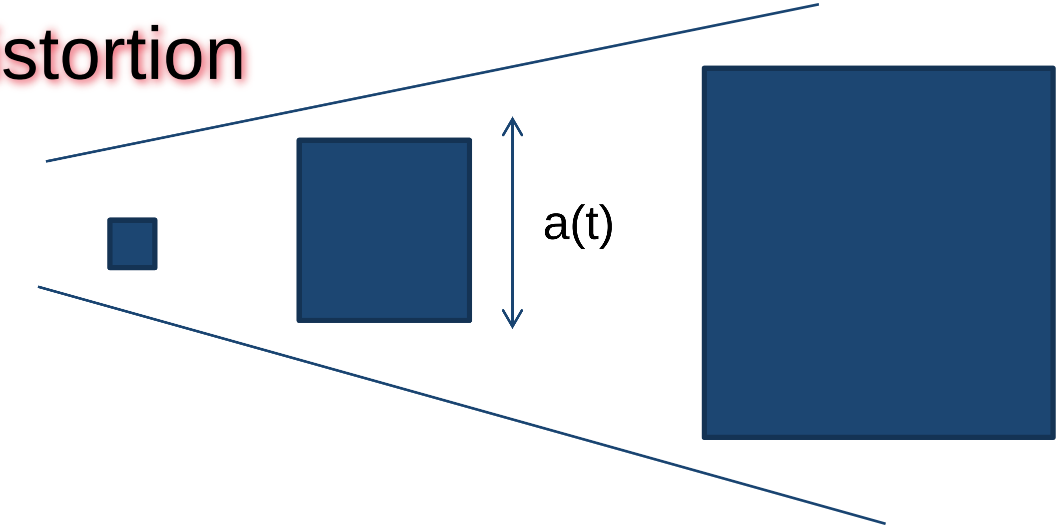
Redshift

The sun

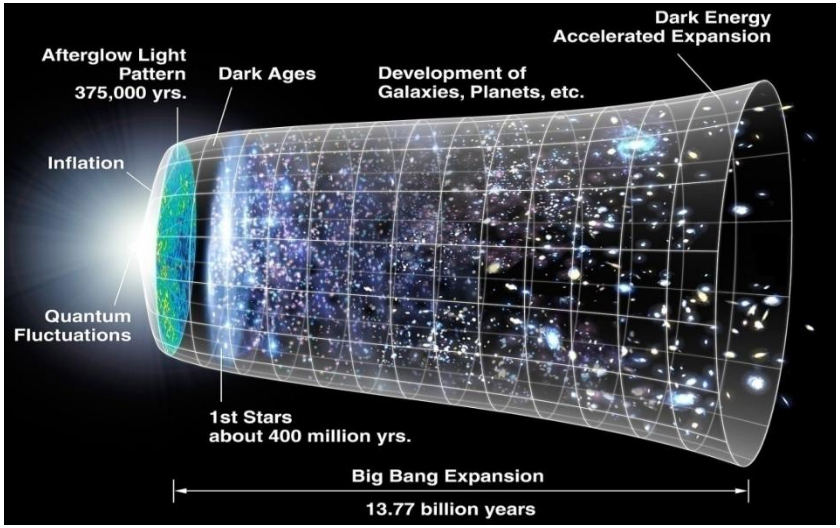


A distant star

Part. 5 Redshift distortion



$$\begin{cases} \partial_\tau \mathbf{v} + (\mathbf{v}\cdot\nabla_x)\mathbf{v} = -\dfrac{3}{2\tau}(\nabla_x\phi + \mathbf{v}) \\ \partial_\tau \rho + \nabla_x \cdot (\rho\mathbf{v}) = 0 \\ \Delta\phi = 4\pi\mathcal{G}\dfrac{\rho - 1}{\tau} \end{cases}$$



Part. 5 Redshift distortion

$$\mathbf{s}_i = \mathbf{x}_i + \beta(\mathbf{v}_i \cdot \hat{\mathbf{x}}_i)\hat{\mathbf{x}}_i$$

Where we think
the galaxy is (taking
into account only
the expansion of the
Universe)

Part. 5 Redshift distortion

$$\mathbf{s}_i = \mathbf{x}_i + \beta(\mathbf{v}_i \cdot \hat{\mathbf{x}}_i)\hat{\mathbf{x}}_i$$

Where we think
the galaxy is (taking
into account only
the expansion of the
Universe)

Where the galaxy is

Part. 5 Redshift distortion

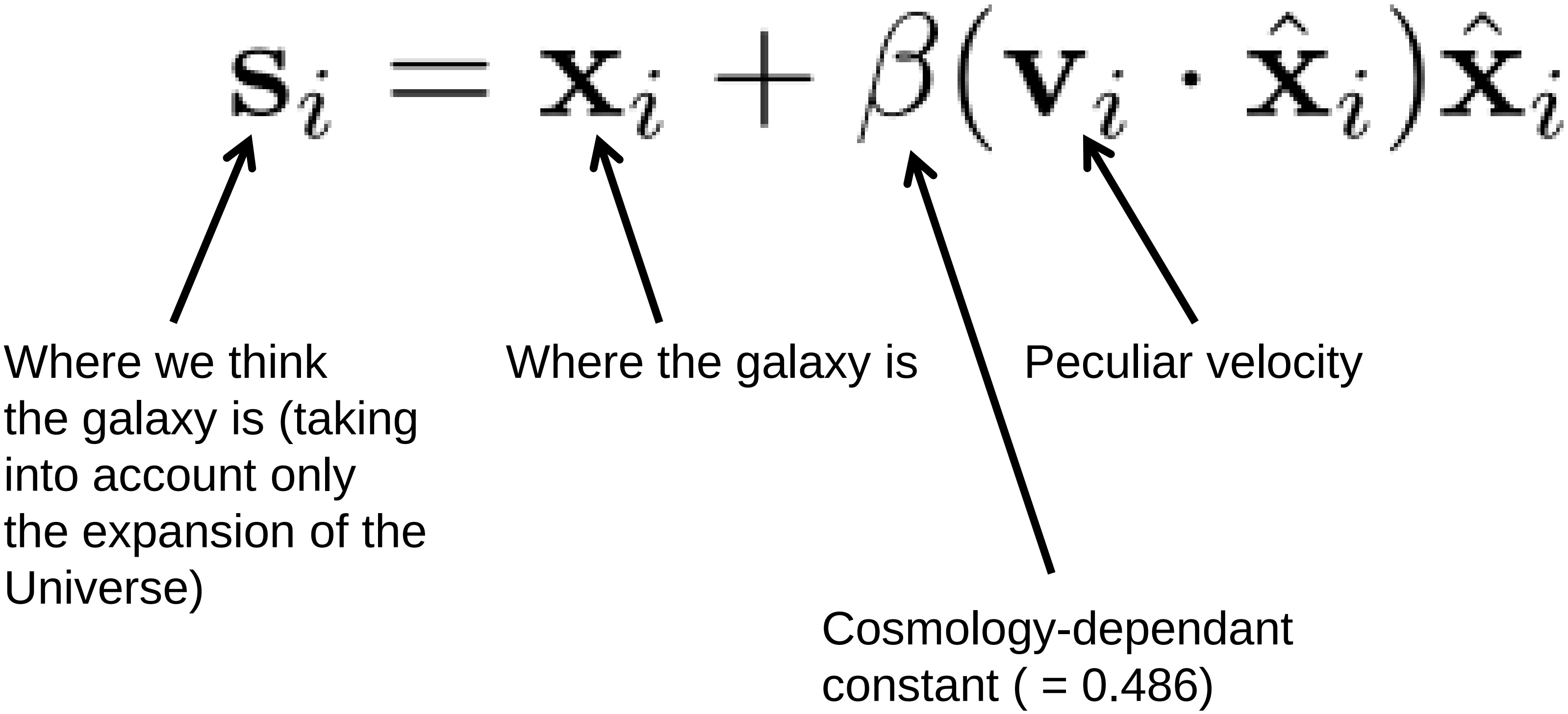
$$\mathbf{s}_i = \mathbf{x}_i + \beta(\mathbf{v}_i \cdot \hat{\mathbf{x}}_i)\hat{\mathbf{x}}_i$$

Where we think the galaxy is (taking into account only the expansion of the Universe)

Where the galaxy is

Peculiar velocity

Part. 5 Redshift distortion



$$\mathbf{s}_i = \mathbf{x}_i + \beta(\mathbf{v}_i \cdot \hat{\mathbf{x}}_i)\hat{\mathbf{x}}_i$$

Where we think
the galaxy is (taking
into account only
the expansion of the
Universe)

Where the galaxy is

Peculiar velocity

Cosmology-dependant
constant (= 0.486)

Part. 5 Redshift distortion

$$\mathbf{s}_i = \mathbf{x}_i + \beta(\mathbf{v}_i \cdot \hat{\mathbf{x}}_i)\hat{\mathbf{x}}_i$$

Where we think
the galaxy is (taking
into account only
the expansion of the
Universe)

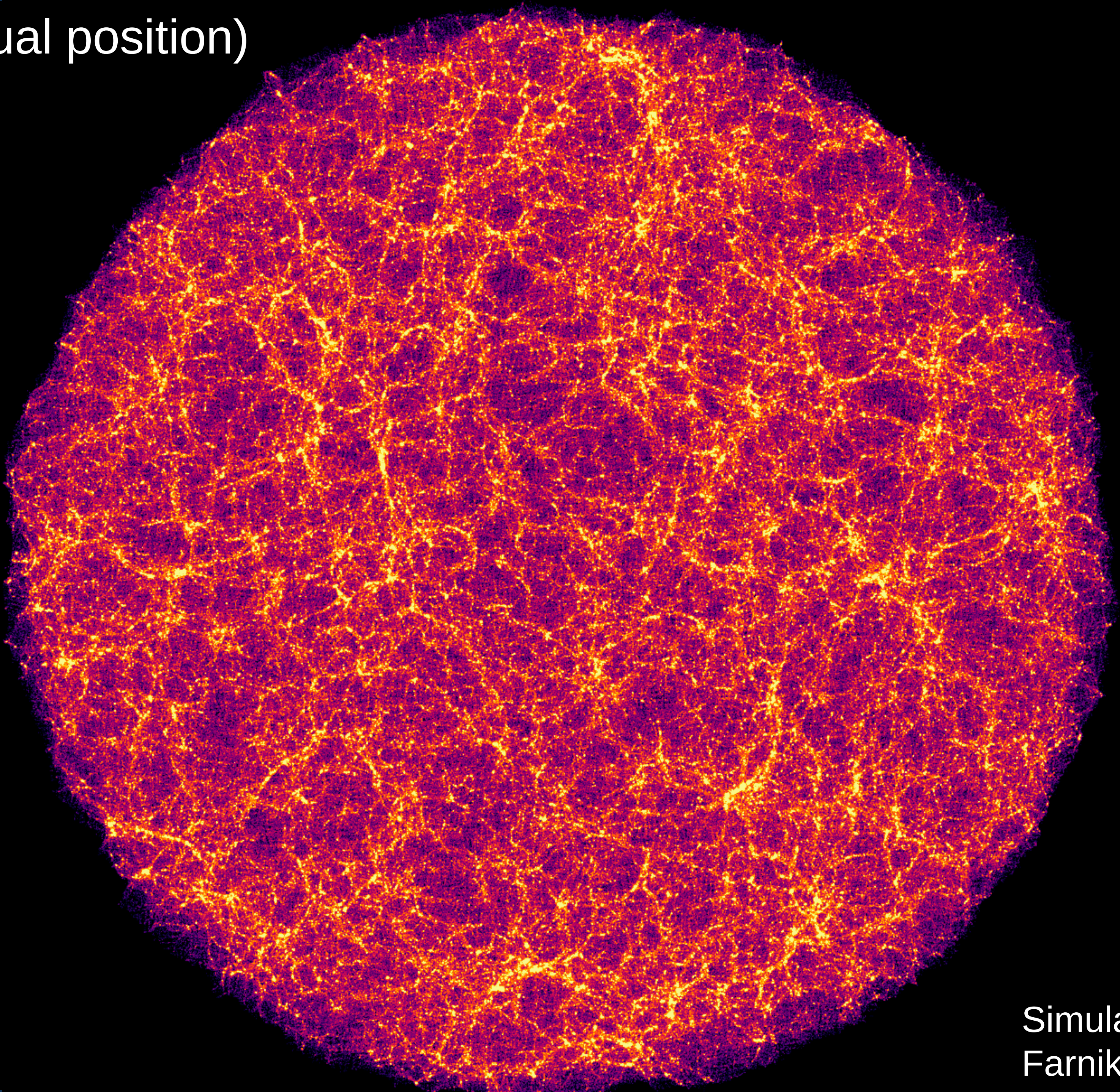
Where the galaxy is

Peculiar velocity

Cosmology-dependant
constant (= 0.486)

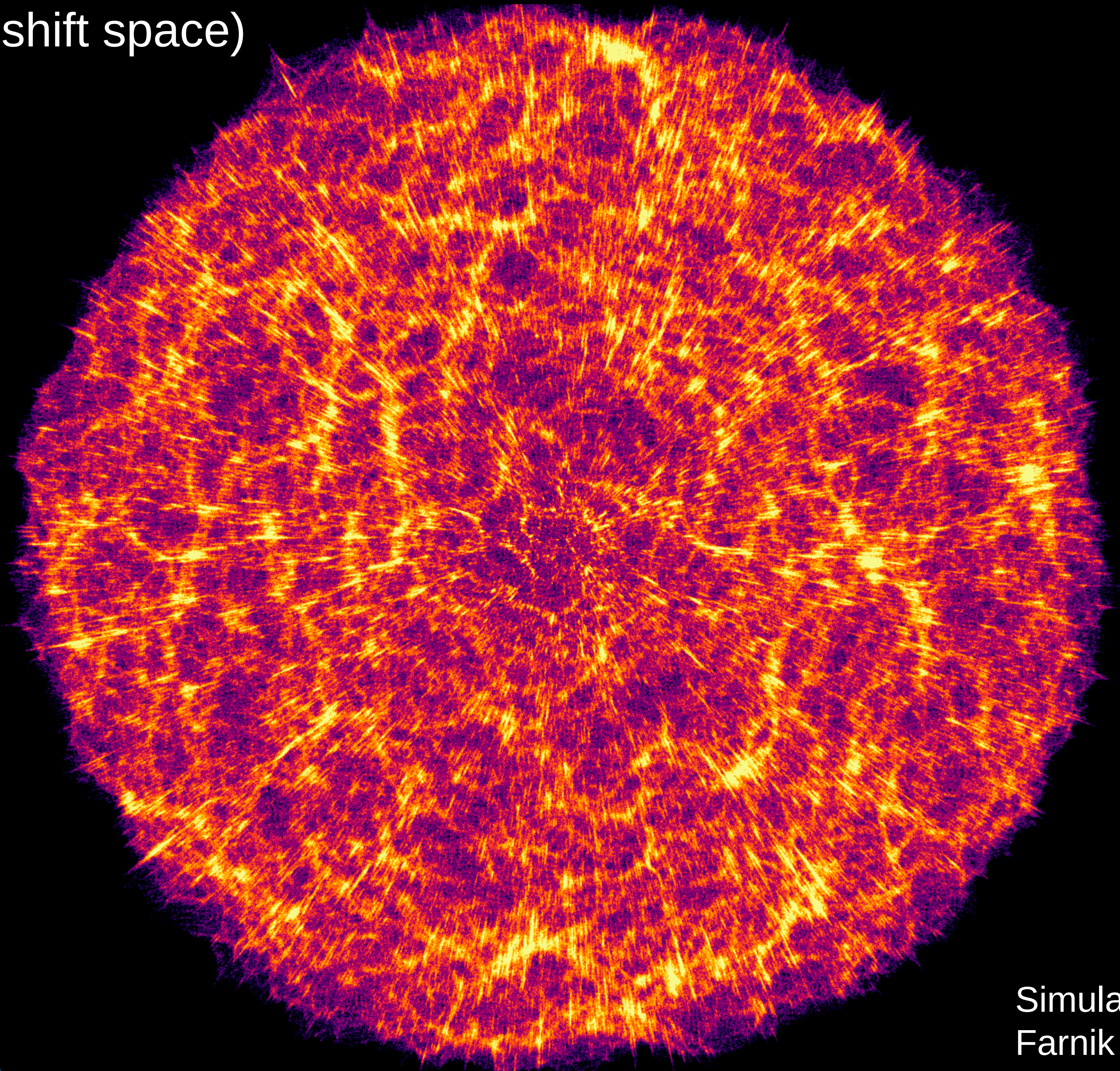
Unit radial vector

X (actual position)

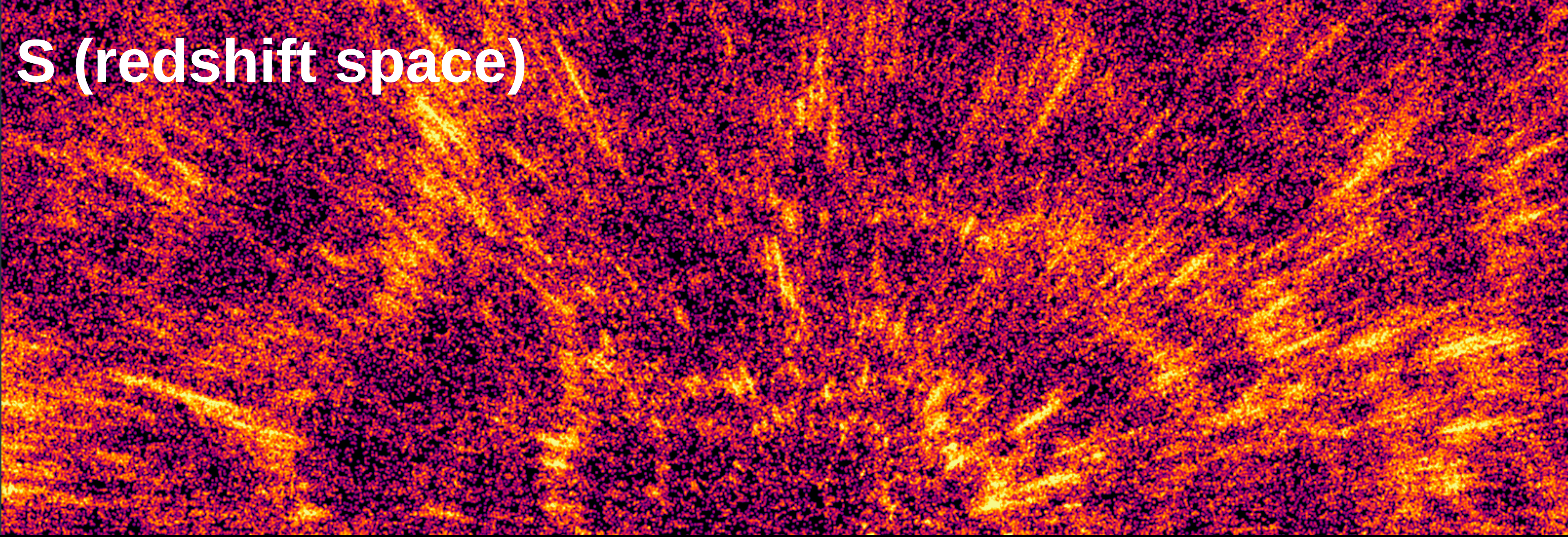


Simulation
Farnik Nikhaktar

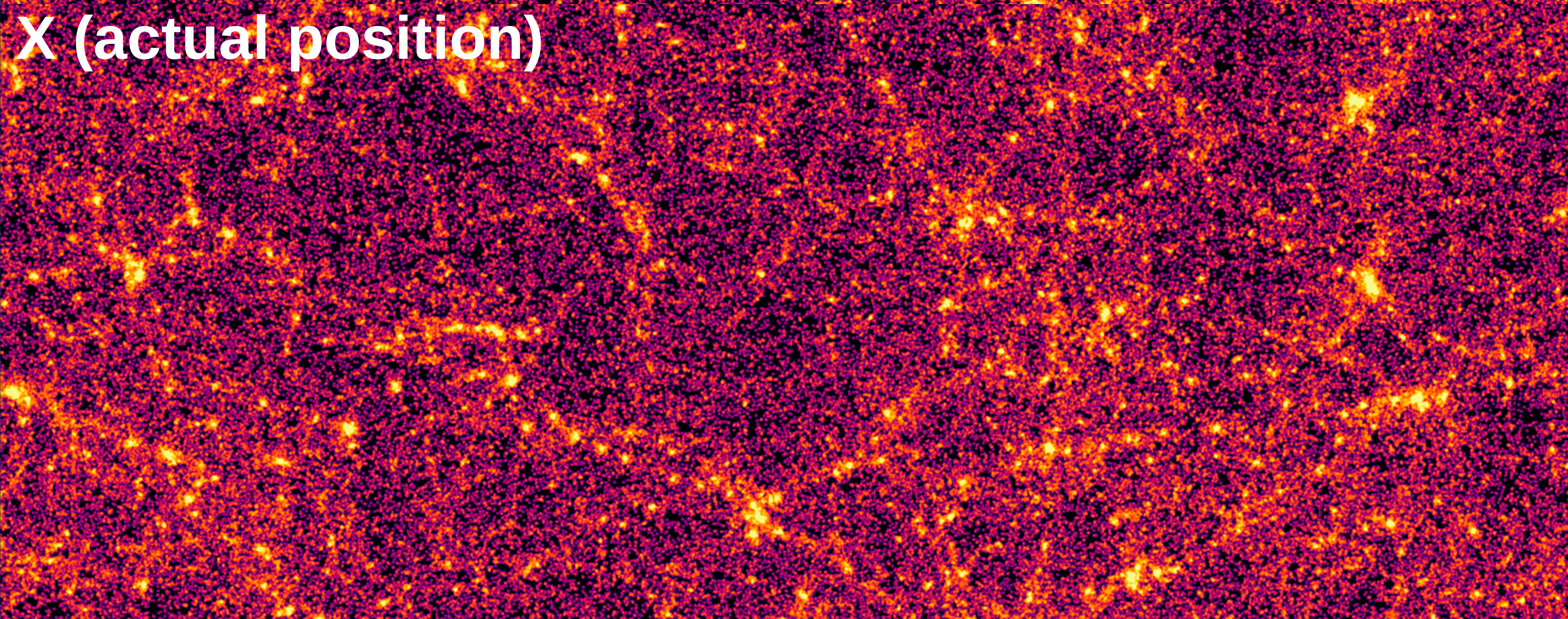
S (redshift space)



Simulation
Farnik Nikhaktar



S (redshift space)



X (actual position)

Part. 5 Redshift distortion

$$\mathbf{s}_i = \mathbf{x}_i + \beta(\mathbf{v}_i \cdot \hat{\mathbf{x}}_i)\hat{\mathbf{x}}_i$$

Part. 5 Redshift distortion

Average velocity

$$\mathbf{s}_i = \mathbf{x}_i + \beta \left(\left(\mathbf{x}_i - \mathbf{q}_i \right) \cdot \hat{\mathbf{x}}_i \right) \hat{\mathbf{x}}_i$$

Initial position
reconstructed by OT

Part. 5 Redshift distortion

$$\hat{\mathbf{S}}(\mathbf{X}) = \mathbf{S}\big(\mathbf{X}, \mathbf{Q}(\mathbf{X}, \mathbf{\Psi}^*(\mathbf{X}))\big) = \mathbf{S}_{\mathrm{catalog}}$$

```
$\mathbf{X}^{(0)} \leftarrow \mathbf{S}_{\mathrm{catalog}}$
while $\left\|\hat{\mathbf{S}}(\mathbf{X}^{(k)}) - \mathbf{S}_{\mathrm{catalog}}\right\| > \epsilon$
    solve for $\delta\mathbf{X}^{(k)}$ in $(d_{\mathbf{X}}\hat{\mathbf{S}})\ \delta\mathbf{X}^{(k)} = \mathbf{S}_{\mathrm{catalog}} - \hat{\mathbf{S}}(\mathbf{X}^{(k)})$
    $\mathbf{X}^{(k+1)} \leftarrow \mathbf{X}^{(k)} + \delta\mathbf{X}^{(k)}$
    $k \leftarrow k + 1$
end//while
```

Newton-Raphson

Part. 5 Redshift distortion

$$\hat{\mathbf{S}}(\mathbf{X}) = \mathbf{S}\big(\mathbf{X}, \mathbf{Q}(\mathbf{X}, \mathbf{\Psi}^*(\mathbf{X}))\big) = \mathbf{S}_{\text{catalog}}$$

```
$\mathbf{X}^{(0)} \leftarrow \mathbf{S}_{\text{catalog}}$
**while** $\left\| \hat{\mathbf{S}}(\mathbf{X}^{(k)}) - \mathbf{S}_{\text{catalog}} \right\| > \epsilon$
    solve for $\delta\mathbf{X}^{(k)}$ in $\boxed{(d_{\mathbf{X}}\hat{\mathbf{S}})}\,\delta\mathbf{X}^{(k)} = \mathbf{S}_{\text{catalog}} - \hat{\mathbf{S}}(\mathbf{X}^{(k)})$
    $\mathbf{X}^{(k+1)} \leftarrow \mathbf{X}^{(k)} + \delta\mathbf{X}^{(k)}$
    $k \leftarrow k + 1$
**end**$//while$
```

Newton-Raphson

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\mathbf{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}}S + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{X}}\mathbf{Q} + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{\Psi}}\mathbf{Q}\ \partial_{\mathbf{X}}\mathbf{\Psi}^*$$

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\mathbf{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}} S + \partial_{\mathbf{Q}} S \ \partial_{\mathbf{X}} \mathbf{Q} + \partial_{\mathbf{Q}} S \ \partial_{\mathbf{\Psi}} \mathbf{Q} \boxed{\partial_{\mathbf{X}} \mathbf{\Psi}^*}$$

$$\mathbf{\Psi}^*(\mathbf{X}) \quad = \quad \arg\max_{\mathbf{\Psi}} \left[K(\mathbf{\Psi},\mathbf{X},\mathbf{m})\right]$$

Kantorovich dual

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X}, \mathbf{Q}(\mathbf{X}, \boldsymbol{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}} S + \partial_{\mathbf{Q}} S \ \partial_{\mathbf{X}} \mathbf{Q} + \partial_{\mathbf{Q}} S \ \partial_{\boldsymbol{\Psi}} \mathbf{Q} \boxed{\partial_{\mathbf{X}} \boldsymbol{\Psi}^*}$$

state function **F** is defined by:

$$\mathbf{F}(\mathbf{X}, \boldsymbol{\Psi}) := \partial_{\boldsymbol{\Psi}} K(\boldsymbol{\Psi}, \mathbf{X}).$$

Kantorovich dual

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\mathbf{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}}S + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{X}}\mathbf{Q} + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{\Psi}}\mathbf{Q}\ \boxed{\partial_{\mathbf{X}}\mathbf{\Psi}^*}$$

state function $\mathbf{F}$ is defined by:

$$\mathbf{F}(\mathbf{X},\mathbf{\Psi}) := \partial_{\mathbf{\Psi}}K(\mathbf{\Psi},\mathbf{X}).$$

$$d_{\mathbf{X}}\mathbf{F} = 0$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\boldsymbol{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}}S + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{X}}\mathbf{Q} + \partial_{\mathbf{Q}}S\ \partial_{\boldsymbol{\Psi}}\mathbf{Q}\, \boxed{\partial_{\mathbf{X}}\boldsymbol{\Psi}^*}$$

state function **F** is defined by:

$$\mathbf{F}(\mathbf{X},\boldsymbol{\Psi}) := \partial_{\boldsymbol{\Psi}}K(\boldsymbol{\Psi},\mathbf{X}).$$

$$\begin{aligned} d_{\mathbf{X}}\mathbf{F} = 0 \quad &= \quad \partial_{\mathbf{X}}\mathbf{F} + \partial_{\boldsymbol{\Psi}}\mathbf{F}\ \partial_{\mathbf{X}}\boldsymbol{\Psi}^* \\ \text{or: }\ \partial_{\boldsymbol{\Psi}}\mathbf{F}\partial_{\mathbf{X}}\boldsymbol{\Psi}^* \quad &= \quad -\partial_{\mathbf{X}}\mathbf{F} \end{aligned}$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\mathbf{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}}S + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{X}}\mathbf{Q} + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{\Psi}}\mathbf{Q}\ \boxed{\partial_{\mathbf{X}}\mathbf{\Psi}^*}$$

state function **F** is defined by:

$$\mathbf{F}(\mathbf{X},\mathbf{\Psi}) := \partial_{\mathbf{\Psi}}K(\mathbf{\Psi},\mathbf{X}).$$

$$\begin{aligned} d_{\mathbf{X}}\mathbf{F} = 0 &= \partial_{\mathbf{X}}\mathbf{F} + \partial_{\mathbf{\Psi}}\mathbf{F}\ \partial_{\mathbf{X}}\mathbf{\Psi}^* \\ \text{or: } \partial_{\mathbf{\Psi}}\mathbf{F}\partial_{\mathbf{X}}\mathbf{\Psi}^* &= -\partial_{\mathbf{X}}\mathbf{F} \end{aligned}$$

adjoint **P**, a $3N \times N$ matrix, defined as the solution of

$$\mathbf{P}\ \partial_{\mathbf{\Psi}}\mathbf{F} = -\partial_{\mathbf{Q}}\mathbf{S}\ \partial_{\mathbf{\Psi}}\mathbf{Q},$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\mathbf{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}}S + \partial_{\mathbf{Q}}S\ \partial_{\mathbf{X}}\mathbf{Q} + \boxed{\partial_{\mathbf{Q}}S\ \partial_{\mathbf{\Psi}}\mathbf{Q}\ \partial_{\mathbf{X}}\mathbf{\Psi}^*}$$

$$\partial_{\mathbf{Q}}\mathbf{S}\ \partial_{\mathbf{\Psi}}\mathbf{Q}\,\partial_{\mathbf{X}}\mathbf{\Psi}^* \ =$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\mathbf{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}} S + \partial_{\mathbf{Q}} S \; \partial_{\mathbf{X}}\mathbf{Q} + \boxed{\partial_{\mathbf{Q}} S \; \partial_{\mathbf{\Psi}}\mathbf{Q} \; \partial_{\mathbf{X}}\mathbf{\Psi}^*}$$

$$\underbrace{\partial_{\mathbf{Q}}\mathbf{S} \; \partial_{\mathbf{\Psi}}\mathbf{Q}}_{\downarrow \text{ Adjoint equation}} \partial_{\mathbf{X}}\mathbf{\Psi}^* =$$

$$-\mathbf{P}\,\partial_{\mathbf{\Psi}}\mathbf{F} \;\; \partial_{\mathbf{X}}\mathbf{\Psi}^* =$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$d_{\mathbf{X}}\mathbf{S}(\mathbf{X},\mathbf{Q}(\mathbf{X},\boldsymbol{\Psi}^*(\mathbf{X}))) = \partial_{\mathbf{X}}S + \partial_{\mathbf{Q}}S\;\partial_{\mathbf{X}}\mathbf{Q} + \boxed{\partial_{\mathbf{Q}}S\;\partial_{\boldsymbol{\Psi}}\mathbf{Q}\;\partial_{\mathbf{X}}\boldsymbol{\Psi}^*}$$

$$\underbrace{\partial_{\mathbf{Q}}\mathbf{S}\;\partial_{\boldsymbol{\Psi}}\mathbf{Q}}_{\downarrow\ \textit{Adjoint equation}}\,\partial_{\mathbf{X}}\boldsymbol{\Psi}^* =$$

$$-\mathbf{P}\,\underbrace{\partial_{\boldsymbol{\Psi}}\mathbf{F}\quad\partial_{\mathbf{X}}\boldsymbol{\Psi}^*}_{\downarrow\ \textit{State equation}} =$$

$$\mathbf{P}\;\partial_{\mathbf{X}}\mathbf{F}$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

$$\underbrace{d_{\mathbf{X}}\mathbf{S}}_{3N\times 3N} = \underbrace{\partial_{\mathbf{X}}\mathbf{S}}_{3N\times 3N} + \underbrace{\partial_{\mathbf{Q}}\mathbf{S}}_{3N\times 3N}\ \underbrace{\partial_{\mathbf{X}}\mathbf{Q}}_{3N\times 3N} + \underbrace{\mathbf{P}}_{3N\times N}\ \underbrace{\partial^2_{\mathbf{\Psi},\mathbf{X}}K}_{N\times 3N}$$

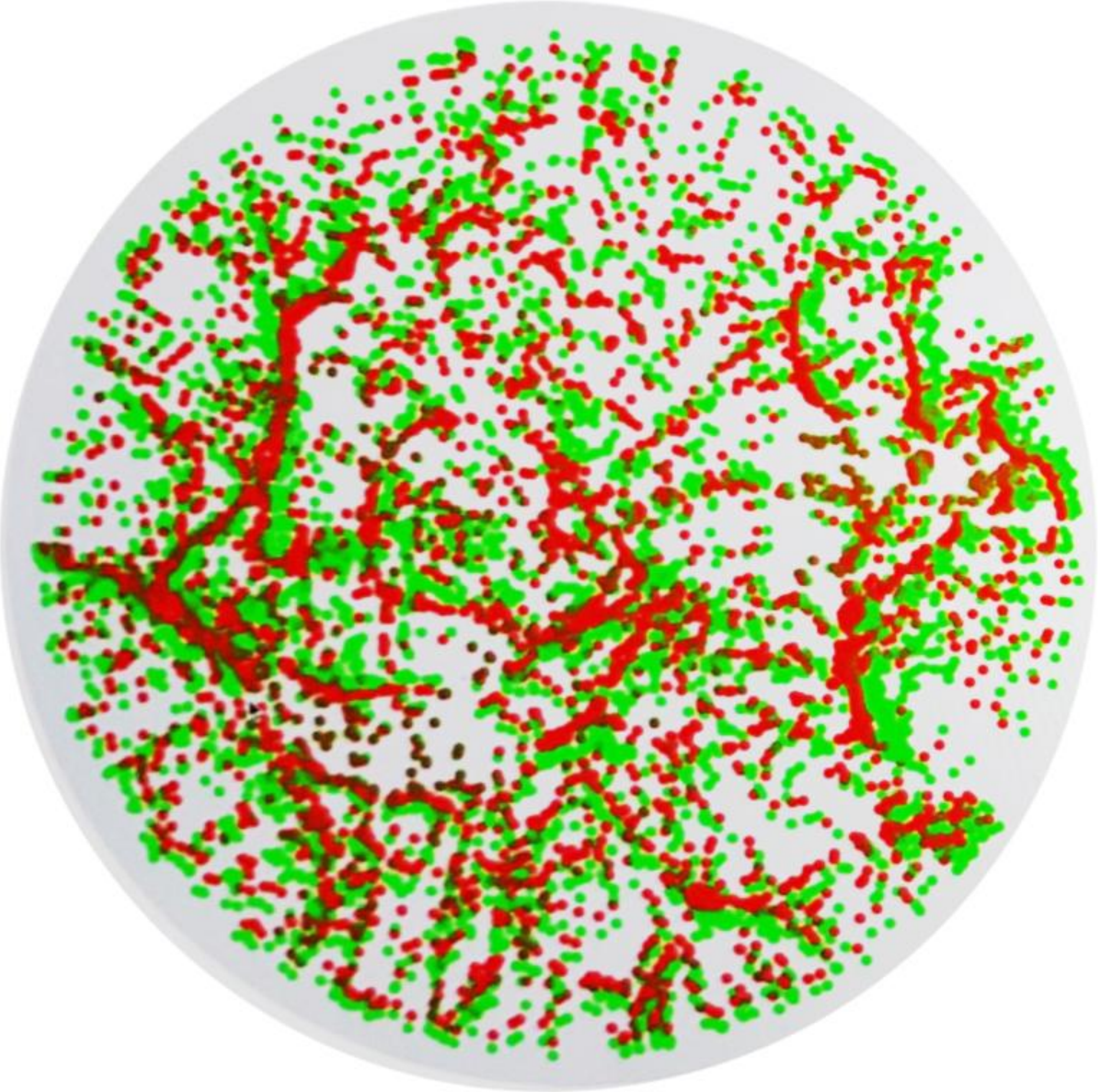
where:

$$\underbrace{\mathbf{P}}_{3N\times N}\ \underbrace{\partial^2_{\mathbf{\Psi},\mathbf{\Psi}}K}_{N\times N} = -\ \underbrace{\partial_{\mathbf{Q}}\mathbf{S}}_{3N\times 3N}\ \underbrace{\partial_{\mathbf{\Psi}}\mathbf{Q}}_{3N\times N}$$

[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

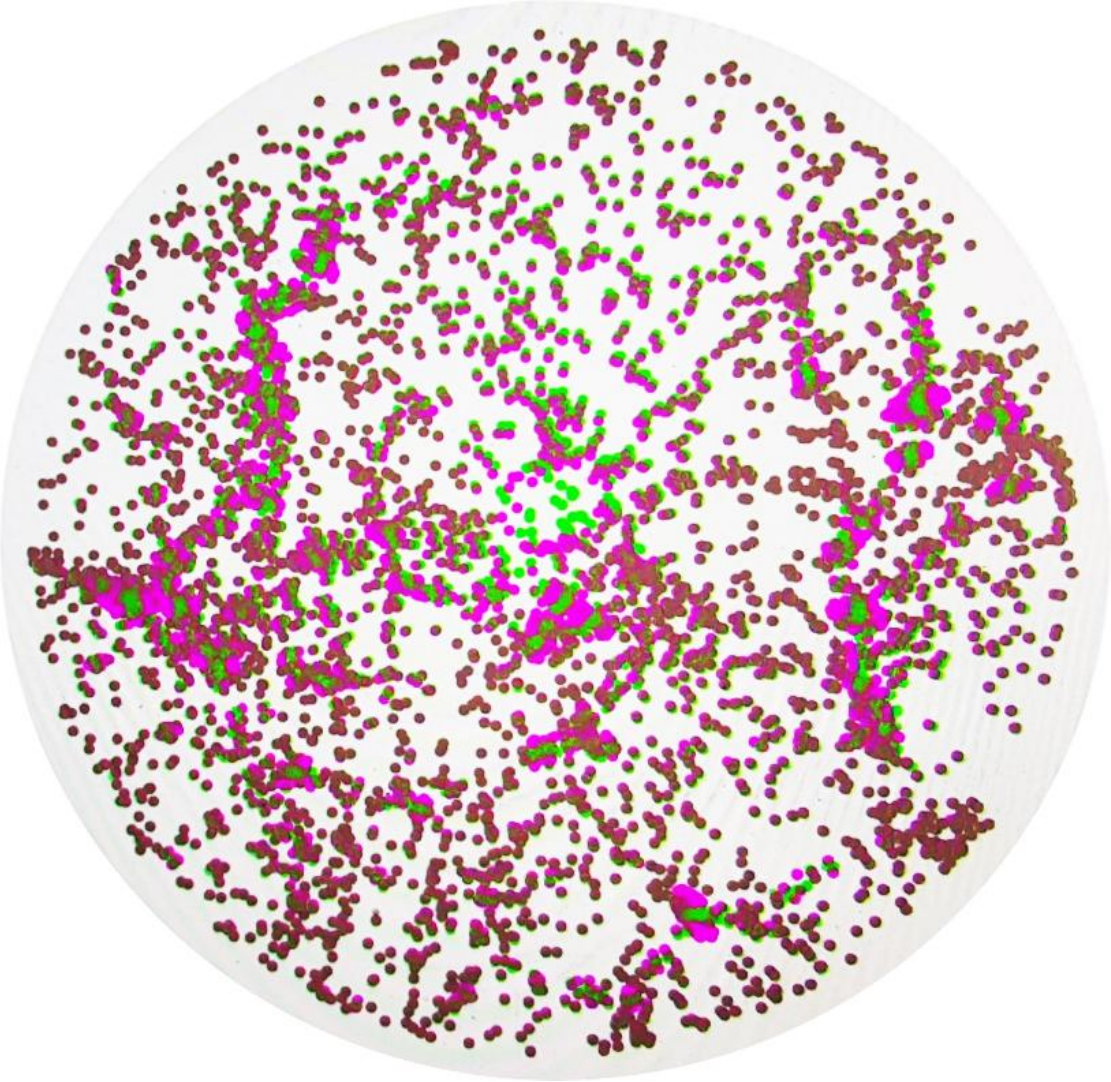
Early numerical experiments in 2D



[Dapogny, Oudet, **L**]

Part. 5 Redshift distortion

Early numerical experiments in 2D



[Dapogny, Oudet, **L**]

6

Brenier-Monge-Ampere gravitation

1. Newton

$$F = -\mathcal{G}\frac{m_1 m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

$$\begin{cases} F & = & \nabla\phi \\ \Delta\phi & = & 4\pi\mathcal{G}(\rho - \bar{\rho}) \end{cases}$$

2. Brenier-Monge-Ampère

$$\begin{cases} F & = & \nabla\Phi \\ \Delta\Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{cases}$$

3. Optimal Transport

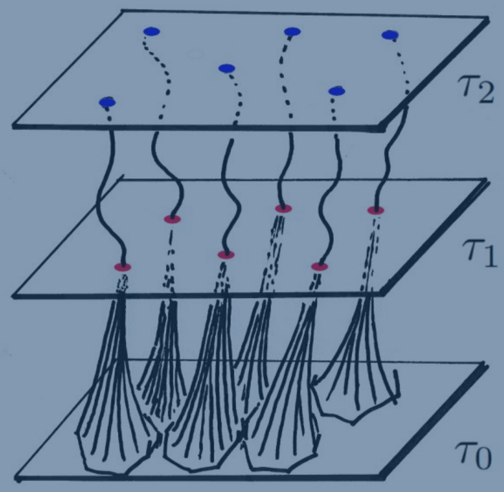
$$T \quad = \quad \nabla\Phi$$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

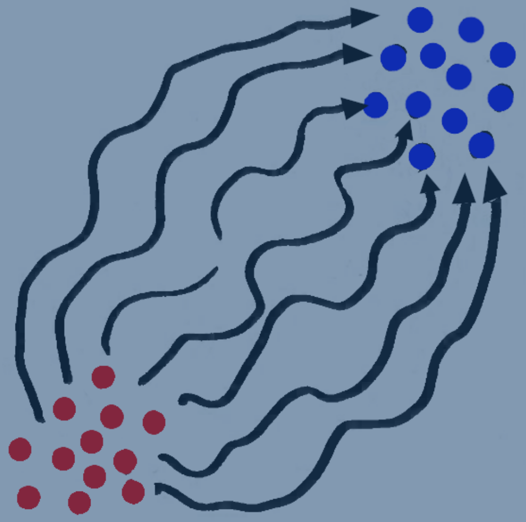
subject to:

$$\int_B \bar{\rho} d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

6. The Path Bundle Method

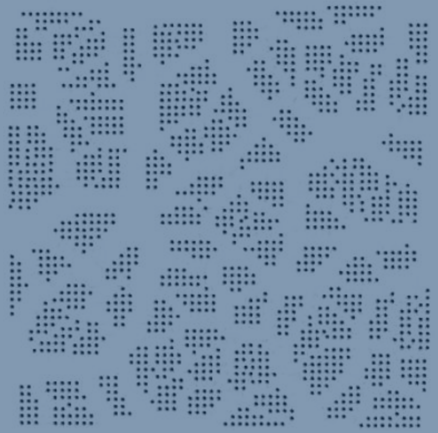


5. Large Deviations Pple.



4. Discrete Optimal Transp.

$$\inf_{\sigma \in S_N} \left[\left| \mathbf{r}_i - \mathbf{q}_{\sigma(i)} \right|^2 \right]$$



1. Newton-Poisson

$\rho(\mathbf{x}, t)$

Gravity for a density field ?
Eulerian coordinates

(F=ma)

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} \quad = \quad \nabla\phi$$

$$\Delta\phi = 4\pi\mathcal{G}(\rho - \boxed{\bar{\rho})}$$

$$\partial_t \rho + \nabla \cdot (\rho\mathbf{u}) \quad = \quad 0$$

(Mass conservation *continuity eqn*)

1. Newton

$$F = -\mathcal{G}\frac{m_1 m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

$$\left\{\begin{array}{lcl} F &=& \nabla\phi \\ \Delta\phi &=& 4\pi\mathcal{G}(\rho - \bar{\rho}) \end{array}\right.$$

2. Brenier-Monge-Ampère

$$\left\{\begin{array}{lcl} F &=& \nabla\Phi \\ \Delta\Phi &=& \frac{\rho}{\bar{\rho}} \\ \Phi &=& \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{array}\right.$$

3. Optimal Transport

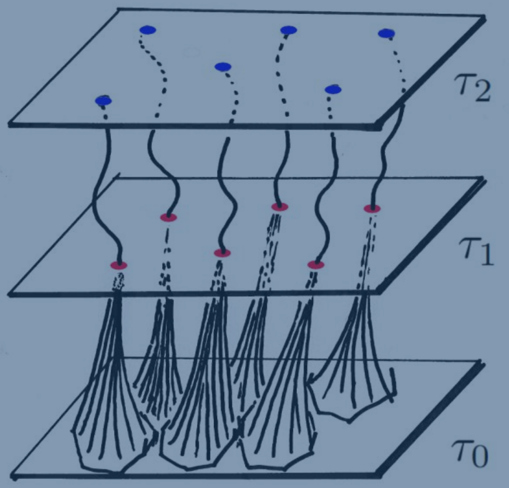
$$T \quad = \quad \nabla\Phi$$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r}\right]$$

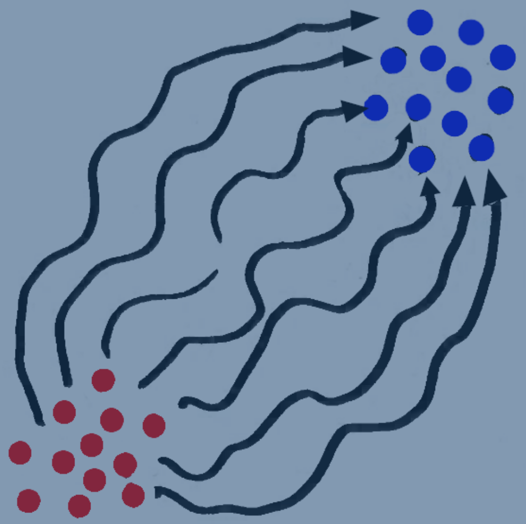
subject to:

$$\int_B \bar{\rho}\, d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

6. The Path Bundle Method

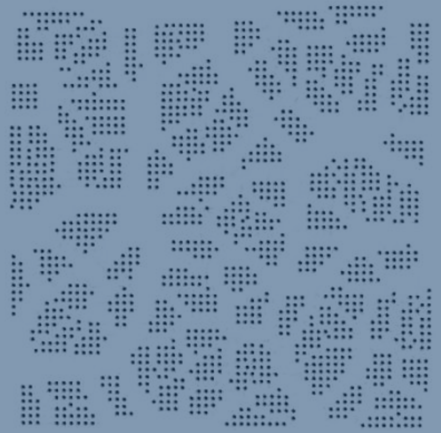


5. Large Deviations Pple.



4. Discrete Optimal Transp.

$$\inf_{\sigma \in S_N} \left[\left|\mathbf{r}_i - \mathbf{q}_{\sigma(i)}\right|^2\right]$$



2. Brenier-Monge-Ampère

Taylor expansion of the determinant of a matrix around the identity:

$$\det(1 + \varepsilon A) = 1 + \varepsilon \mathrm{tr}(A) + O(\varepsilon^2)$$

2. Brenier-Monge-Ampère

Taylor expansion of the determinant of a matrix around the identity:

$$\det(1 + \varepsilon A) = 1 + \varepsilon \mathrm{tr}(A) + O(\varepsilon^2)$$

$$\varepsilon A = \left[\frac{\partial^2 \phi}{\partial x_i \partial x_j} \right]$$

2. Brenier-Monge-Ampère

Taylor expansion of the determinant of a matrix around the identity:

$$\det(1 + \varepsilon A) = 1 + \varepsilon \mathrm{tr}(A) + O(\varepsilon^2)$$

$$\varepsilon A = \left[\frac{\partial^2 \phi}{\partial x_i \partial x_j} \right]$$

$$\varepsilon \mathrm{trace}(A) = \mathrm{trace}(D^2 \phi)$$

2. Brenier-Monge-Ampère

Taylor expansion of the determinant of a matrix around the identity:

$$\det(1 + \varepsilon A) = 1 + \varepsilon \mathrm{tr}(A) + O(\varepsilon^2)$$

$$\varepsilon A = \left[\frac{\partial^2 \phi}{\partial x_i \partial x_j} \right]$$

$$\begin{aligned} \varepsilon \mathrm{trace}(A) &= \mathrm{trace}(D^2 \phi) \\ &= \Delta \phi \end{aligned}$$

2. Brenier-Monge-Ampère

Taylor expansion of the determinant of a matrix around the identity:

$$\det(1+\varepsilon A) = 1 + \varepsilon \mathrm{tr}(A) + O(\varepsilon^2)$$

$$\varepsilon A = \left[\frac{\partial^2 \phi}{\partial x_i \partial x_j} \right]$$

$$\begin{aligned} \varepsilon \mathrm{trace}(A) &= \mathrm{trace}(D^2\phi) \\ &= \Delta\phi \end{aligned}$$

$$\det(1+\varepsilon A) = \det(D^2\phi + 1) = \det\left(D^2(\phi + \mathbf{r}^2/2)\right)$$

2. Brenier-Monge-Ampère

Taylor expansion of the determinant of a matrix around the identity:

$$\det(1 + \varepsilon A) = 1 + \varepsilon \mathrm{tr}(A) + O(\varepsilon^2)$$

$$\varepsilon A = \left[\frac{\partial^2 \phi}{\partial x_i \partial x_j} \right]$$

$$\begin{aligned} \varepsilon \mathrm{trace}(A) &= \mathrm{trace}(D^2 \phi) \\ &= \Delta \phi \end{aligned}$$

$$\begin{aligned} \det(1 + \varepsilon A) = \det(D^2 \phi + 1) &= \det \left(D^2 (\phi + \mathbf{r}^2 / 2) \right) \\ &= \Delta\!\!\!\Delta (\phi + \mathbf{r}^2 / 2) \end{aligned}$$

Newton-Poisson

Brenier-Monge-Ampère

$$\begin{cases} F & = & \nabla\phi \\ \Delta\phi & = & 4\pi\mathcal{G}(\rho-\bar{\rho}) \end{cases}$$

$$\begin{cases} F & = & \nabla\Phi \\ \Delta\Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{cases}$$

$$\Delta\Phi = \det D^2\Phi$$

$$\det(1+\varepsilon A) = 1 + \varepsilon\mathrm{tr}(A) + O(\varepsilon^2)$$

1. Newton

$$F = -\mathcal{G}\frac{m_1 m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

$$\left\{\begin{array}{lcl} F & = & \nabla\phi \\ \Delta\phi & = & 4\pi\mathcal{G}(\rho - \bar{\rho}) \end{array}\right.$$

2. Brenier-Monge-Ampère

$$\left\{\begin{array}{lcl} F & = & \nabla\Phi \\ \Delta\Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{array}\right.$$

3. Optimal Transport

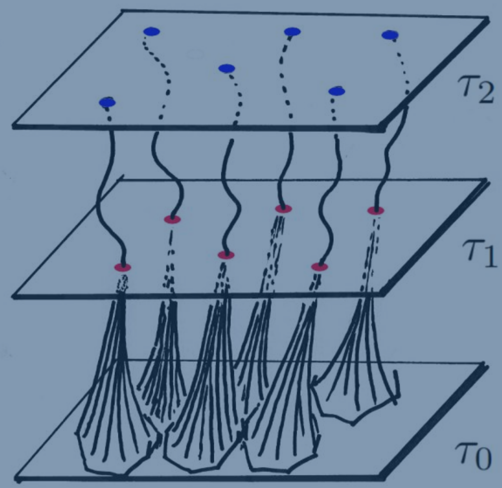
$$T = \nabla\Phi$$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r}\right]$$

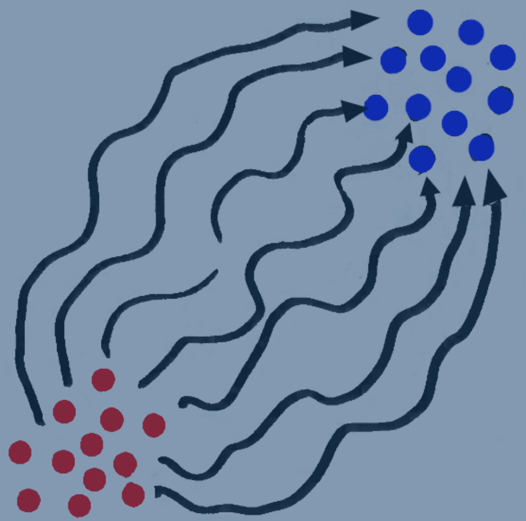
subject to:

$$\int_B \bar{\rho} d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

6. The Path Bundle Method

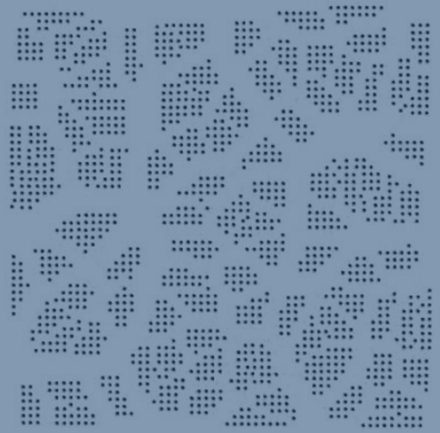


5. Large Deviations Pple.



4. Discrete Optimal Transp.

$$\inf_{\sigma \in S_N}\left[\left|\mathbf{r}_i - \mathbf{q}_{\sigma(i)}\right|^2\right]$$



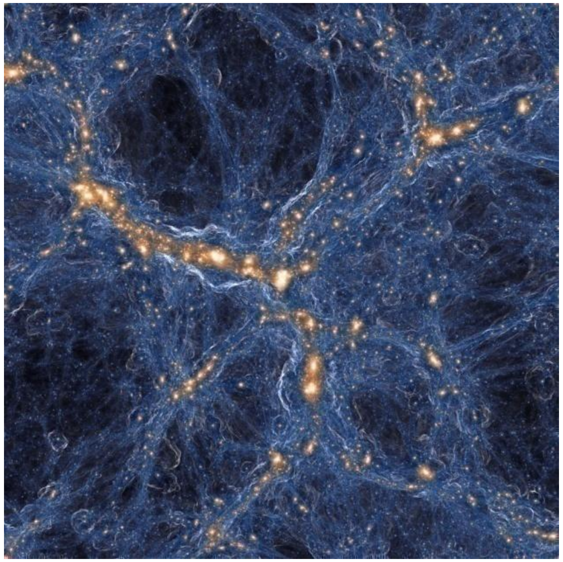
3. Optimal Transport and Monge-Ampère

$$\Delta\Phi = \frac{\rho}{\bar{\rho}}$$

3. Optimal Transport and Monge-Ampère

$$\bar{\rho}\Delta\Phi = \rho$$

3. Optimal Transport and Monge-Ampère

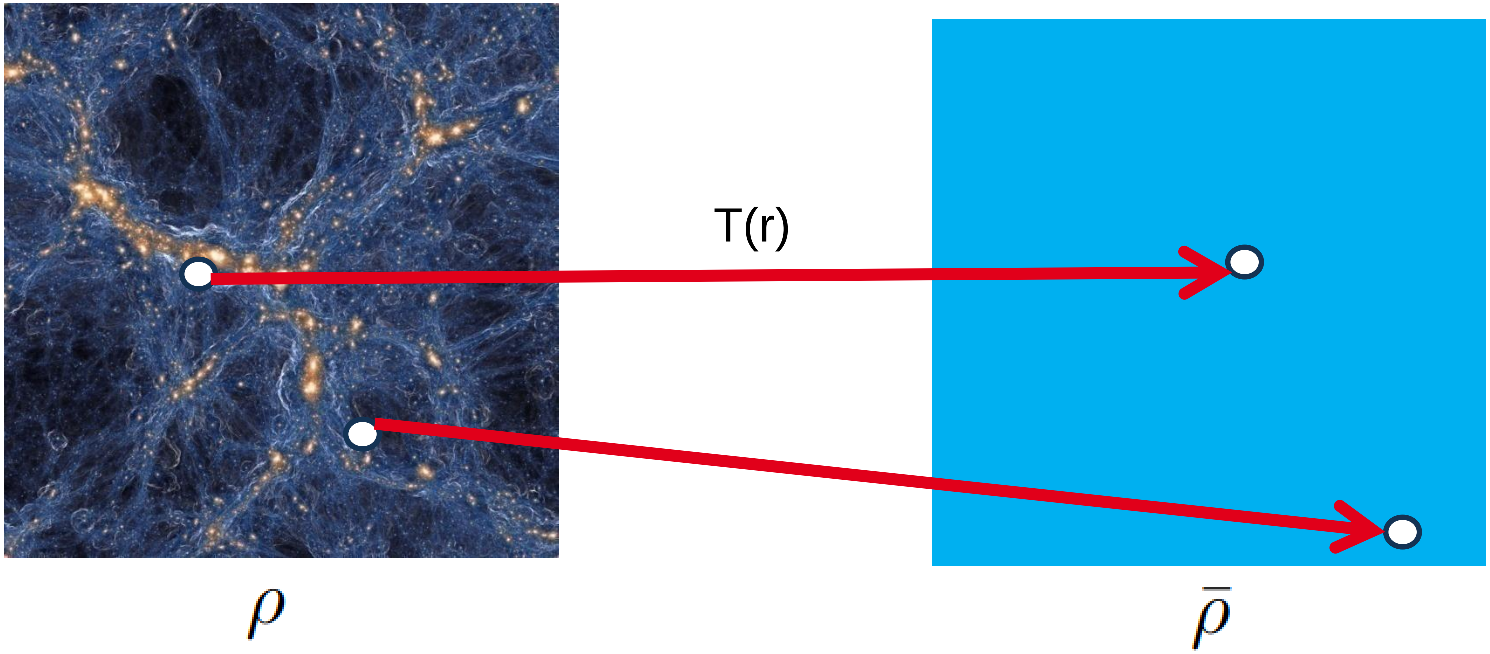


ρ

$\bar{\rho}$

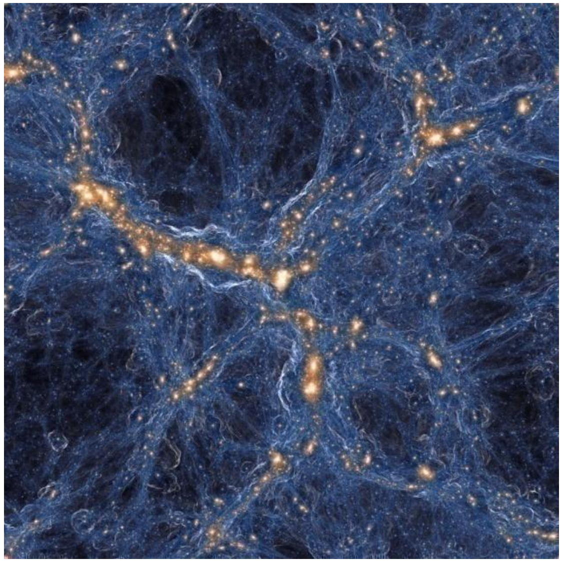
$$\bar{\rho}\Delta\!\!\!\Delta\Phi = \rho$$

3. Optimal Transport and Monge-Ampère

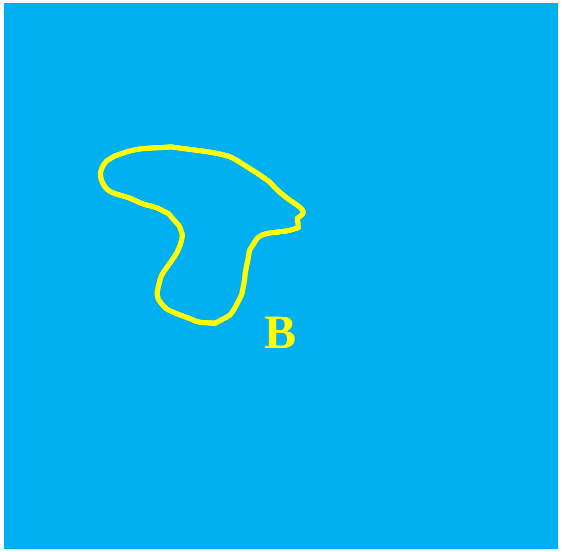


$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

3. Optimal Transport and Monge-Ampère



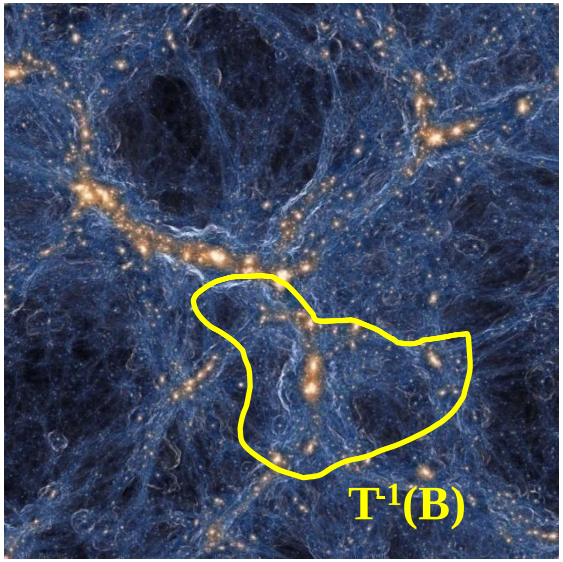
ρ



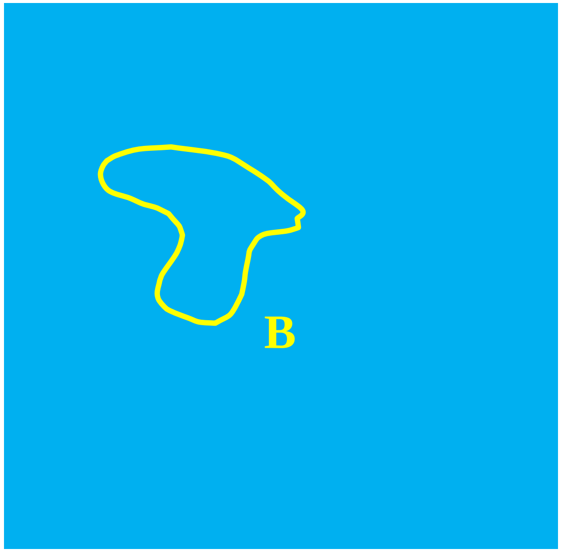
$\bar{\rho}$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

3. Optimal Transport and Monge-Ampère



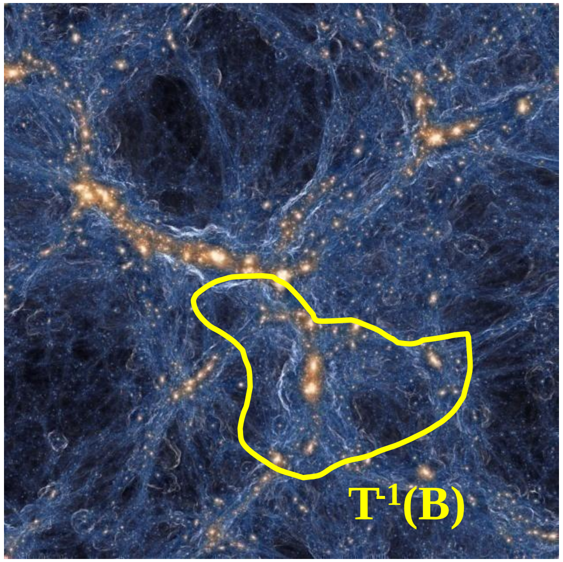
ρ



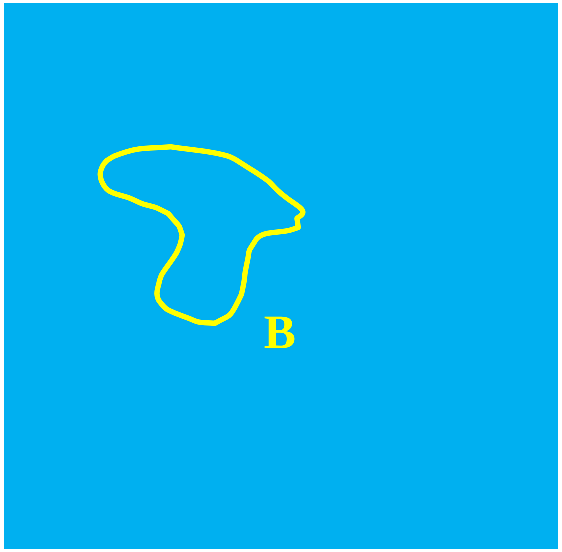
$\bar{\rho}$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

3. Optimal Transport and Monge-Ampère



ρ



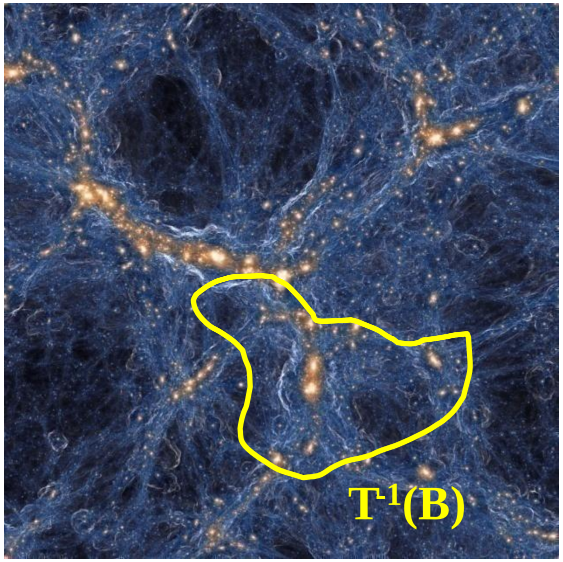
$\bar{\rho}$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

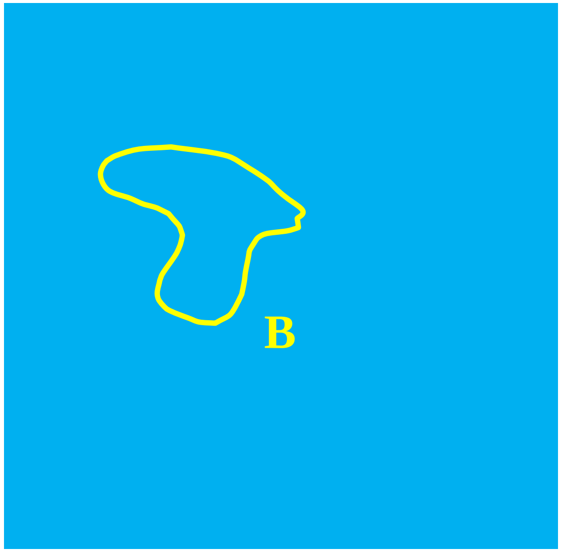
subject to:

$$\int_B \bar{\rho} d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

3. Optimal Transport and Monge-Ampère



ρ



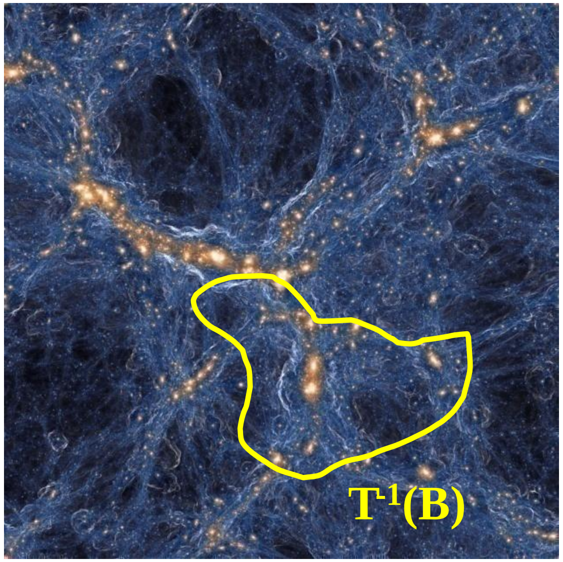
$\bar{\rho}$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

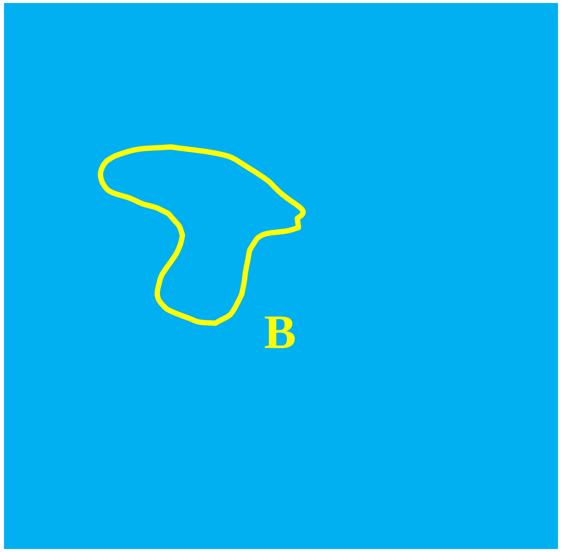
subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

3. Optimal Transport and Monge-Ampère



ρ



$\bar{\rho}$

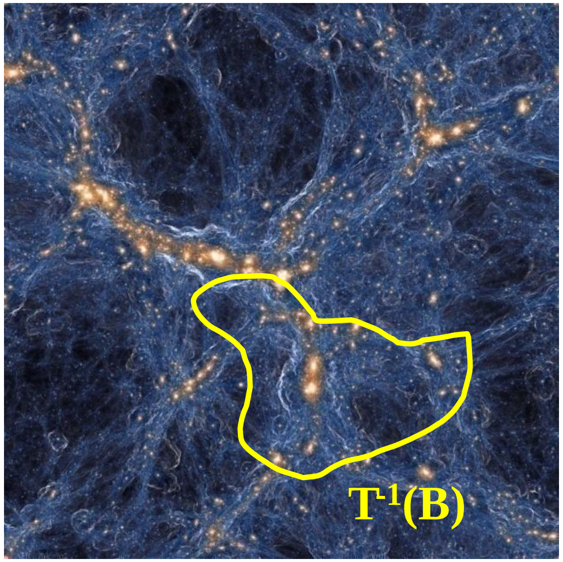
$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

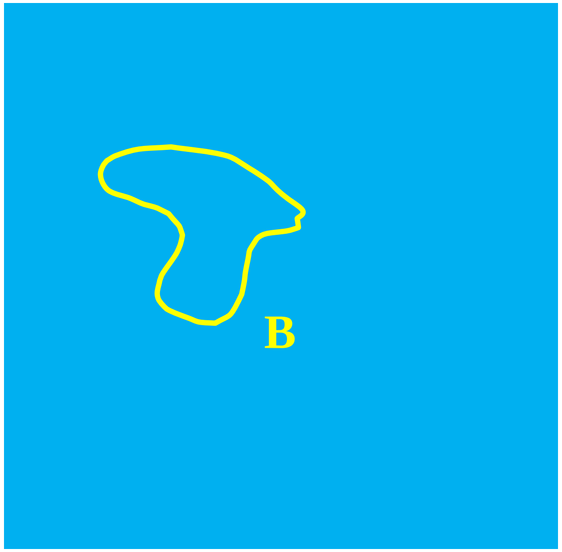
$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\ \mathcal{L}(T, \Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} \ + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \ - \int \Psi(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \ \Big]$$

3. Optimal Transport and Monge-Ampère



ρ



$\bar{\rho}$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\; \mathcal{L}(T, \boxed{\Psi}) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} - \int \Psi(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \Big]$$

Lagrange multiplier associated with the constraint

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\ \mathcal{L}(T,\Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \ - \int \Psi(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \ \Big]$$

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\ \mathcal{L}(T, \Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \ - \int \Psi(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \ \Big]$$

Optimality conditions

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\; \mathcal{L}(T, \Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \; - \int \Psi(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \Big]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla \Psi(T(\mathbf{r}))$$

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \left[\mathcal{L}(T, \Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} - \int \Psi(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \right]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla \Psi(T(\mathbf{r}))$$

$$\frac{\partial^2 \mathcal{L}}{\partial T^2} \geq 0 \quad \Rightarrow \quad \Psi \text{ is a convex function}$$

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r}\right]$$

subject to:

$$\int g(\mathbf{q})\bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r}))\rho(\mathbf{r})d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\ \mathcal{L}(T,\Psi) = \int \rho(\mathbf{r})T(\mathbf{r}) \cdot \mathbf{r}d\mathbf{r} + \int \bar{\rho}\Psi(\mathbf{q})d\mathbf{q} \ - \int \Psi(T(\mathbf{r}))\rho(\mathbf{r})d\mathbf{r} \ \Big]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla\Psi(T(\mathbf{r}))$$

$$\frac{\partial^2 \mathcal{L}}{\partial T^2} \geq 0 \quad \Rightarrow \quad \Psi \text{ is a convex function}$$

$$\begin{array}{rcl} T(\mathbf{r}) & = & \nabla\Phi(\mathbf{r}), \quad \text{where:} \\ \Phi(\mathbf{r}) & = & \Psi^*(\mathbf{r}) = \inf_{\mathbf{q}} [\mathbf{q} \cdot \mathbf{r} - \Psi(\mathbf{q})] \end{array}$$

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\ \mathcal{L}(T,\Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \ - \int \Psi(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \ \Big]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla \Psi(T(\mathbf{r}))$$

$$\frac{\partial^2 \mathcal{L}}{\partial T^2} \geq 0 \quad \Rightarrow \quad \Psi \text{ is a convex function}$$

$$\begin{aligned} T(\mathbf{r}) &= \nabla \Phi(\mathbf{r}), \quad \text{where:} \\ \Phi(\mathbf{r}) &= \Psi^*(\mathbf{r}) = \inf_{\mathbf{q}} \left[\mathbf{q} \cdot \mathbf{r} - \Psi(\mathbf{q}) \right] \end{aligned}$$

Legendre-Fenchel dual

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q})\bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

Insert into constraint:

$$\bar{\rho} \int g(\nabla\Phi(\mathbf{r}))|\mathrm{D}^2\Phi(\mathbf{r})| d\mathbf{r} \;=\; \int g(\nabla\Phi(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r}$$

$$\sup_T \inf_\Psi \Big[\; \mathcal{L}(T,\Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} \; + \int \bar{\rho}\Psi(\mathbf{q}) d\mathbf{q} \; - \int \Psi(T(\mathbf{r}))\rho(\mathbf{r}) d\mathbf{r} \Big]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla\Psi(T(\mathbf{r}))$$

$$\frac{\partial^2 \mathcal{L}}{\partial T^2} \geq 0 \quad \Rightarrow \quad \Psi \text{ is a convex function}$$

$$\begin{aligned} T(\mathbf{r}) &= \nabla\Phi(\mathbf{r}), \quad \text{where:} \\ \Phi(\mathbf{r}) &= \Psi^*(\mathbf{r}) = \inf_{\mathbf{q}} [\mathbf{q}\cdot\mathbf{r} - \Psi(\mathbf{q})] \end{aligned}$$

Legendre-Fenchel dual

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

$$\sup_T \inf_\Psi \Big[\ \mathcal{L}(T, \Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \ - \int \Psi(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \ \Big]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla \Psi(T(\mathbf{r}))$$

$$\frac{\partial^2 \mathcal{L}}{\partial T^2} \geq 0 \quad \Rightarrow \quad \Psi \text{ is a convex function}$$

$$T(\mathbf{r}) \ = \ \nabla \Phi(\mathbf{r}), \quad \text{where:}$$

$$\Phi(\mathbf{r}) \ = \ \Psi^*(\mathbf{r}) = \inf_{\mathbf{q}} [\mathbf{q} \cdot \mathbf{r} - \Psi(\mathbf{q})]$$

Legendre-Fenchel dual

Insert into constraint:

$$\bar{\rho} \int g(\nabla \Phi(\mathbf{r})) |\mathrm{D}^2 \Phi(\mathbf{r})| d\mathbf{r} \ = \ \int g(\nabla \Phi(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r}$$

Pointwise:

$$\bar{\rho} \det D^2 \Phi \ = \ \rho(\mathbf{r})$$

3. Optimal Transport and Monge-Ampère

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

$$\int g(\mathbf{q}) \bar{\rho} d\mathbf{q} = \int g(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \quad \forall g$$

Insert into constraint:

$$\bar{\rho} \int g(\nabla\Phi(\mathbf{r})) |\mathrm{D}^2\Phi(\mathbf{r})| d\mathbf{r} \;=\; \int g(\nabla\Phi(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r}$$

Pointwise:

$$\bar{\rho} \det D^2\Phi \;=\; \rho(\mathbf{r})$$

Monge-Ampère equation:

$$\bar{\rho} \Delta \Phi = \rho$$

$$\sup_T \inf_\Psi \Big[\;\mathcal{L}(T,\Psi) = \int \rho(\mathbf{r}) T(\mathbf{r}) \cdot \mathbf{r} d\mathbf{r} \; + \int \bar{\rho} \Psi(\mathbf{q}) d\mathbf{q} \; - \int \Psi(T(\mathbf{r})) \rho(\mathbf{r}) d\mathbf{r} \;\Big]$$

Optimality conditions

$$\frac{\partial \mathcal{L}}{\partial T} = 0 \quad \Rightarrow \quad \mathbf{r} = \nabla\Psi(T(\mathbf{r}))$$

$$\frac{\partial^2 \mathcal{L}}{\partial T^2} \geq 0 \quad \Rightarrow \quad \Psi \text{ is a convex function}$$

$$T(\mathbf{r}) \;=\; \nabla\Phi(\mathbf{r}), \quad \text{where:}$$

$$\Phi(\mathbf{r}) \;=\; \Psi^*(\mathbf{r}) = \inf_{\mathbf{q}} \left[\mathbf{q} \cdot \mathbf{r} - \Psi(\mathbf{q}) \right]$$

Legendre-Fenchel dual

1. Newton

$$F = -\mathcal{G}\frac{m_1 m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

$$\begin{cases} F & = & \nabla\phi \\ \Delta\phi & = & 4\pi\mathcal{G}(\rho - \bar{\rho}) \end{cases}$$

2. Brenier-Monge-Ampère

$$\begin{cases} F & = & \nabla\Phi \\ \Delta\Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{cases}$$

3. Optimal Transport

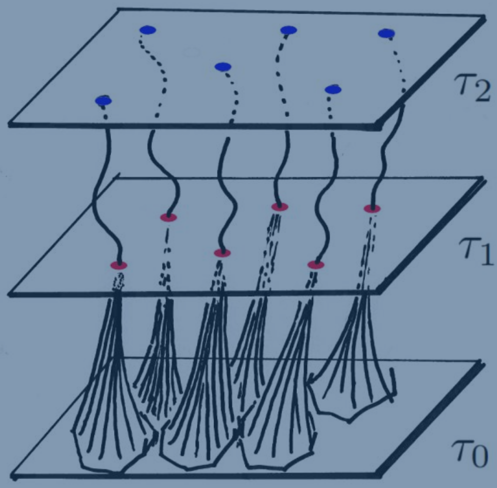
$$T \quad = \quad \nabla\Phi$$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

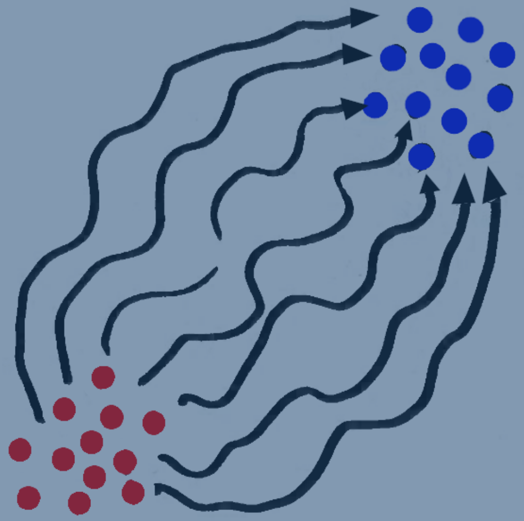
subject to:

$$\int_B \bar{\rho} d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

6. The Path Bundle Method

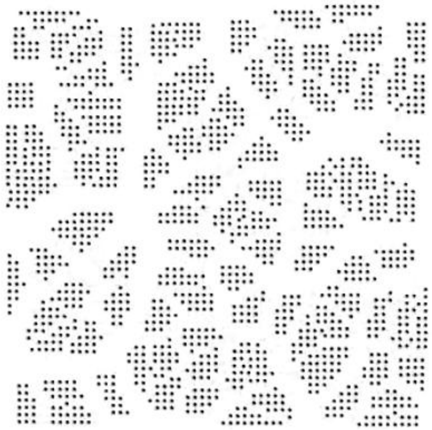


5. Large Deviations Pple.

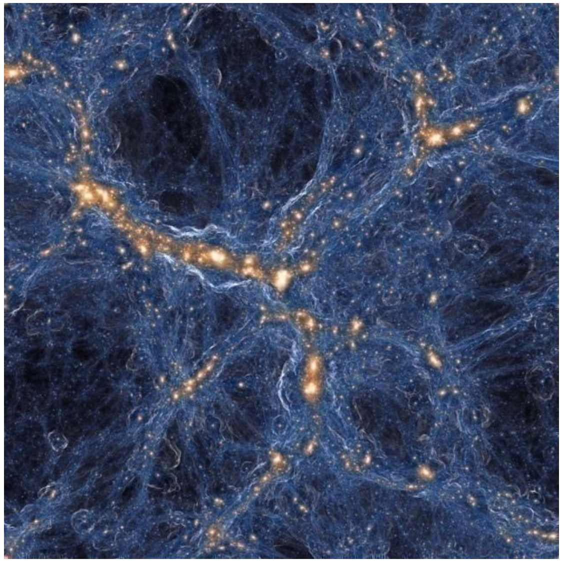


4. Discrete Optimal Transp.

$$\inf_{\sigma \in S_N} \left[\left| \mathbf{r}_i - \mathbf{q}_{\sigma(i)} \right|^2 \right]$$



4. Discrete Optimal Transport

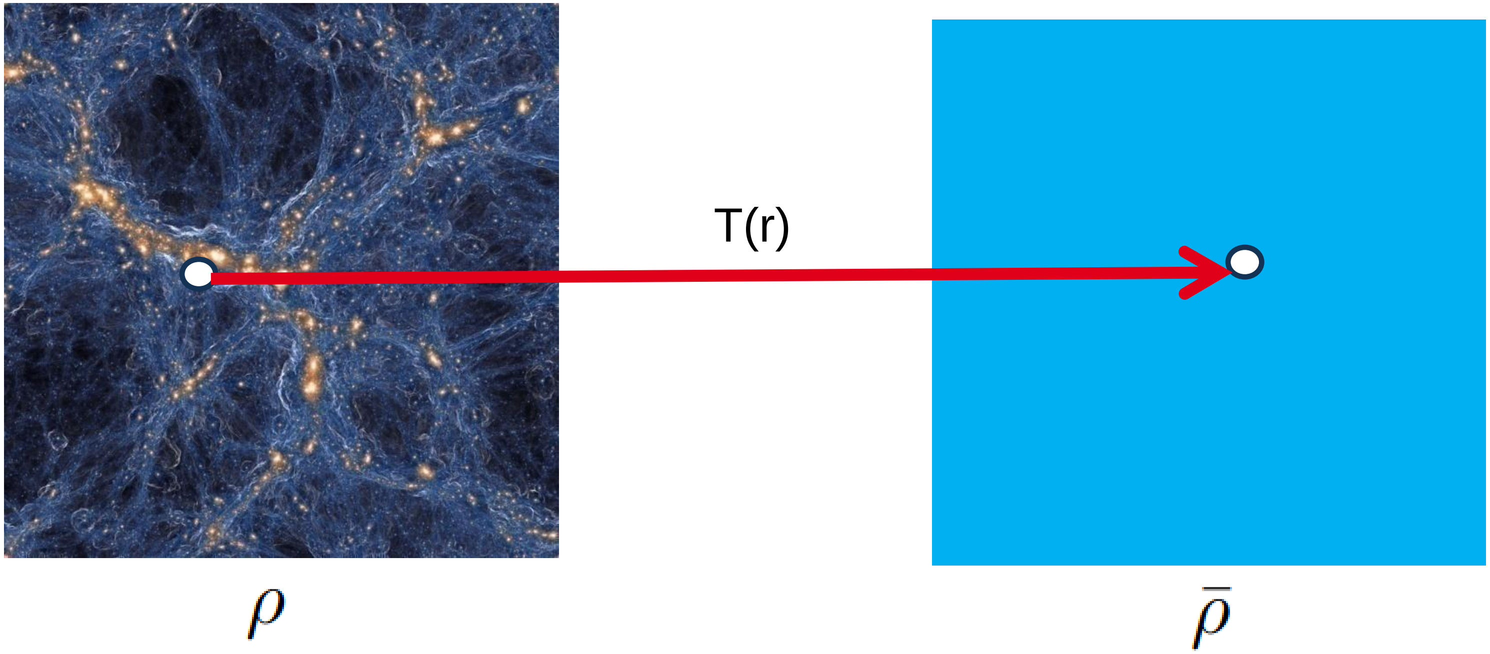


ρ

$\bar{\rho}$

$$\left\{ \begin{array}{lcl} F & = & \nabla \Phi \\ \Delta\!\!\!\Delta \Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi \mathcal{G} \bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{array} \right.$$

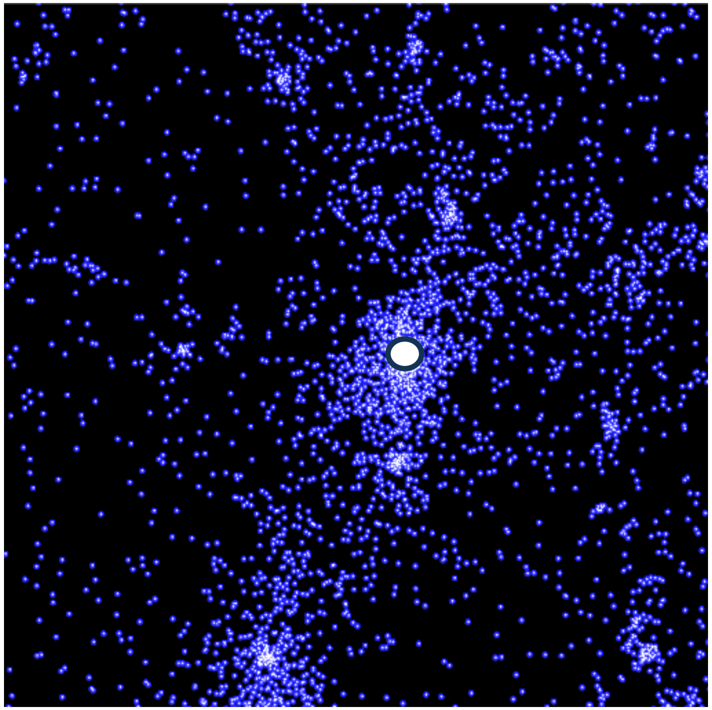
4. Discrete Optimal Transport



$$\begin{cases} F & = & \nabla \Phi \\ \Delta \Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi \mathcal{G} \bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{cases}$$

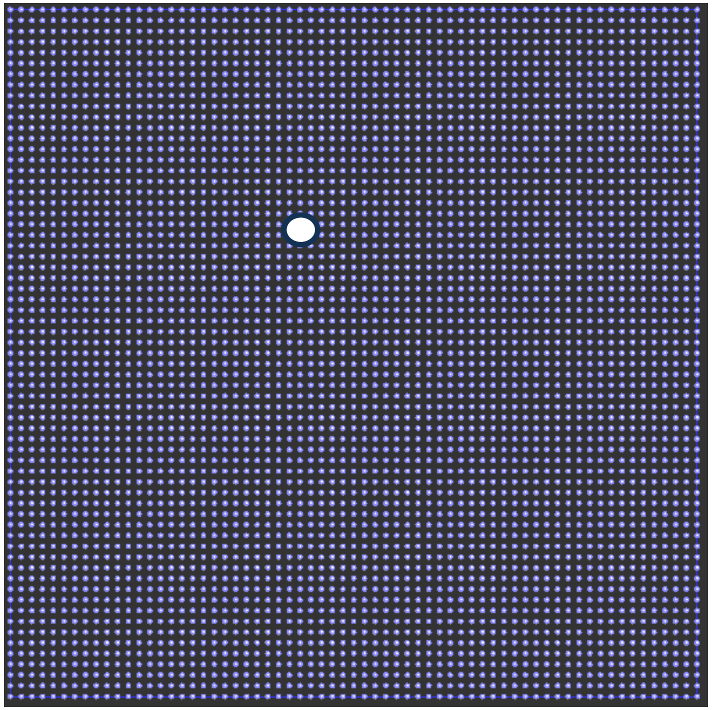
$$F = \frac{1}{4\pi \mathcal{G} \bar{\rho}} (\mathbf{r} - T(\mathbf{r}))$$

4. Discrete Optimal Transport



ρ

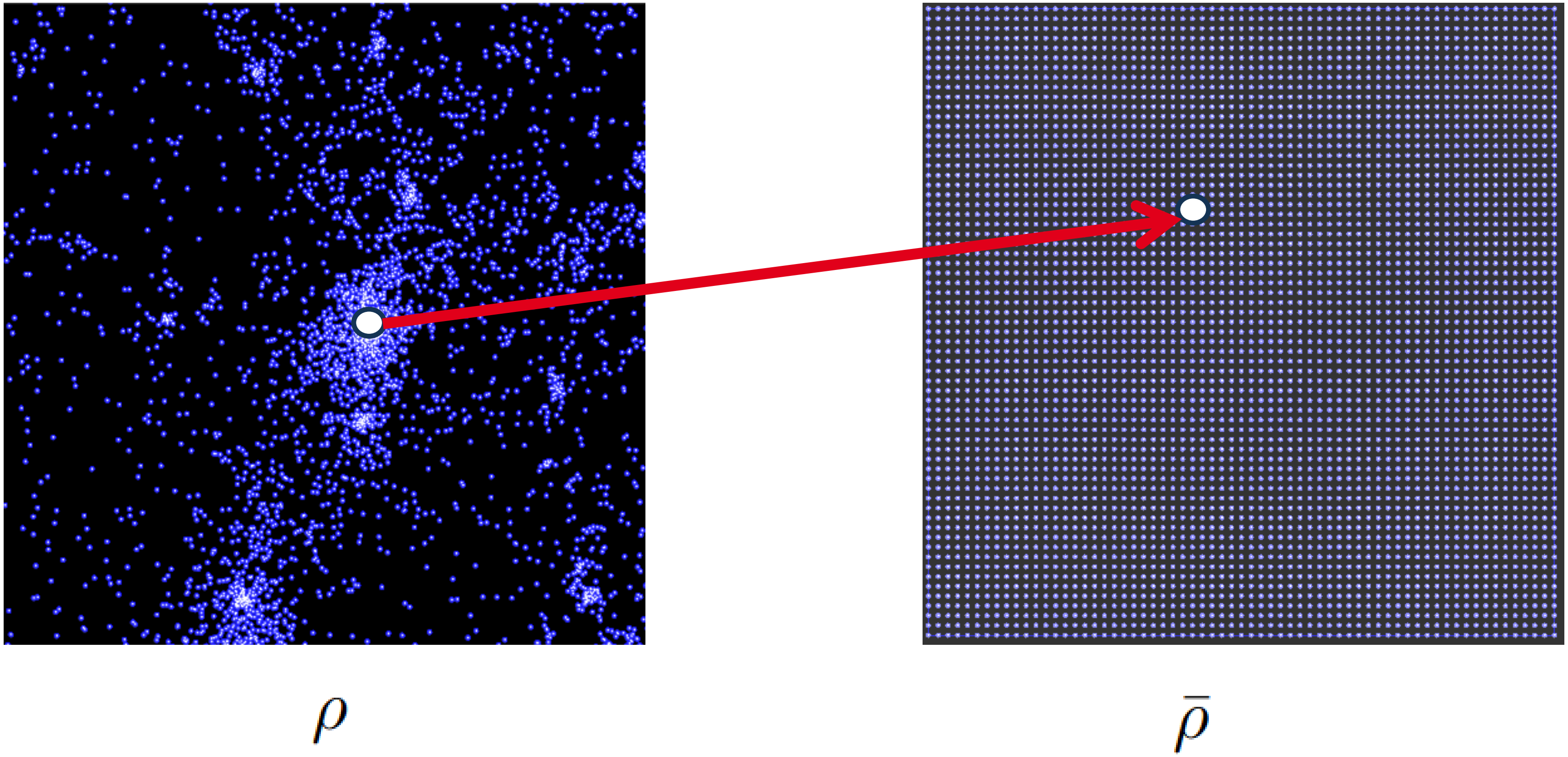
N points $\mathbf{r}_i$



$\bar{\rho}$

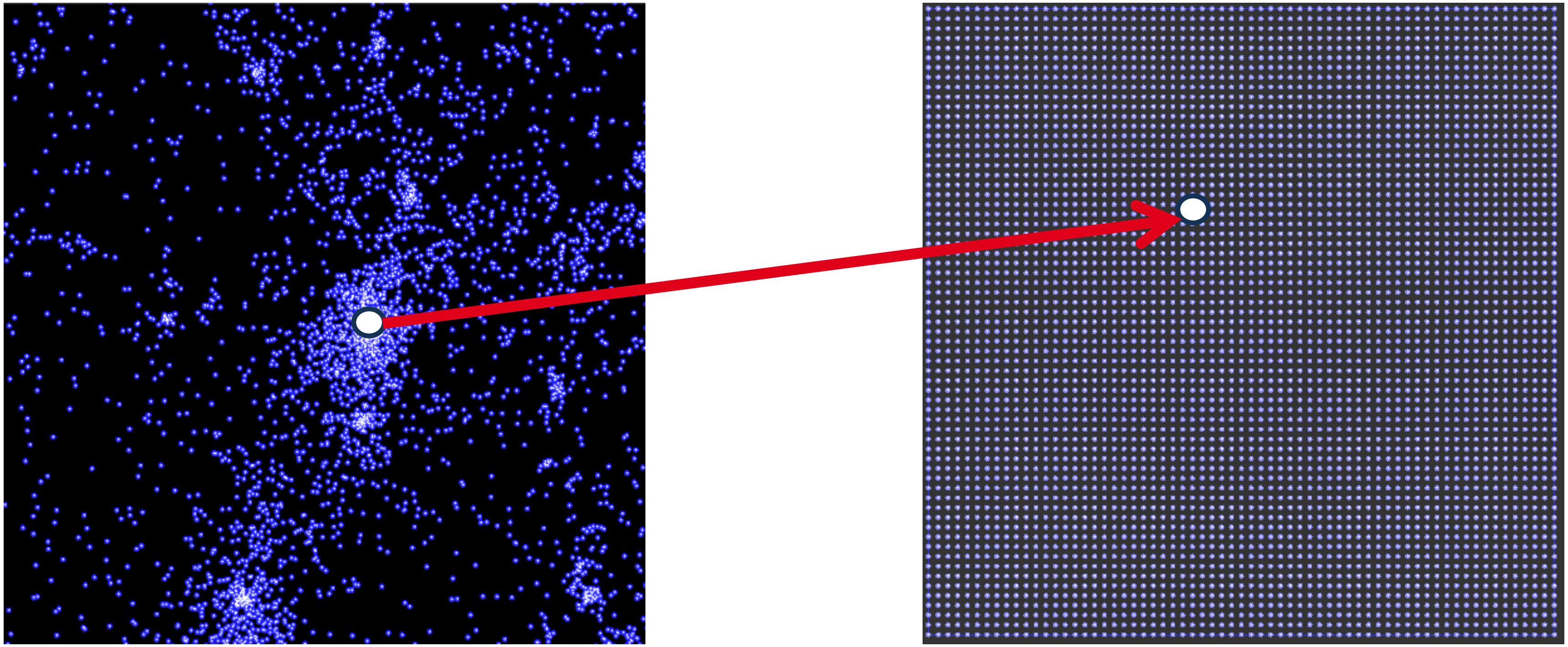
N points $\mathbf{q}_i$

4. Discrete Optimal Transport



$$T(\mathbf{r}_i) = \mathbf{q}_{\sigma(i)}$$

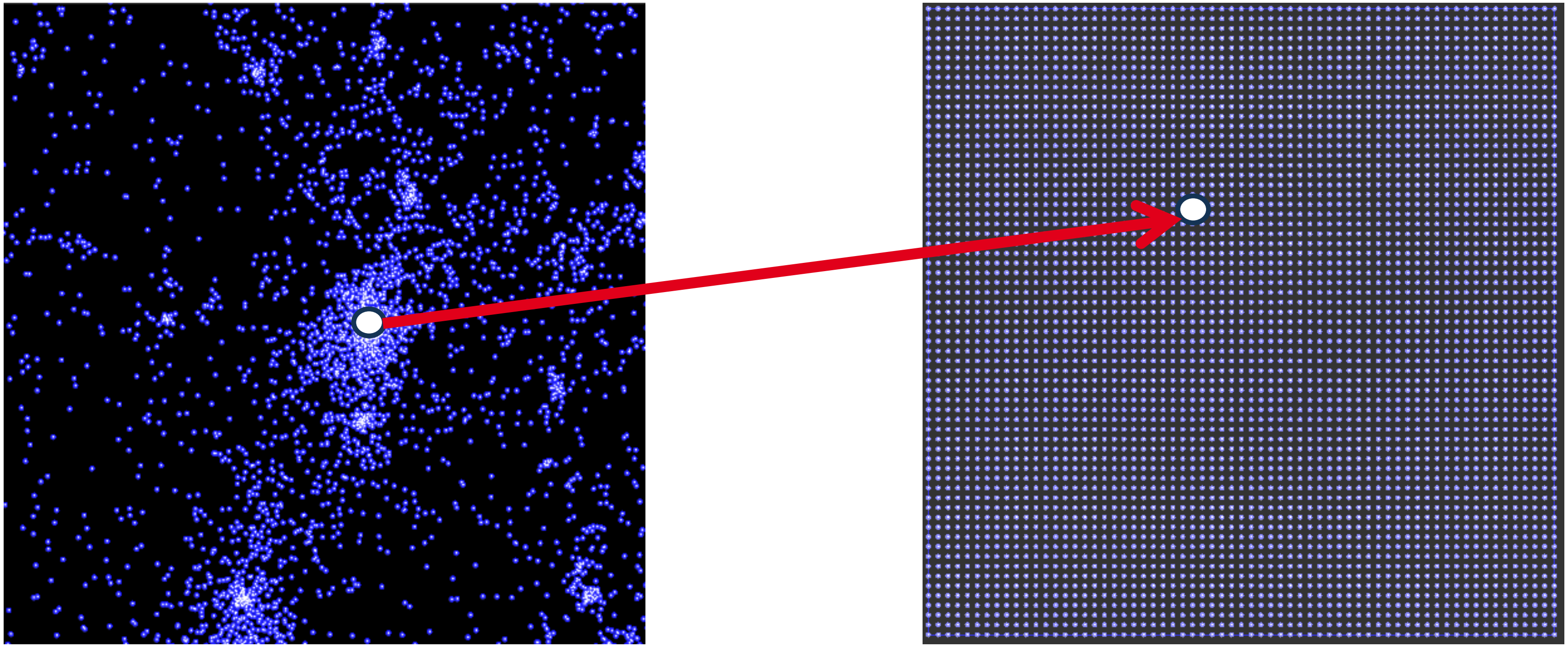
4. Discrete Optimal Transport



$$\mathrm{T}(\mathbf{r}_i) = \mathbf{q}_{\sigma(i)}$$

σ :*The permutation that minimizes* $\left[\left|\mathbf{r}_i - \mathbf{q}_{\sigma(i)}\right|^2\right]$

4. Discrete Optimal Transport

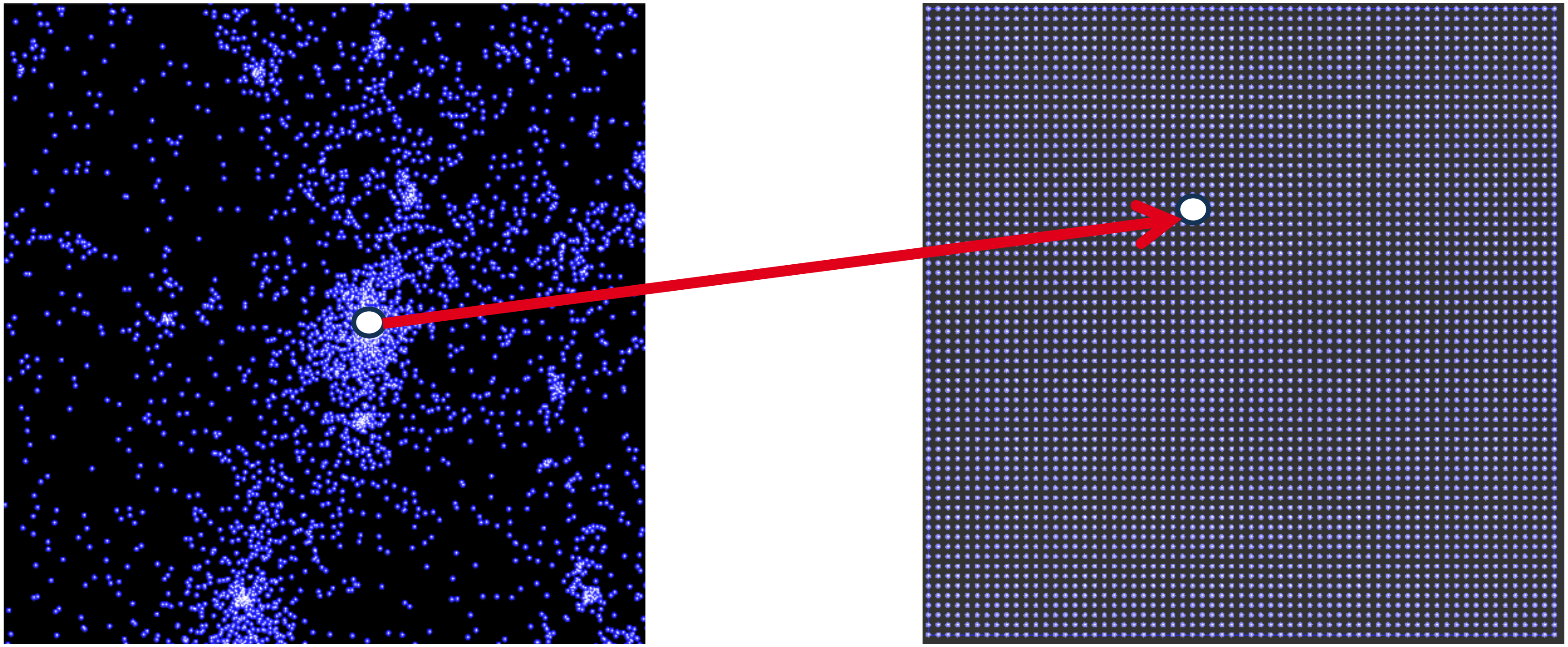


ρ $\quad T(\mathbf{r}_i) = \mathbf{q}_{\sigma(i)}$ $\quad \bar{\rho}$

$$F = \frac{1}{4\pi\mathcal{G}\bar{\rho}}(\mathbf{r} - T(\mathbf{r}))$$

σ :*The permutation that minimizes* $\left[\left| \mathbf{r}_i - \mathbf{q}_{\sigma(i)} \right|^2 \right]$

4. Discrete Optimal Transport



ρ

$T(\mathbf{r}_i) = \mathbf{q}_{\sigma(i)}$

$\bar{\rho}$

$$F_i = \frac{1}{4\pi\mathcal{G}\bar{\rho}}(\mathbf{r}_i - \mathbf{q}_{\sigma(i)})$$

σ :*The permutation that minimizes* $\left[\left|\mathbf{r}_i - \mathbf{q}_{\sigma(i)}\right|^2\right]$

1. Newton

$$F = -\mathcal{G}\frac{m_1 m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

$$\begin{cases} F &= \nabla\phi \\ \Delta\phi &= 4\pi\mathcal{G}(\rho - \bar{\rho}) \end{cases}$$

2. Brenier-Monge-Ampère

$$\begin{cases} F &= \nabla\Phi \\ \Delta\Phi &= \frac{\rho}{\bar{\rho}} \\ \Phi &= \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{cases}$$

3. Optimal Transport

$$T = \nabla\Phi$$

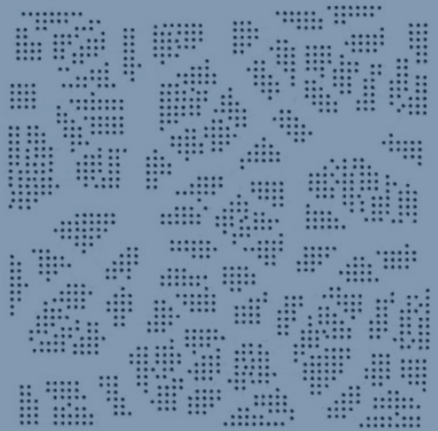
$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

subject to:

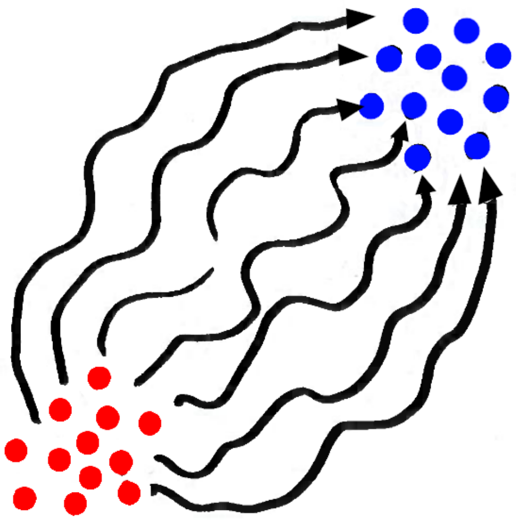
$$\int_B \bar{\rho} d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

4. Discrete Optimal Transp.

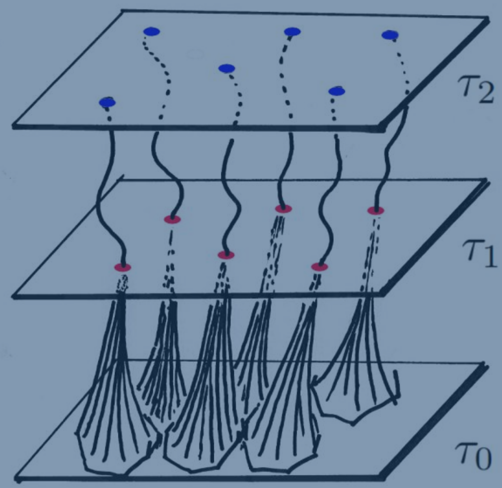
$$\inf_{\sigma \in S_N} \left[\left| \mathbf{r}_i - \mathbf{q}_{\sigma(i)} \right|^2 \right]$$



5. Large Deviations Pple.



6. The Path Bundle Method



5. Large Deviation Principle

$$F_i = \frac{1}{4\pi\mathcal{G}\bar{\rho}}(\mathbf{r}_i - \mathbf{q}_{\sigma(i)})$$

σ :*The permutation that minimizes* $\left[\left|\mathbf{r}_i - \mathbf{q}_{\sigma(i)}\right|^2\right]$

5. Large Deviation Principle

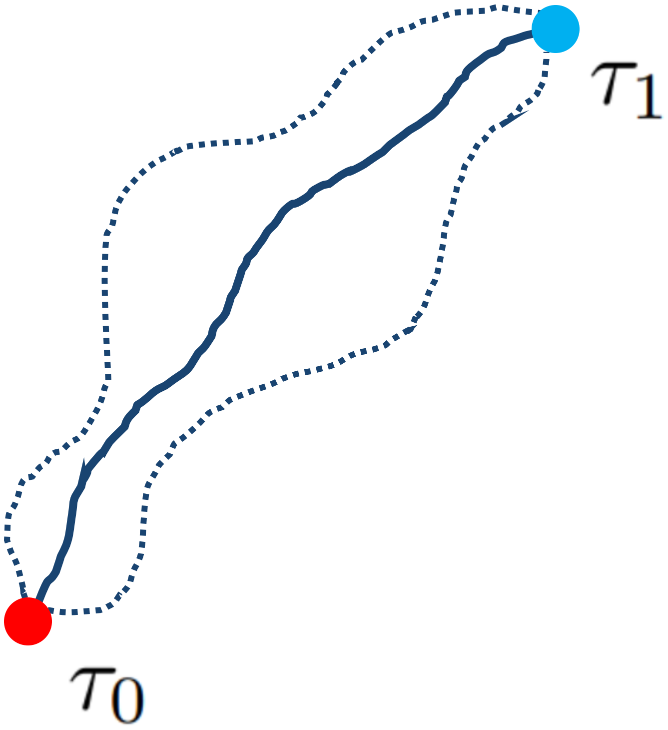
$$F_i = \frac{1}{4\pi\mathcal{G}\bar{\rho}}(\mathbf{r}_i - \mathbf{q}_{\sigma(i)})$$

σ :*The permutation that minimizes* $\left[\left|\mathbf{r}_i - \mathbf{q}_{\sigma(i)}\right|^2\right]$

Why ?

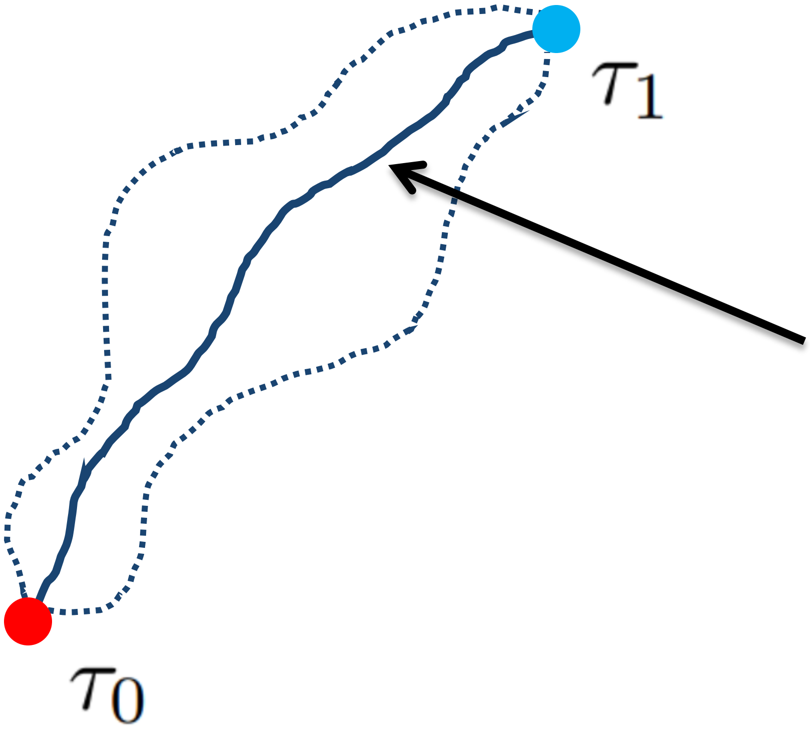
Can we *deduce* this formula from something else ?

5. Large Deviation Principle



Idea has similarities with ***least action***

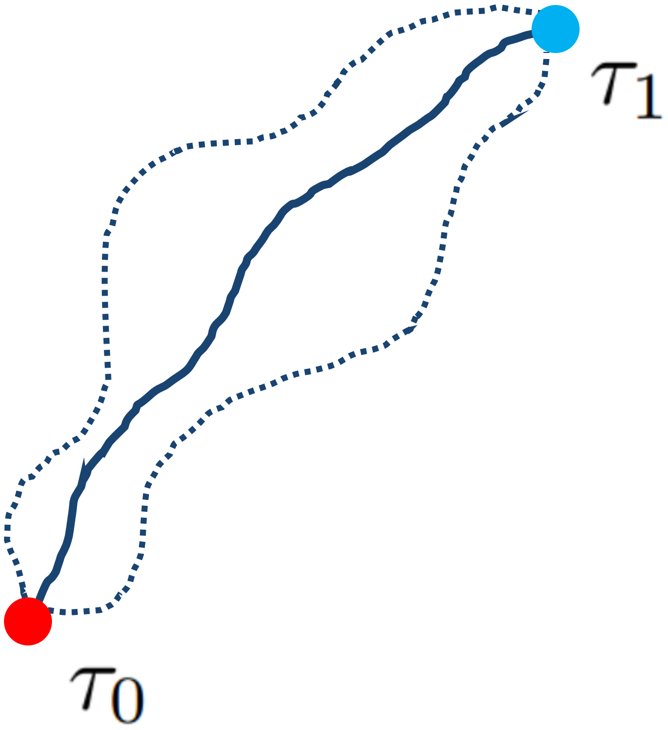
5. Large Deviation Principle



Idea has similarities with ***least action***

Extremize action between ***fixed*** initial and final conditions.

5. Large Deviation Principle

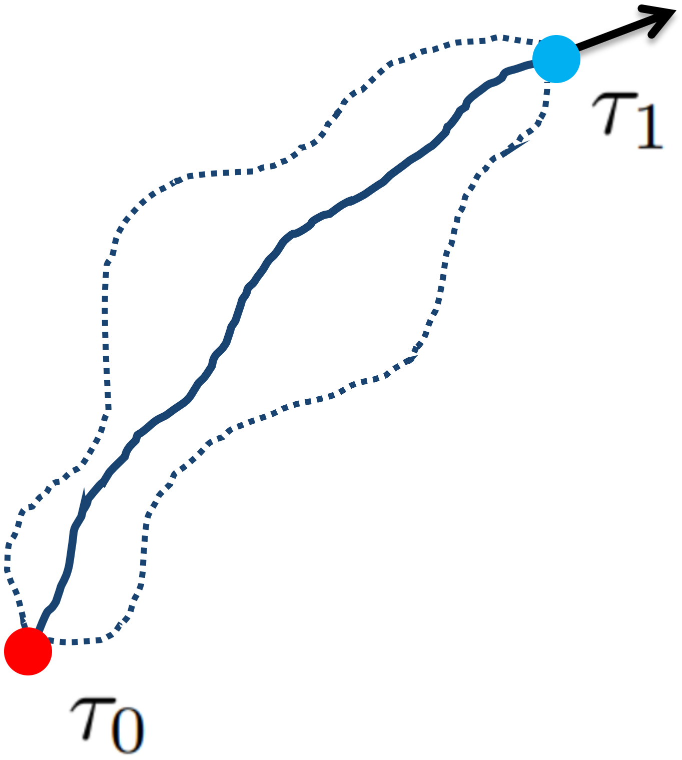


Idea has similarities with ***least action***

Extremize action between ***fixed*** initial and final conditions.

Deduce law of motion (differential relation)

5. Large Deviation Principle



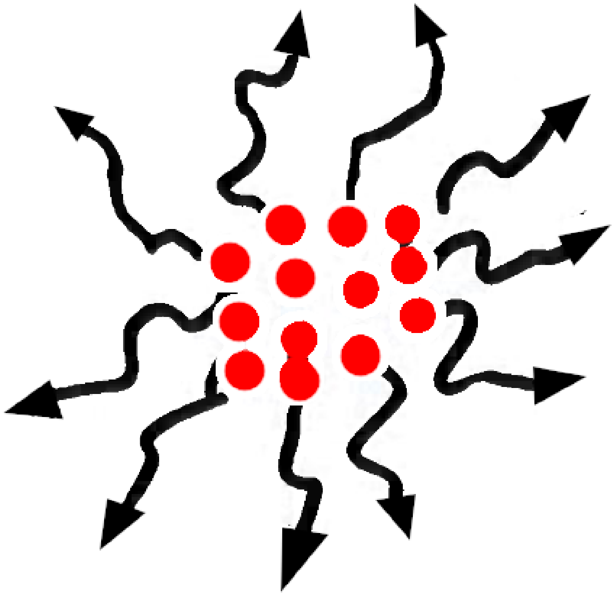
Idea has similarities with ***least action***

Extremize action between ***fixed*** initial and final conditions.

Deduce law of motion (differential relation)

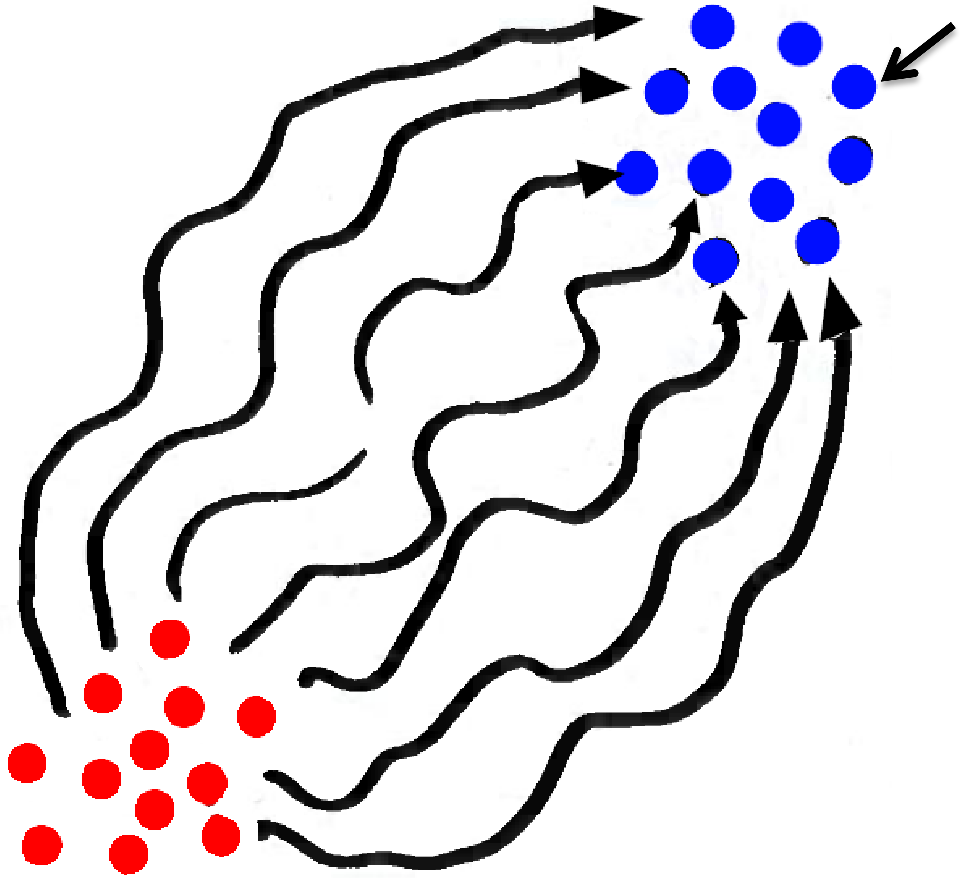
Extrapolate it

5. Large Deviation Principle



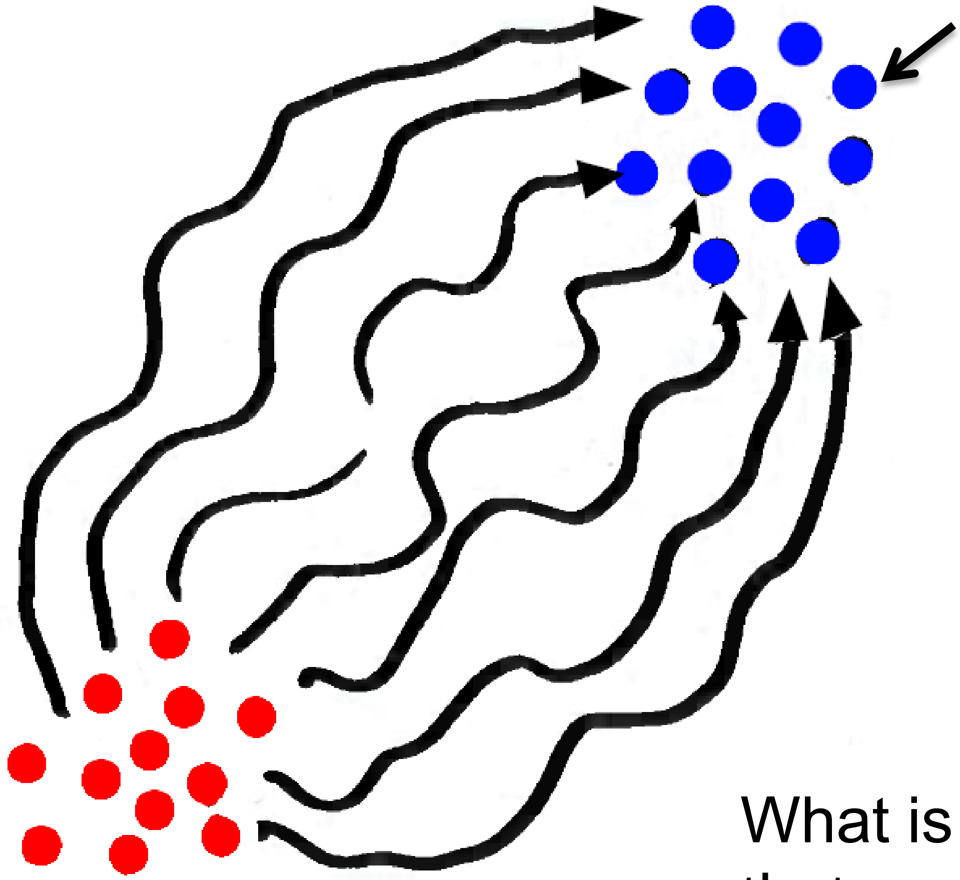
M ***indistinguishable*** particles
Independent Brownian motion
No interaction

5. Large Deviation Principle



We suppose that we observe them here after T seconds

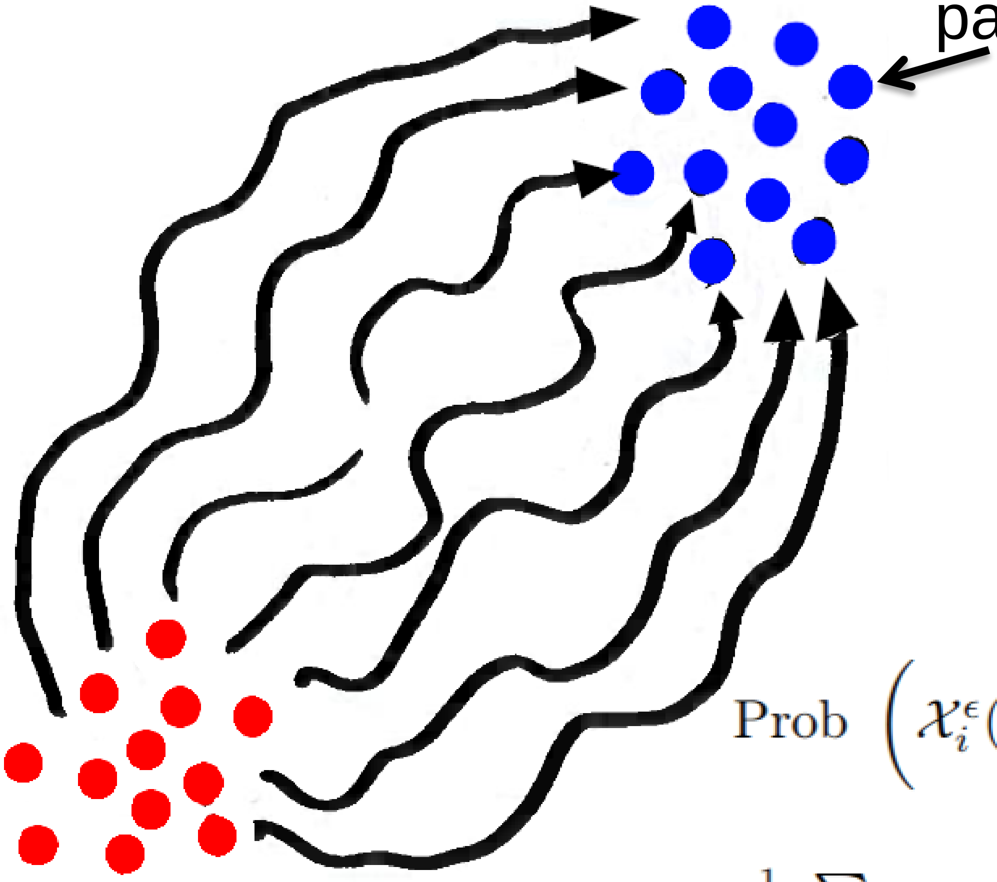
5. Large Deviation Principle



We suppose that we observe them here after T seconds

What is the “most probable” motion that accounts for the observation ?

5. Large Deviation Principle

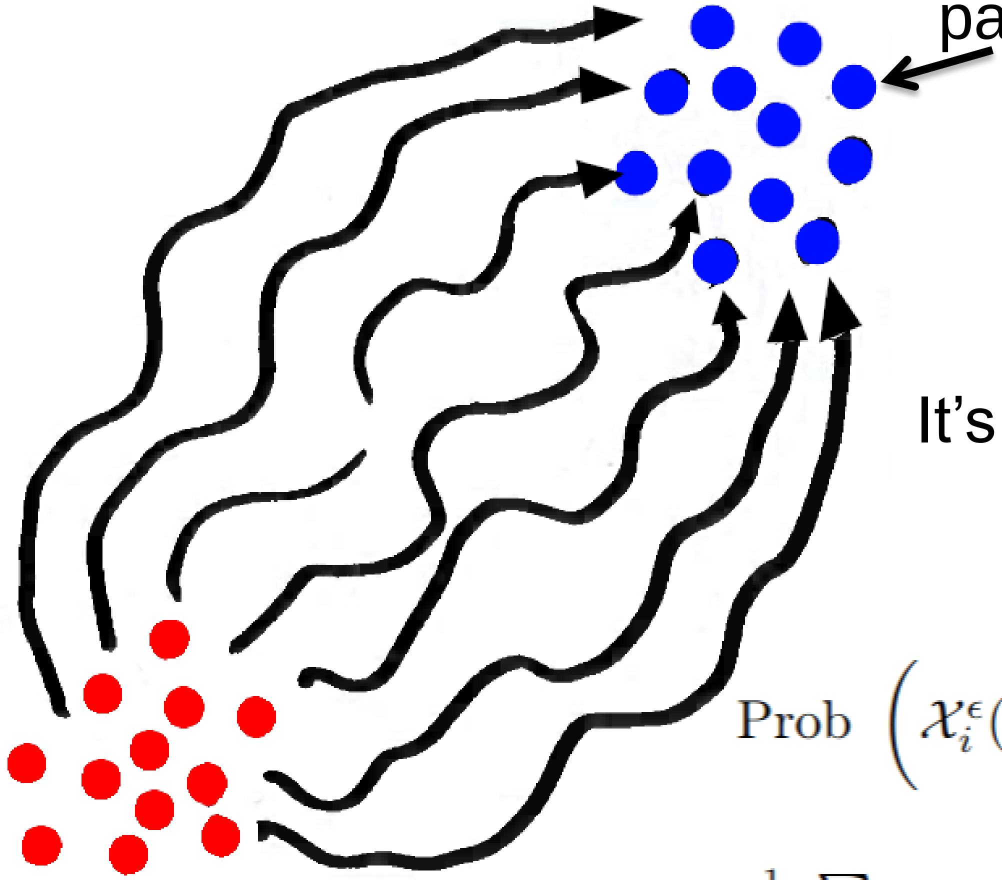


Probability of observing the particles here after T seconds:

$$\text{Prob}\left(\mathcal{X}_i^\epsilon(T) \underset{perm}{\approx} Y\right) \approx$$

$$\frac{1}{M!}\sum_{\sigma\in S_M}\exp\left[\frac{-\sum_i |Y_{\sigma(i)}-X_i^0|^2}{2\epsilon T}\right](2\pi\epsilon T)^{-\frac{3M}{2}}$$

5. Large Deviation Principle



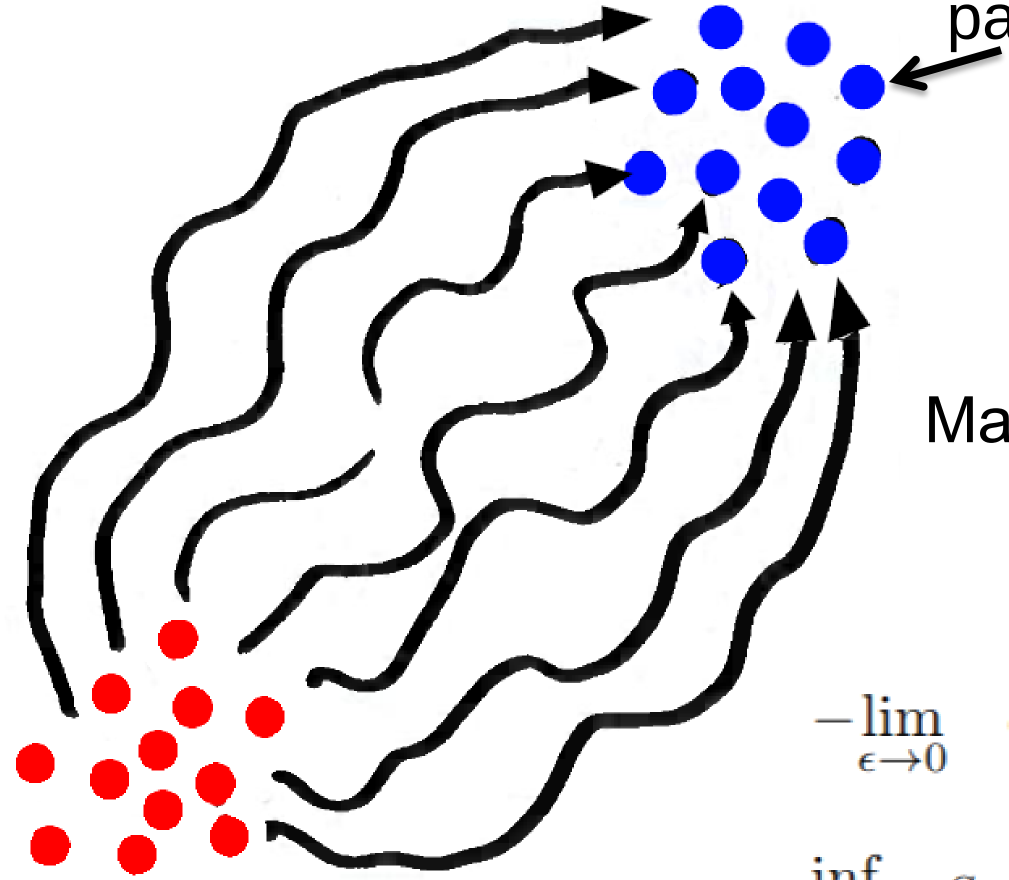
Probability of observing the particles here after T seconds:

It’s a soft inf !

$$\mathrm{Prob}\left(\mathcal{X}_i^\epsilon(T) \underset{perm}{\approx} Y\right) \approx$$

$$\frac{1}{M!}\sum_{\sigma\in S_M}\exp\left[\frac{\boxed{-\sum_i |Y_{\sigma(i)}-X_i^0|^2}}{2\epsilon T}\right](2\pi\epsilon T)^{-\frac{3M}{2}}$$

5. Large Deviation Principle



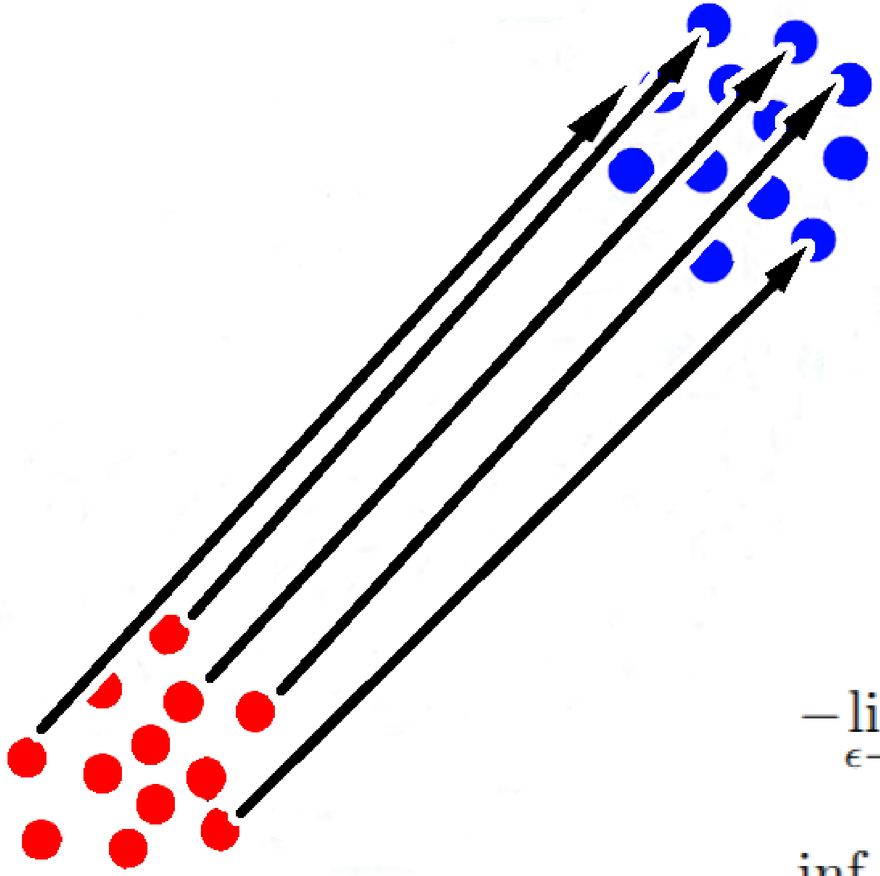
Probability of observing the particles here after T seconds:

Make “temperature” ϵ tend to 0:

$$-\lim_{\epsilon\to 0} \epsilon \log \mathrm{Prob}\left[\mathcal{X}_i^\epsilon(T) \underset{perm}{\approx} Y\right] \approx$$

$$\inf_{\sigma\in S_N}\left[\frac{\sum_i |Y_{\sigma(i)}-X_i^0|^2}{2T}\right]$$

5. Large Deviation Principle

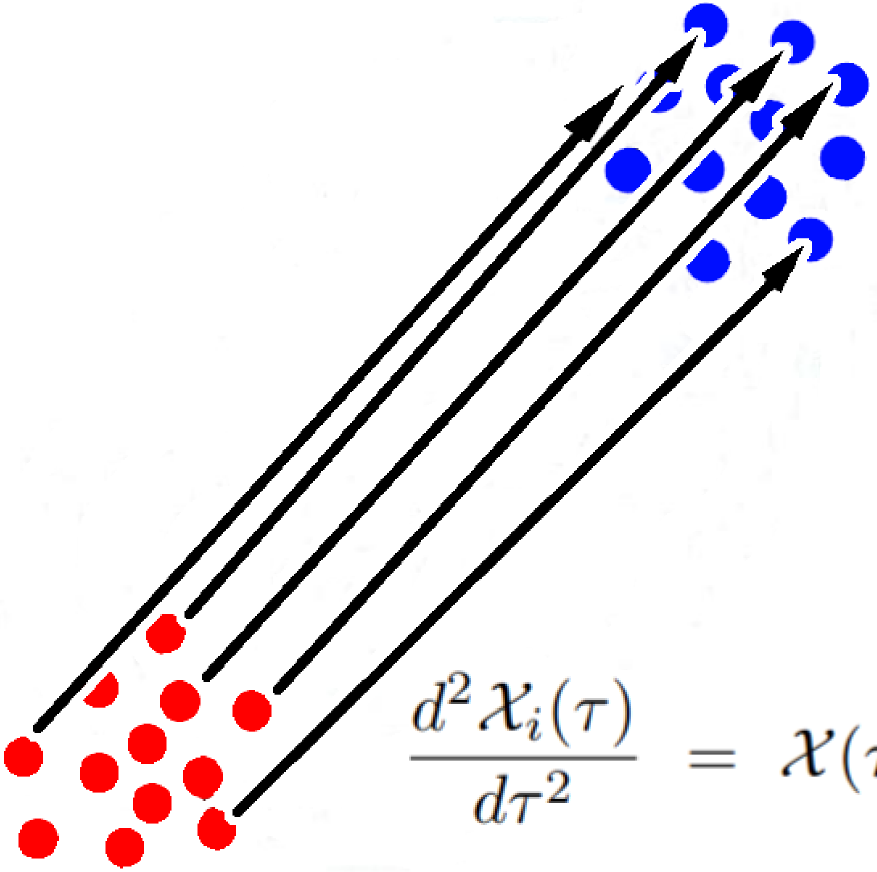


Trajectories become geodesics

$$-\lim_{\epsilon \to 0} \epsilon \log \mathrm{Prob}\left[\mathcal{X}_i^\epsilon(T) \underset{perm}{\approx} Y\right] \approx$$

$$\inf_{\sigma \in S_N}\left[\frac{\sum_i |Y_{\sigma(i)} - X_i^0|^2}{2T}\right]$$

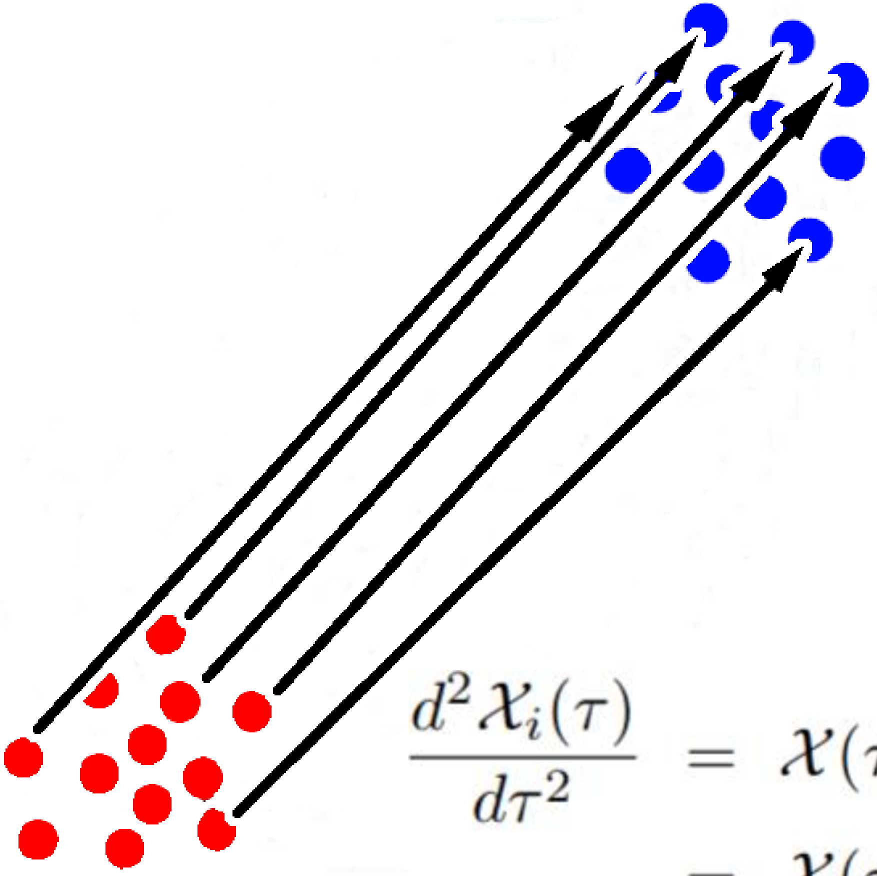
5. Large Deviation Principle



Along these geodesics:

$$\frac{d^2\mathcal{X}_i(\tau)}{d\tau^2} = \mathcal{X}(\tau) - \mathbf{q}_{(\sigma|\mathcal{X}(\tau))(i)}$$

5. Large Deviation Principle



Along these geodesics:

$$\begin{aligned}\frac{d^2\mathcal{X}_i(\tau)}{d\tau^2} &= \mathcal{X}(\tau) - \mathbf{q}_{(\sigma|\mathcal{X}(\tau))(i)} \\ &= \mathcal{X}(\tau) - \nabla\Phi(\mathcal{X}(t)) = -\nabla\phi(\mathcal{X}(\tau))\end{aligned}$$

1. Newton

$$F = -\mathcal{G}\frac{m_1 m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

$$\begin{cases} F & = & \nabla\phi \\ \Delta\phi & = & 4\pi\mathcal{G}(\rho - \bar{\rho}) \end{cases}$$

2. Brenier-Monge-Ampère

$$\begin{cases} F & = & \nabla\Phi \\ \Delta\!\!\Delta\Phi & = & \frac{\rho}{\bar{\rho}} \\ \Phi & = & \frac{\phi}{4\pi\mathcal{G}\bar{\rho}} + \frac{|\mathbf{r}|^2}{2} \end{cases}$$

3. Optimal Transport

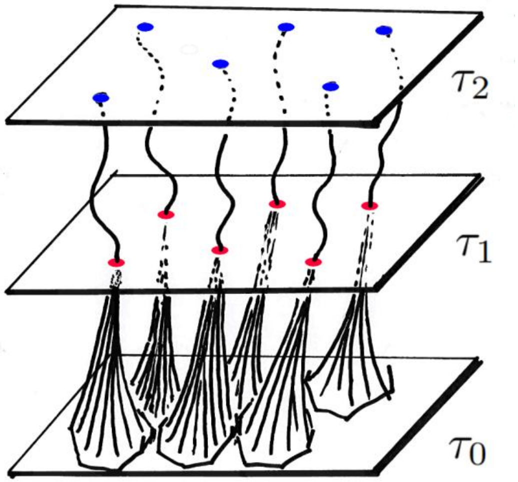
$$T \quad = \quad \nabla\Phi$$

$$\inf_T \left[\int_V |\mathbf{r} - T(\mathbf{r})|^2 \rho(\mathbf{r}) d\mathbf{r} \right]$$

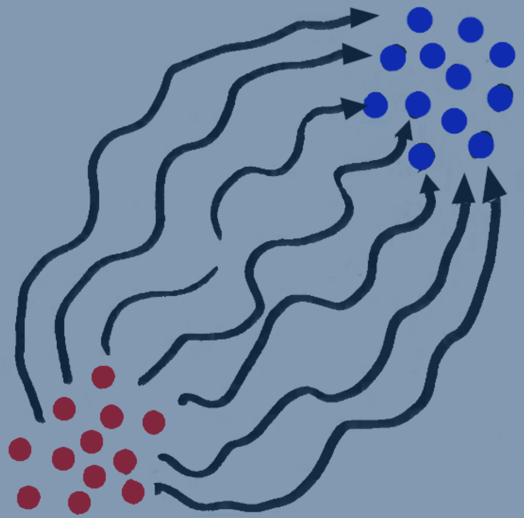
subject to:

$$\int_B \bar{\rho} d\mathbf{q} = \int_{T^{-1}(B)} \rho(\mathbf{r}) d\mathbf{r} \quad \forall B$$

6. The Path Bundle Method

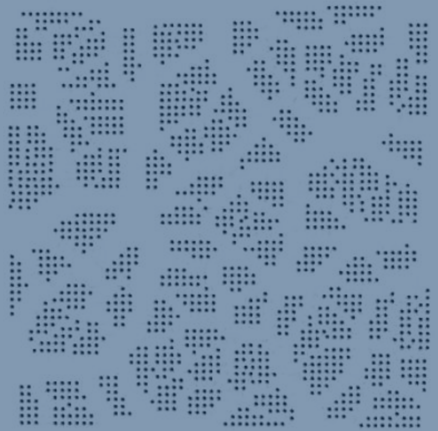


5. Large Deviations Pple.

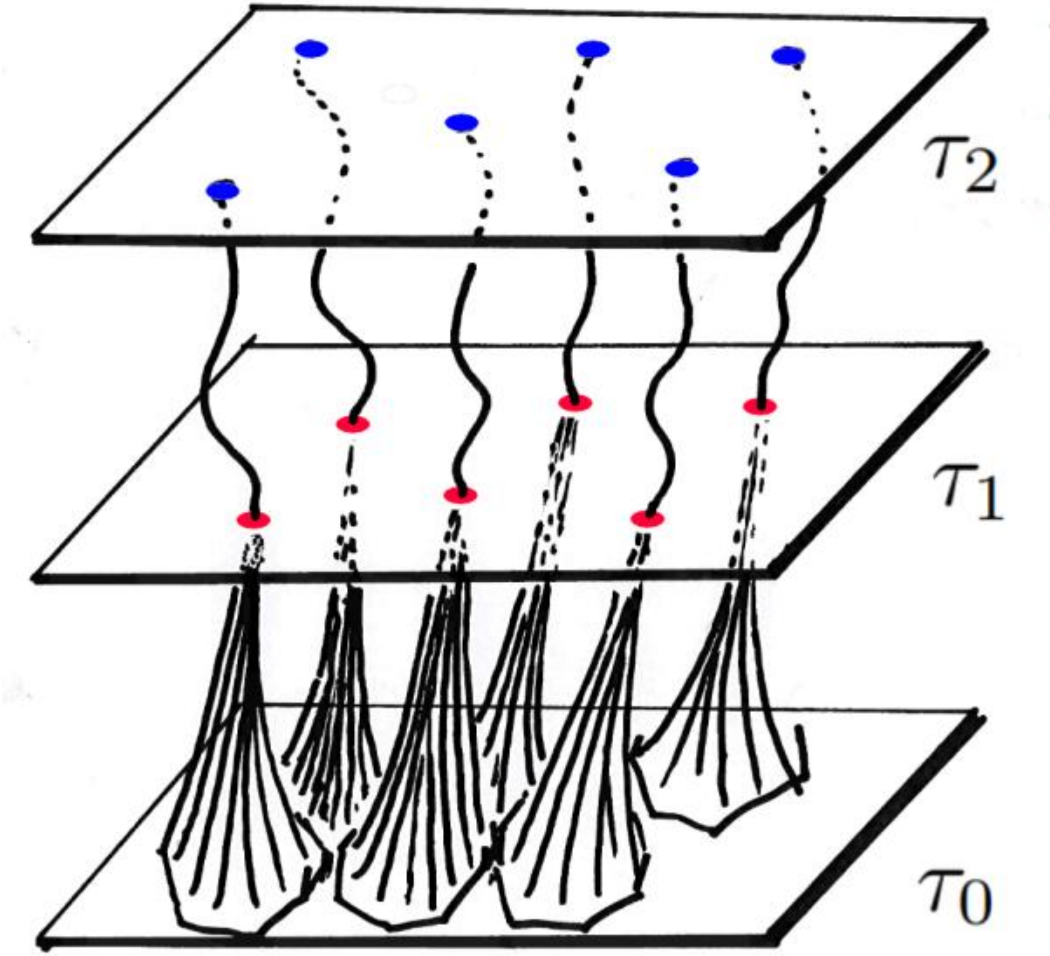


4. Discrete Optimal Transp.

$$\inf_{\sigma \in S_N} \left[\left| \mathbf{r}_i - \mathbf{q}_{\sigma(i)} \right|^2 \right]$$

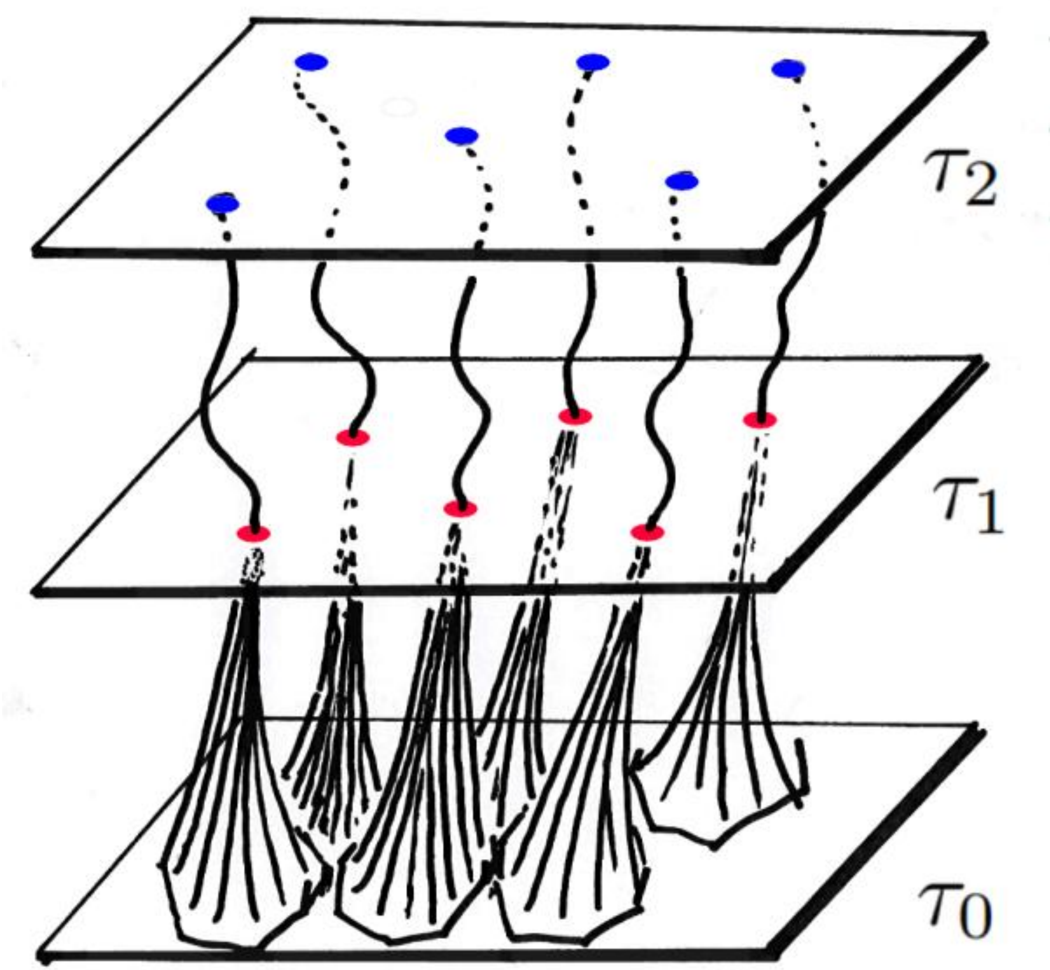


6. The Path Bundle Method



Initial condition (homogeneous)

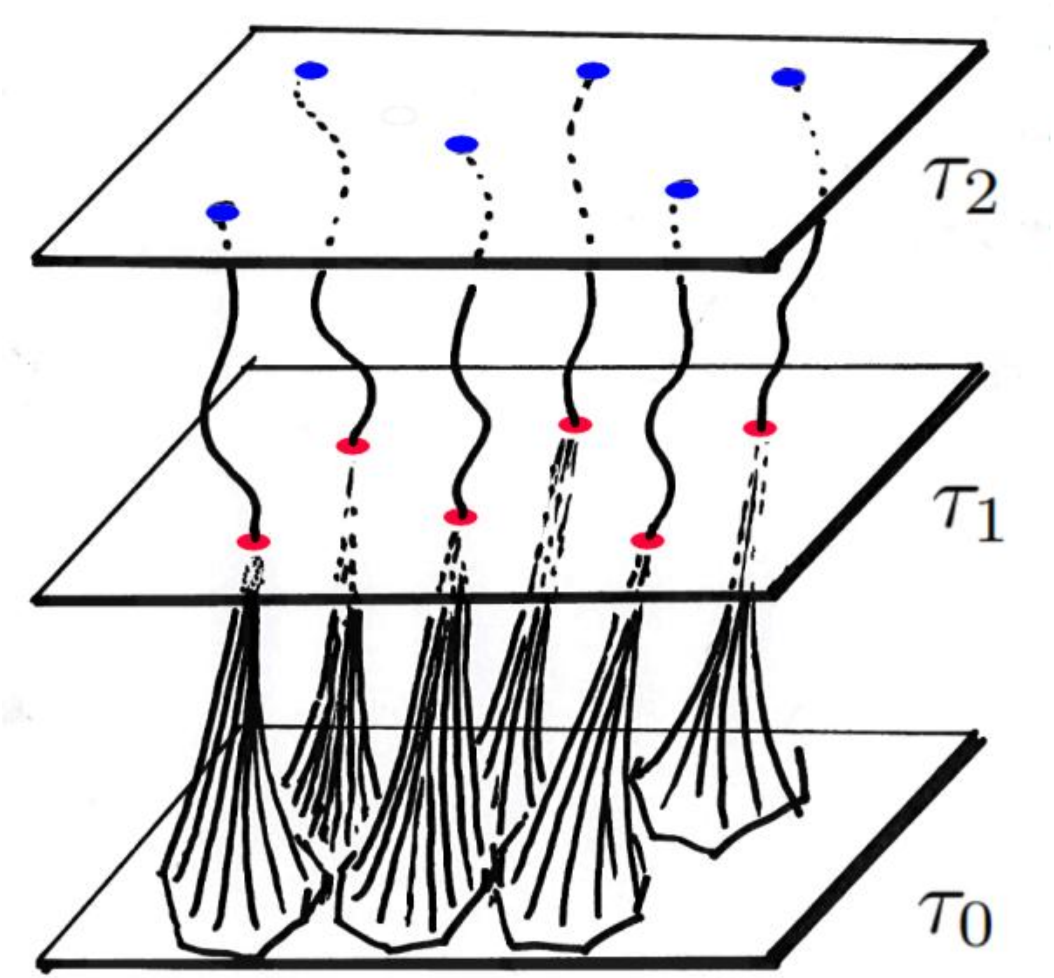
6. The Path Bundle Method



Structures formation

Initial condition (homogeneous)

6. The Path Bundle Method



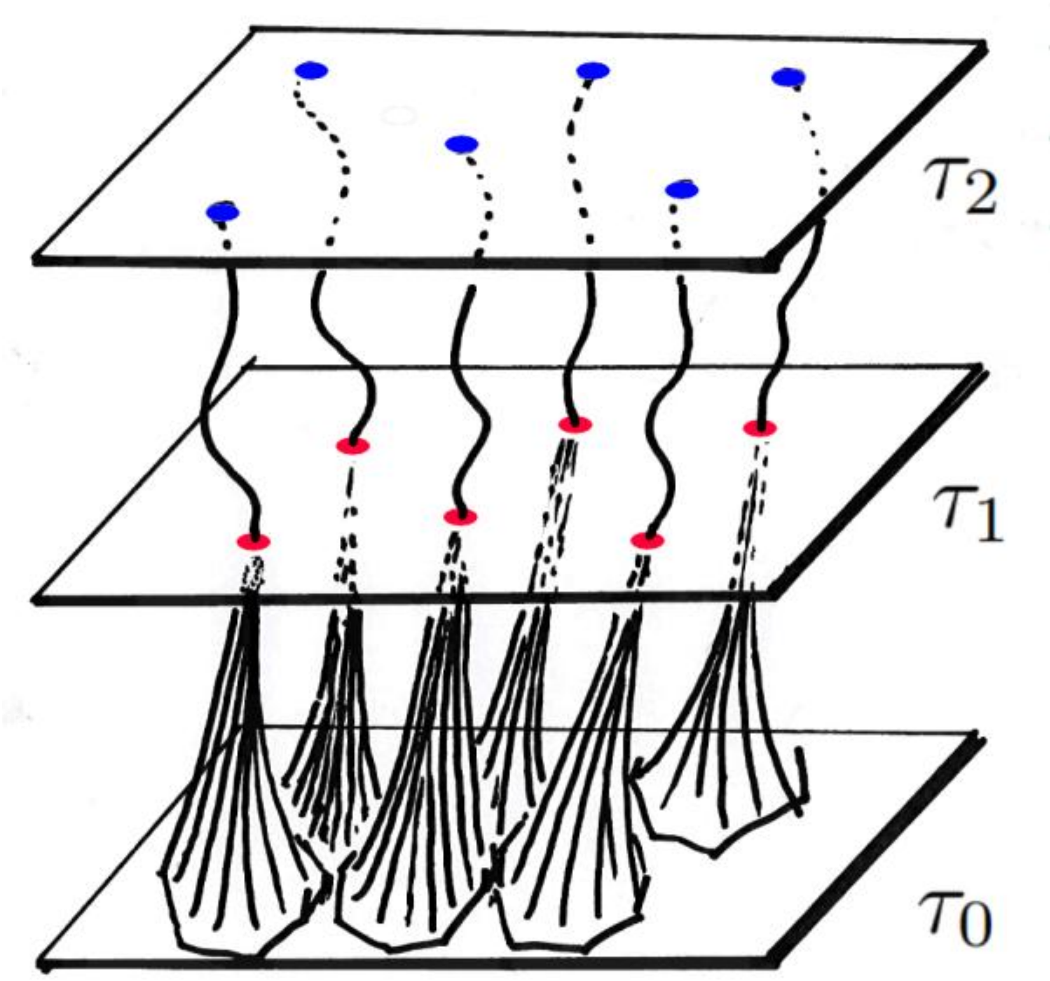
Observation

Structures formation

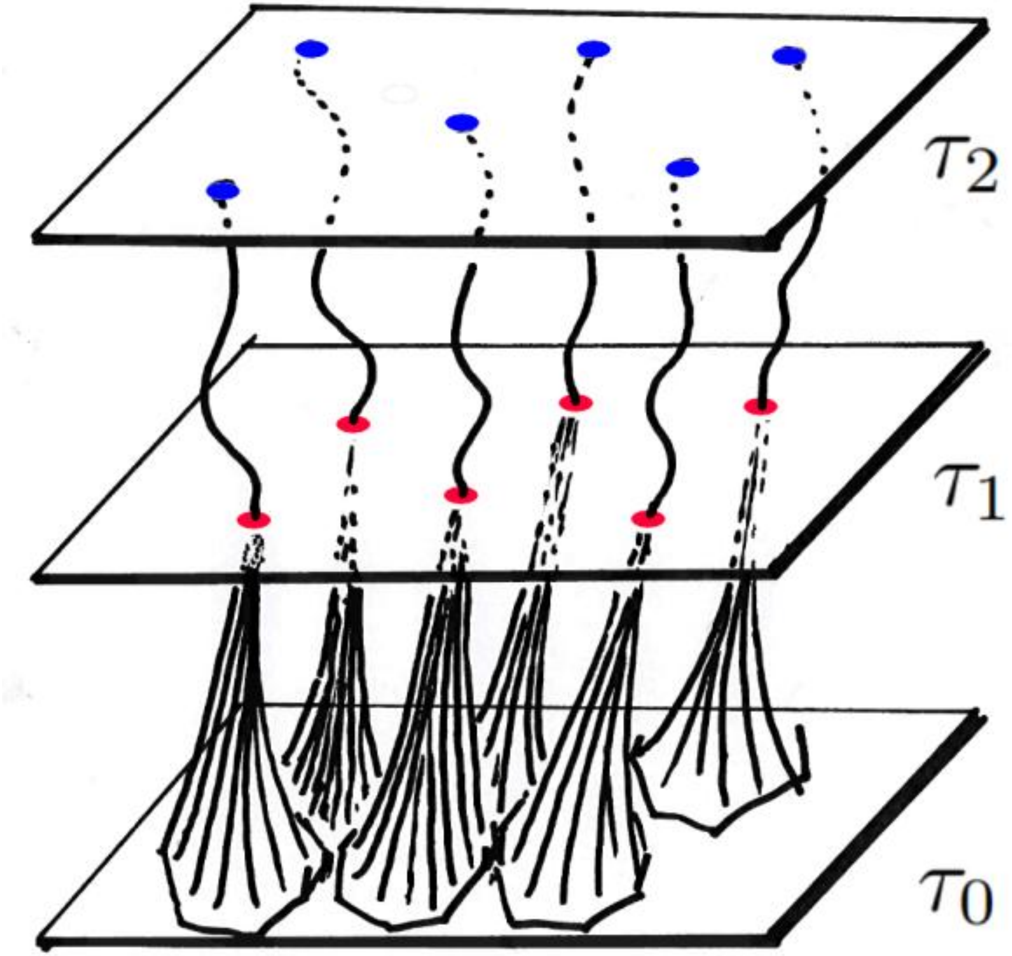
Initial condition (homogeneous)

6. The Path Bundle Method

$$\frac{d^2\mathbf{r}_i(\tau)}{d\tau^2} = F_i(\tau)$$



6. The Path Bundle Method



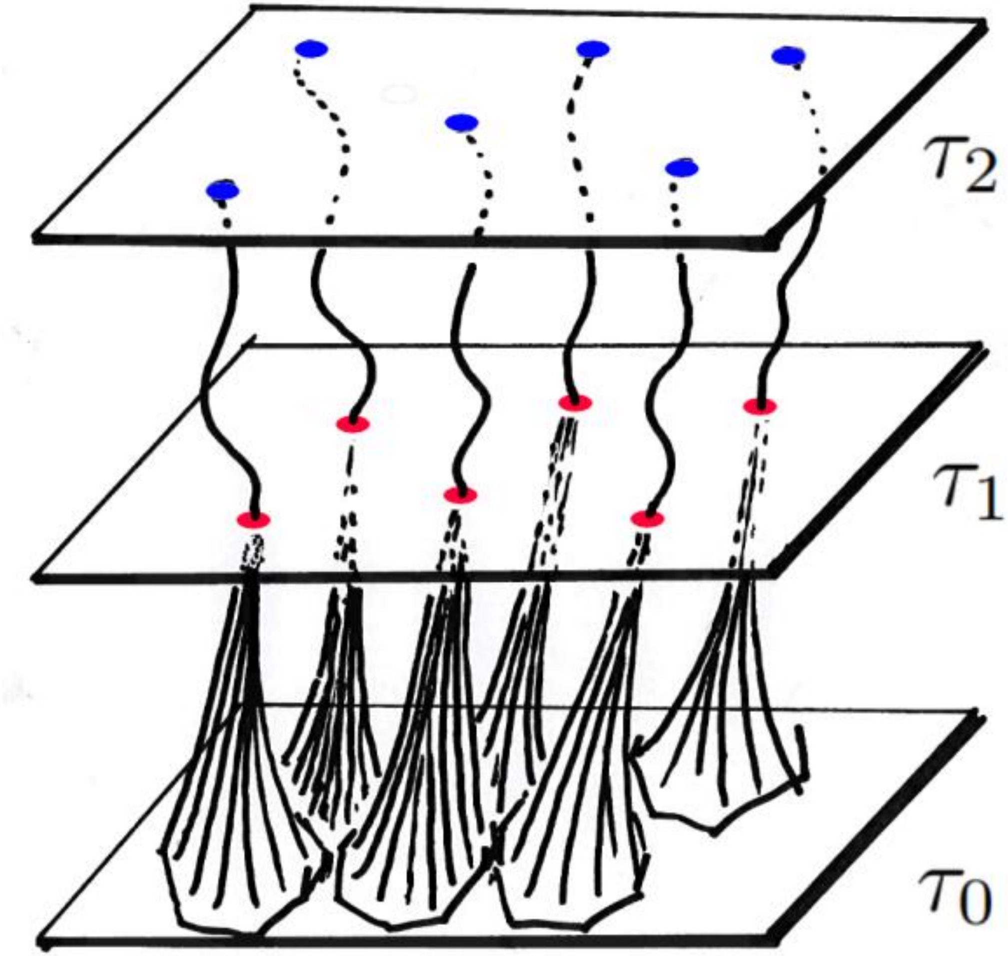
$$\frac{d^2\mathbf{r}_i(\tau)}{d\tau^2} = F_i(\tau)$$

$$\begin{aligned} F_i(\tau) &= -\nabla\phi(\tau) \\ &= \mathbf{r}_i - \nabla\Phi(\mathbf{r}_i, \tau) \end{aligned}$$

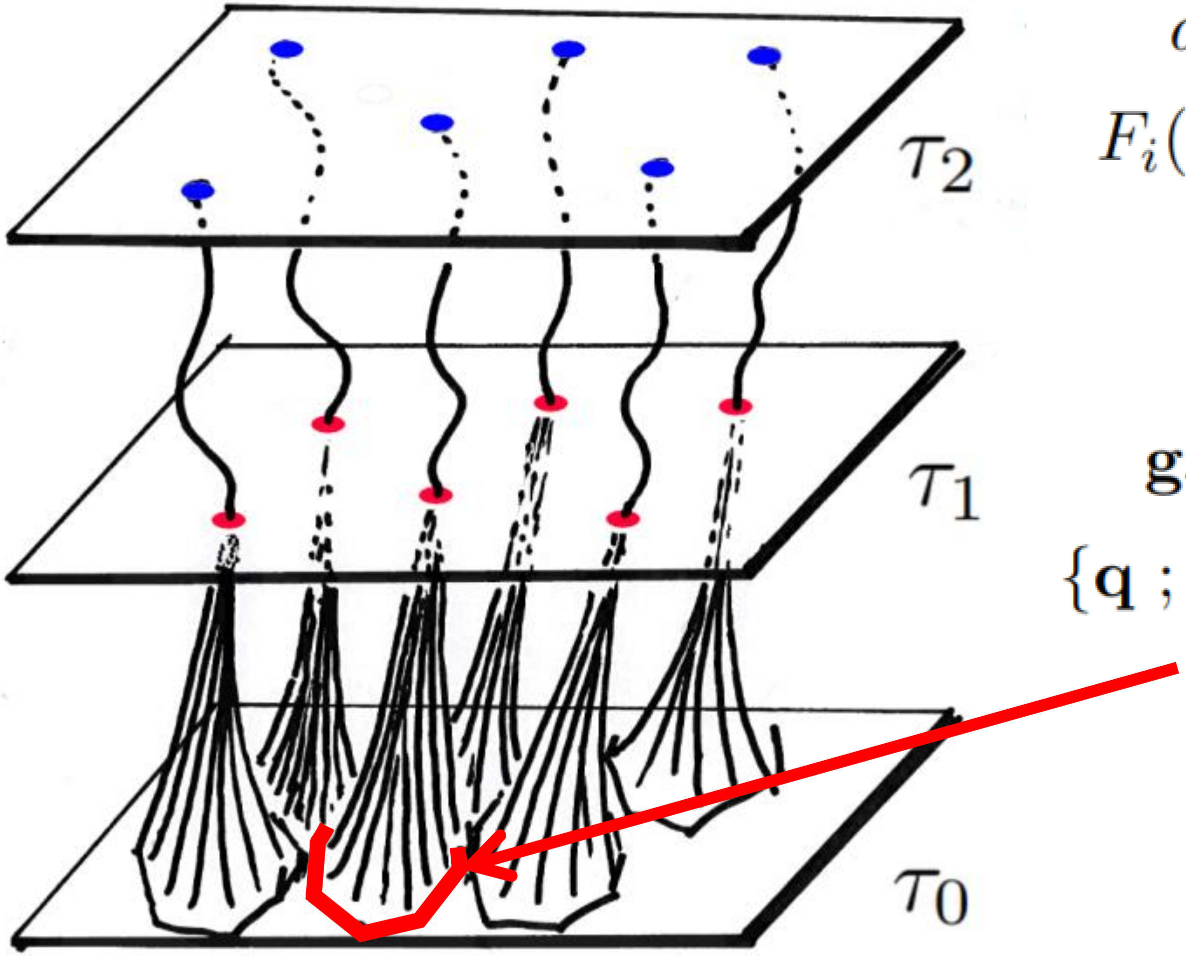
6. The Path Bundle Method

$$\frac{d^2\mathbf{r}_i(\tau)}{d\tau^2} = F_i(\tau)$$

$$\begin{aligned} F_i(\tau) &= -\nabla\phi(\tau) \\ &= \mathbf{r}_i - \nabla\Phi(\mathbf{r}_i, \tau) \\ &= \mathbf{r}_i(\tau) - \mathbf{g}_i(\tau) \end{aligned}$$



6. The Path Bundle Method



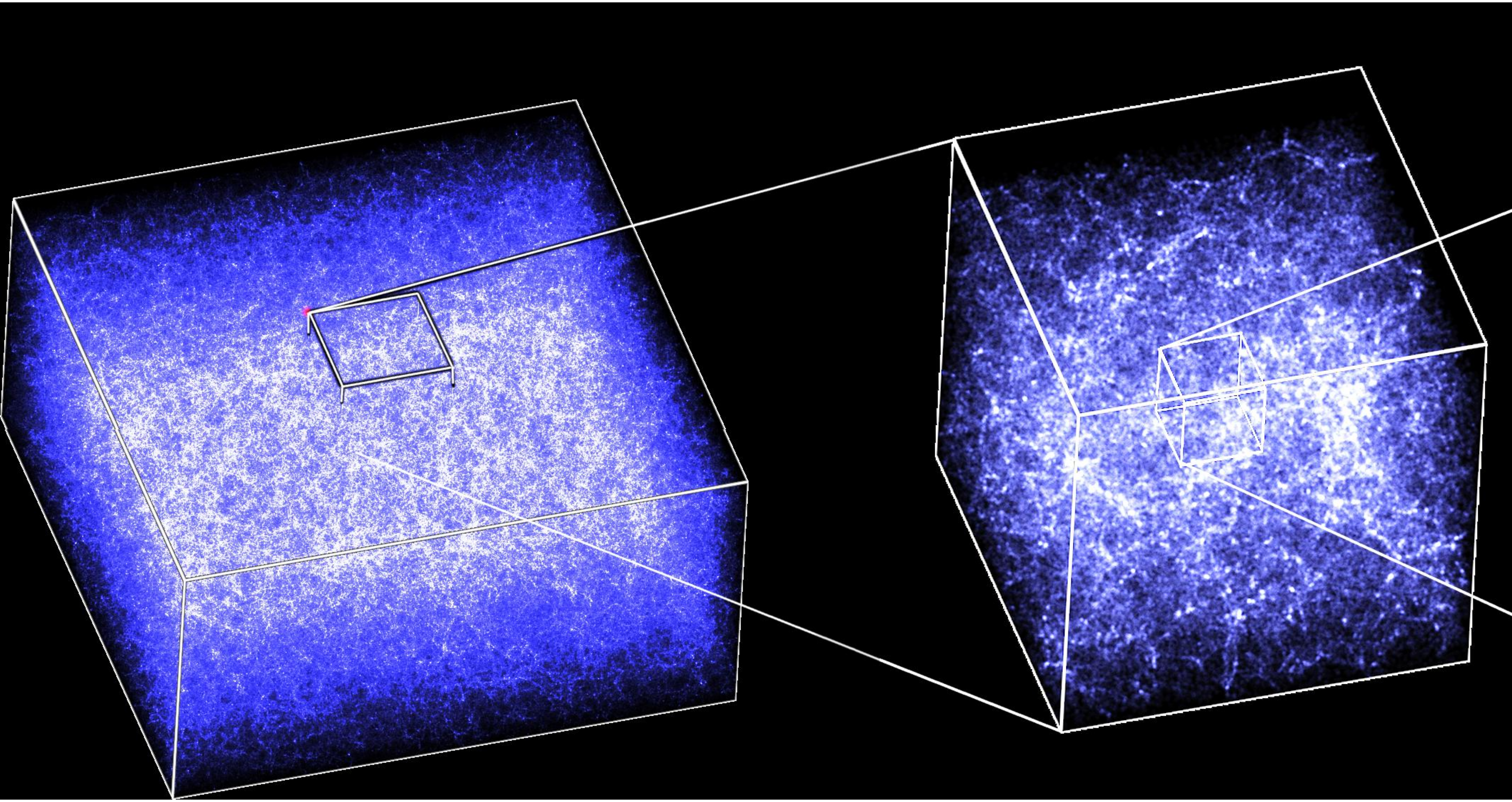
$$\frac{d^2\mathbf{r}_i(\tau)}{d\tau^2} = F_i(\tau)$$

$$\begin{aligned} F_i(\tau) &= -\nabla\phi(\tau) \\ &= \mathbf{r}_i - \nabla\Phi(\mathbf{r}_i,\tau) \\ &= \mathbf{r}_i(\tau) - \mathbf{g}_i(\tau) \end{aligned}$$

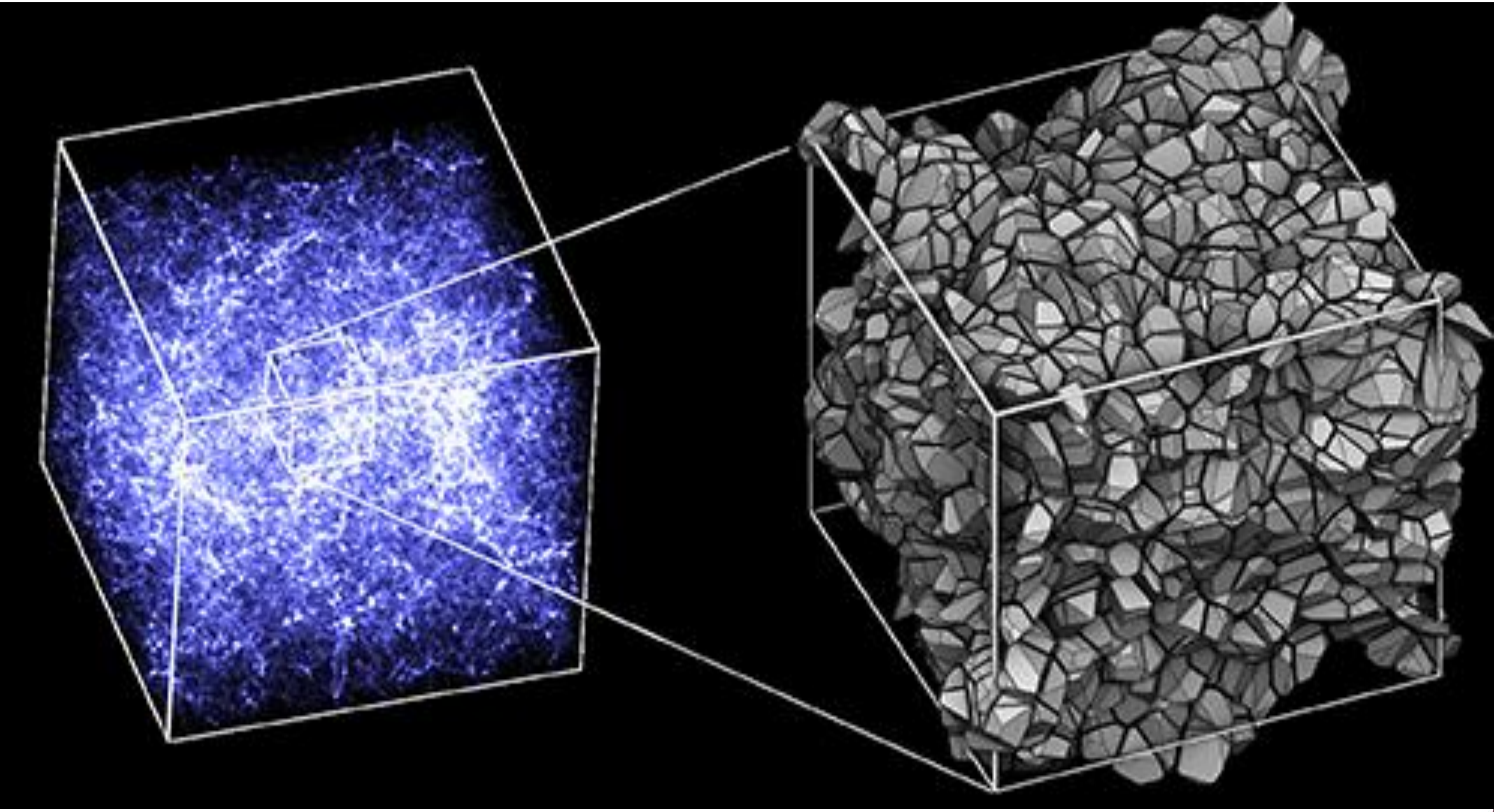
$\mathbf{g}_i(\tau)$: barycenter of

$$\{\mathbf{q}\ ;\ |\mathbf{q}-\mathbf{r}_i|^2 - \phi_i \leq |\mathbf{q}-\mathbf{r}_j|^2 - \phi_j \quad \forall 1 \leq j \leq N\}$$

6. The Path Bundle Method



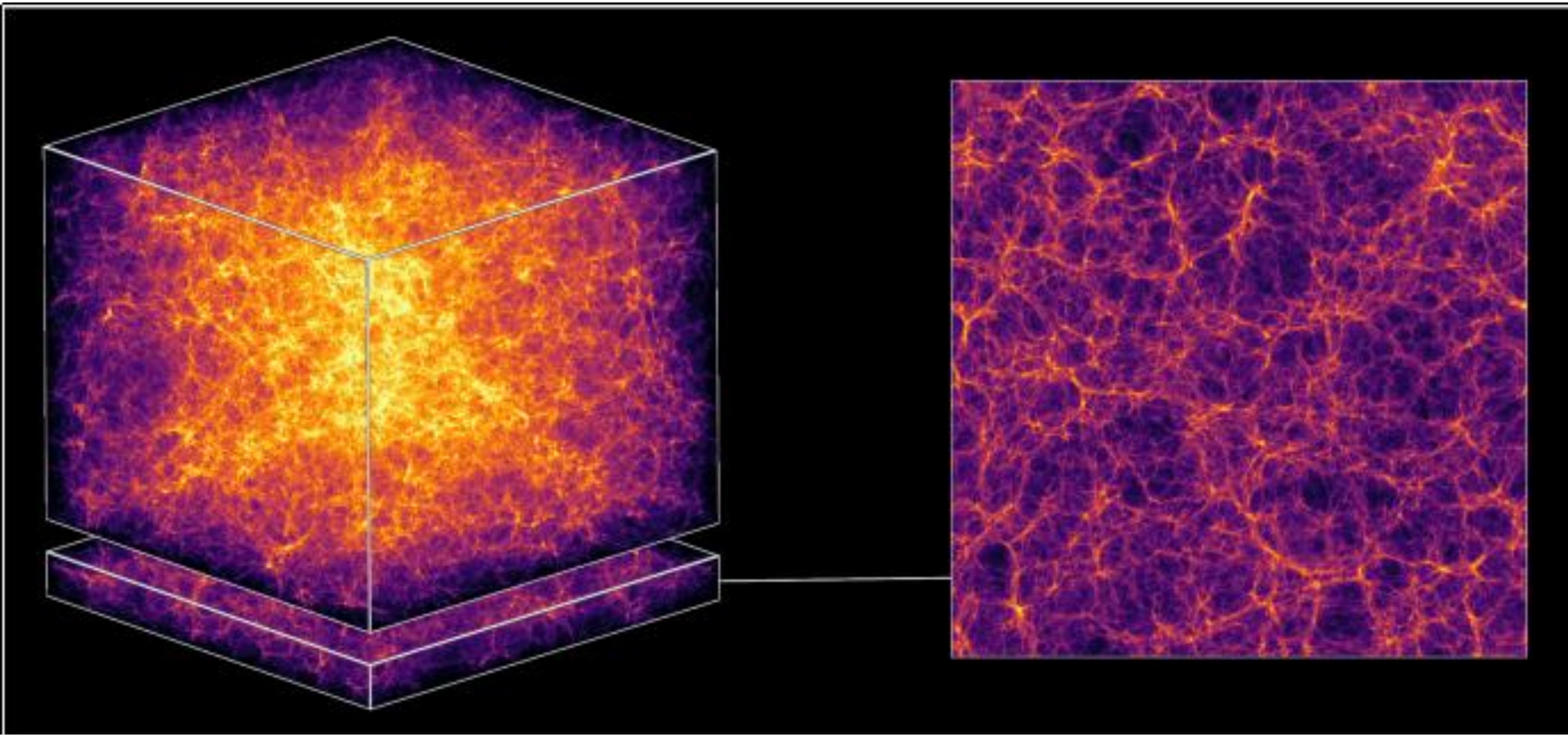
6. The Path Bundle Method



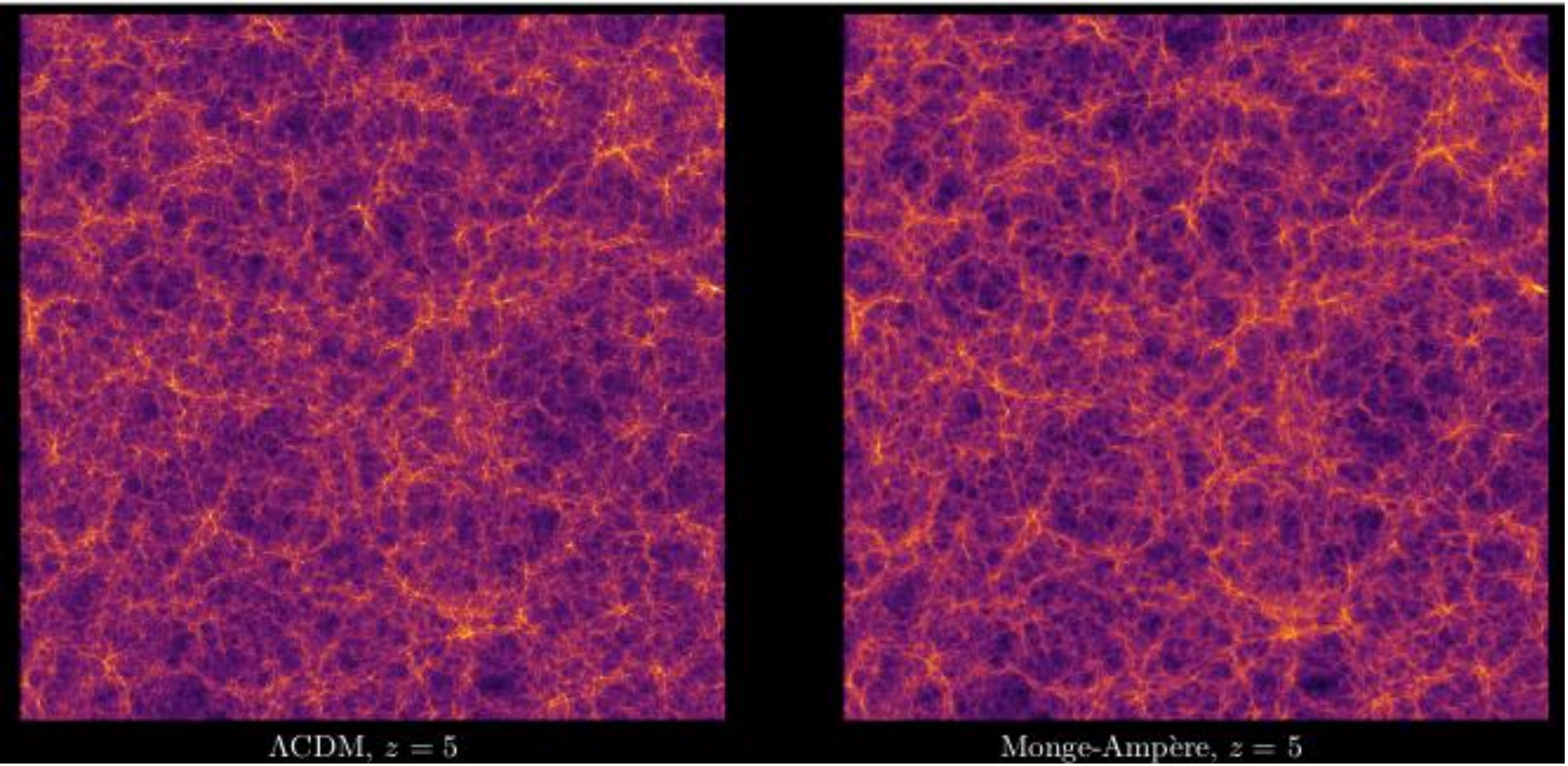
Results – Cosmological simulation

- 150 million particles
- 300 Mpc/h
- Λ-CDM initial conditions [Planck]
- Newton-Poisson and BMAG

Results – Simulation with 300 M cells

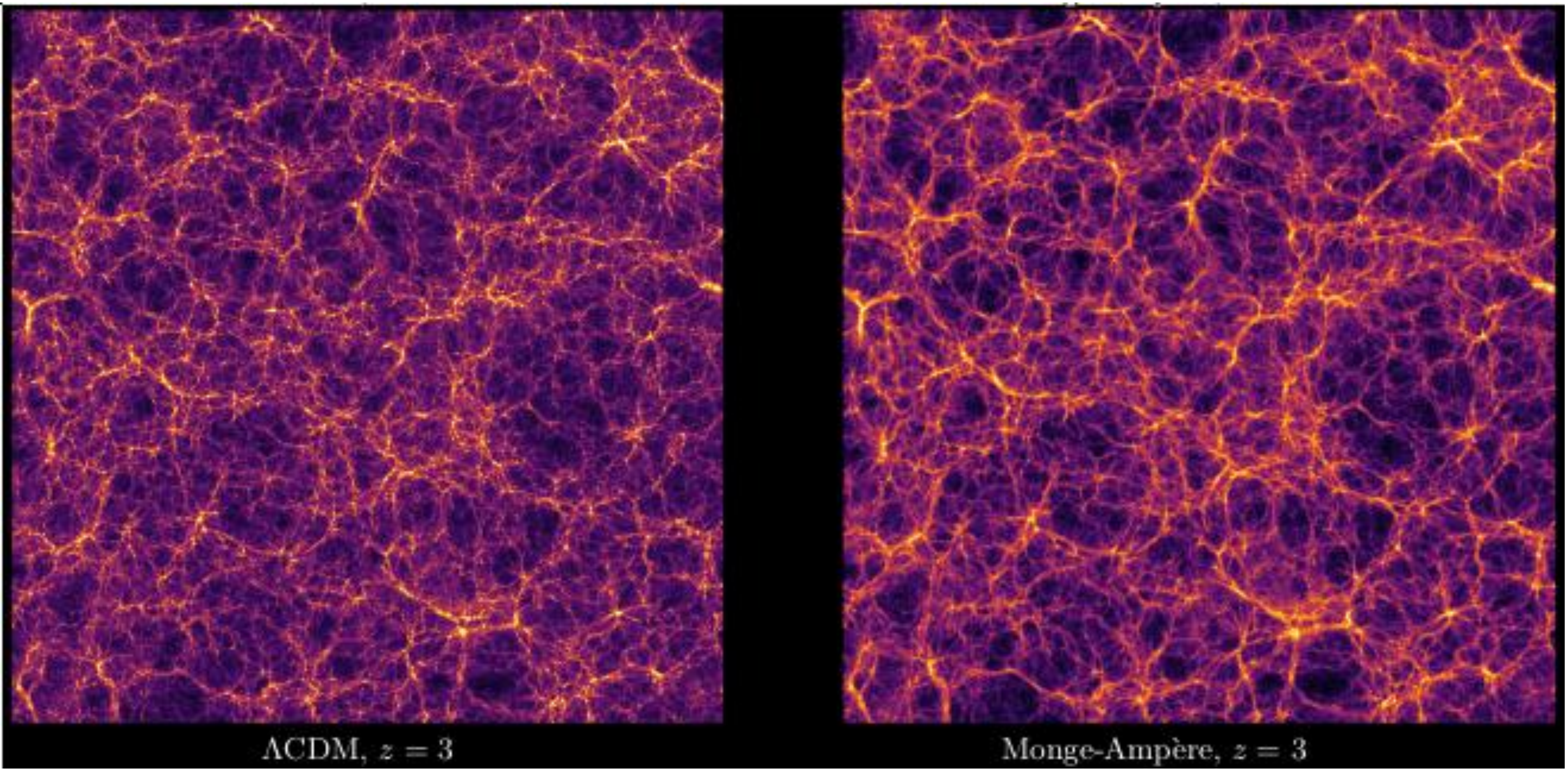


Results – Simulation with 300 M cells

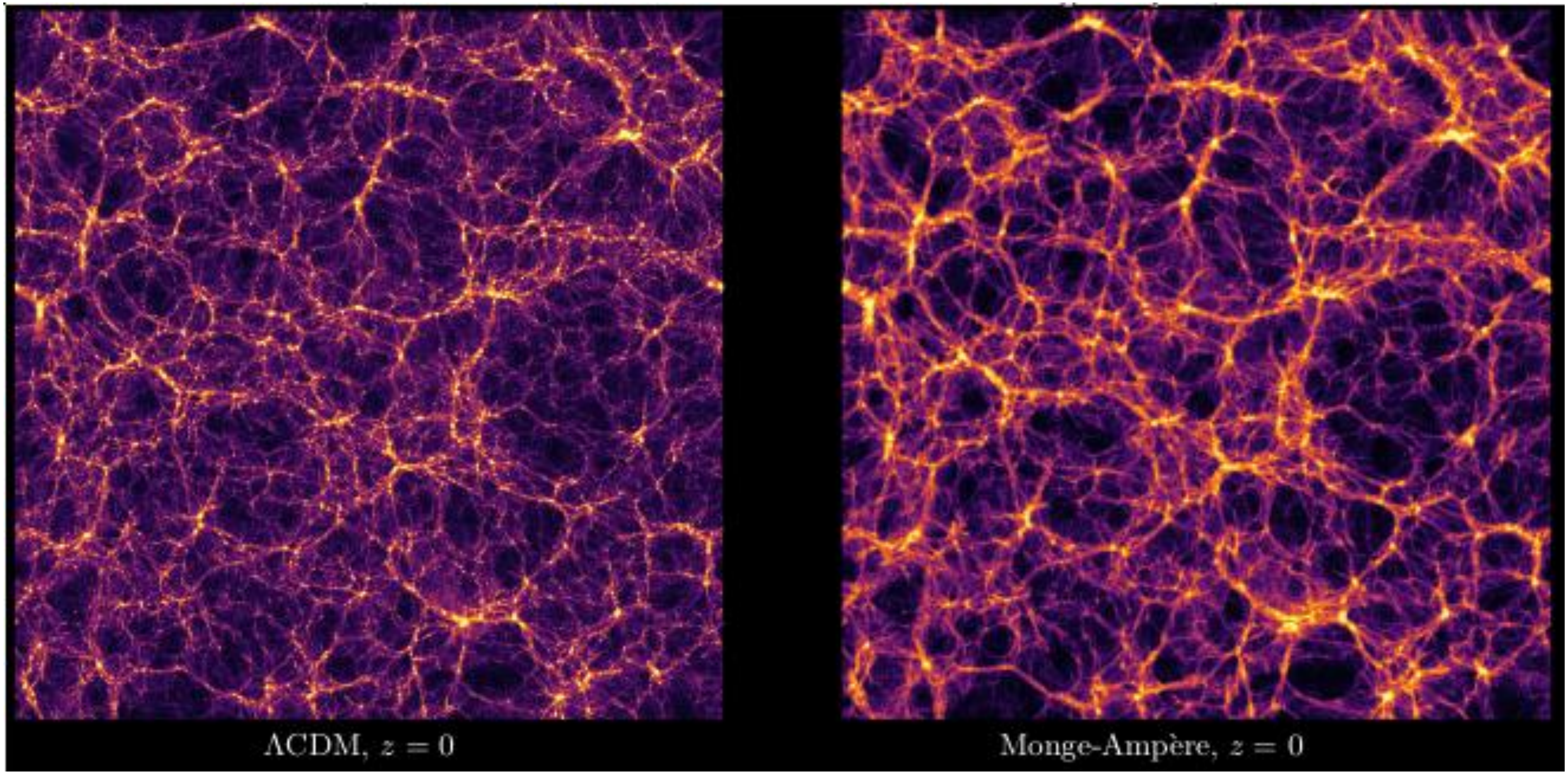


ΛCDM, $z = 5$ Monge-Ampère, $z = 5$

Results – Simulation with 300 M cells



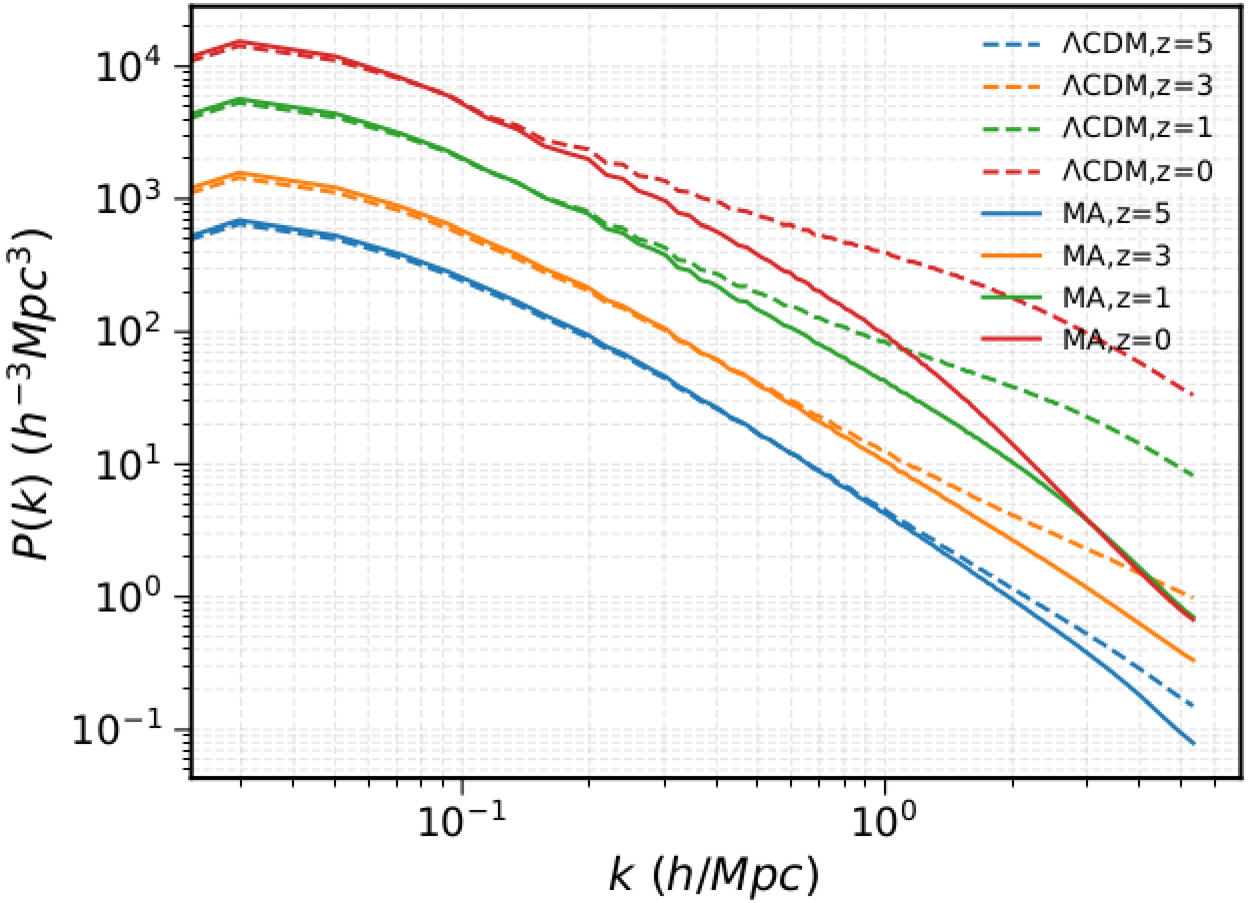
Results – Simulation with 300 M cells

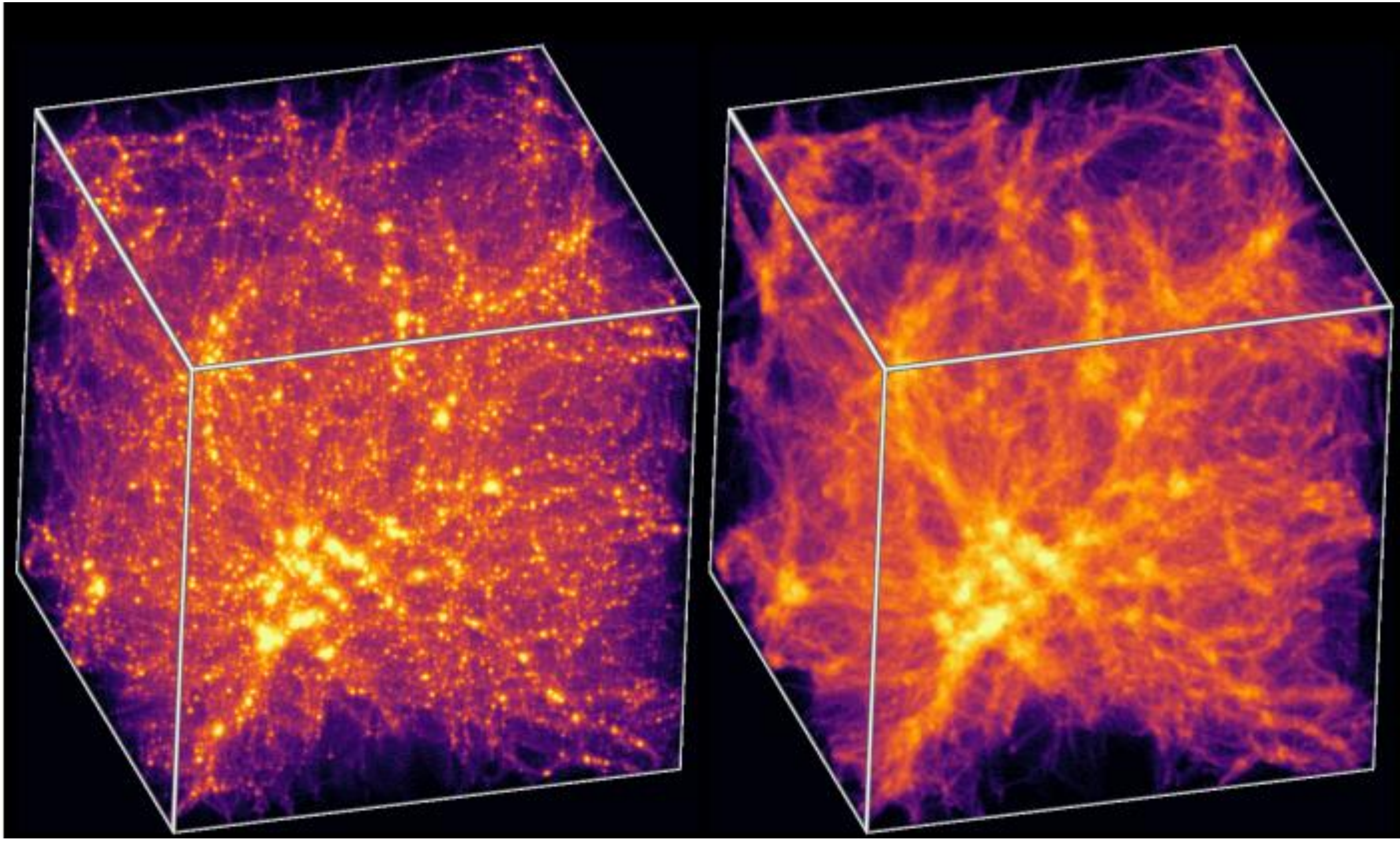


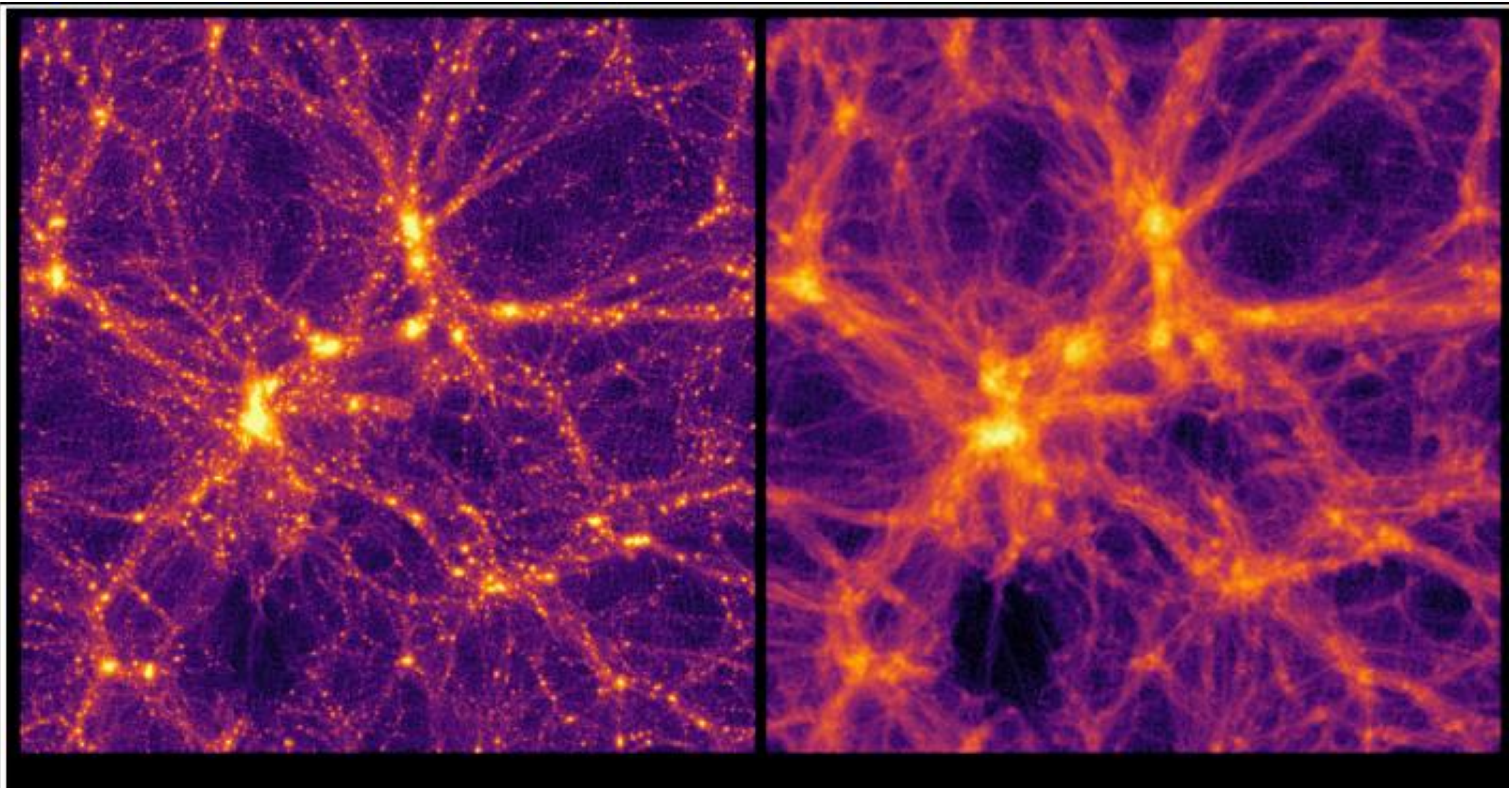
ΛCDM, $z = 0$

Monge-Ampère, $z = 0$

Results – Simulation with 300 M cells







Results – Conclusions

BMAG is a small *non-linear* modification of Newtonian dynamics

Differences:

- Larger number of filaments
- Smaller number of small haloes
- Haloes spin faster. Origin of angular momentum of disk galaxies ?
- Centrail density profile of haloes is flatter
- More power on large scales and less power on small scales

Results – Conclusions

BMAG is a small *non-linear* modification of Newtonian dynamics

Differences:

- Larger number of filaments
- Smaller number of small haloes
- Haloes spin faster. Origin of angular momentum of disk galaxies ?
- Centrail density profile of haloes is flatter
- More power on large scales and less power on small scales

Can be falsified with future observational surveys

Results – Conclusions

BMAG is a small *non-linear* modification of Newtonian dynamics

Differences:

- Larger number of filaments
- Smaller number of small haloes
- Haloes spin faster. Origin of angular momentum of disk galaxies ?
- Centrail density profile of haloes is flatter
- More power on large scales and less power on small scales

Can be falsified with future observational surveys

Questions:

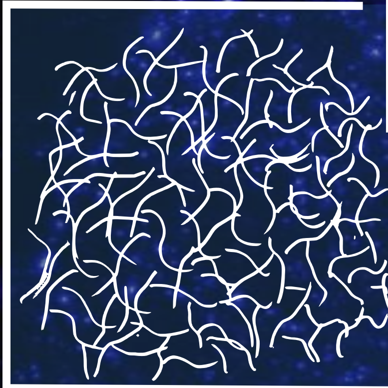
- BMAG as the weak field limit of another strong-field theory ?
- BMAG emerging from GR (or other modified theories of gravity) ?
- Entropic gravity ?

Future works:

Exploring the shape of the Universe

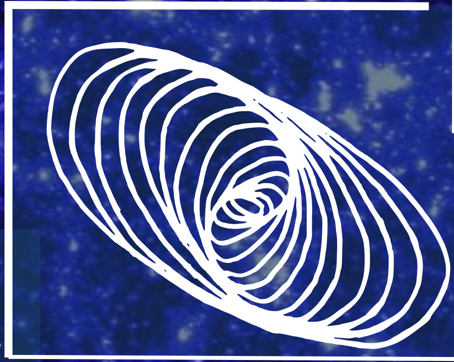
Geometric complexity

A **Large Scale Structure**
3D, Euclidean



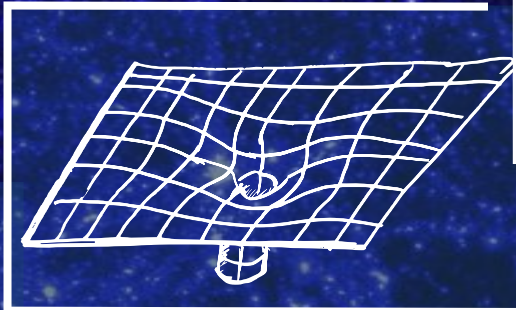
L = 1 GPc/h *N = 10^9*

B **Galactic dynamics**
6D phase space



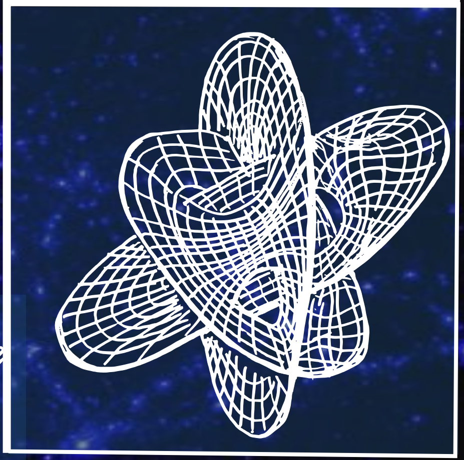
L = 1 kPc/h *N = 10^6*

C **General Relativity**
4D, Riemannian



L = 1 Pc/h *N = 1 … 10*

D **Calabi-Yau Manifolds**
10D, Complex



L = Planck

Scale

References on Cosmology and OT

Nature 2002, Frisch, Matarrese, Mohayaee, Sobolevski
MNRAS 2003, Brenier, Frisch, Henon, Loeper, Matarrese, Mohayaee, Sobolevski
Geom. & Func. Ana., 2004, Brenier
Confluentes Math, 2011, Brenier
Analysis & PDE, 2023, Ambrosio, Baradat and Brenier
JEMS, 2019, Kitagawa, Merigot, Thibert

MNRAS 2021, **L**, Mohayaee, von Hausegger
Physical Review Letters 2021, von Hausegger, **L**, Mohayaee
Journal of Computational Physics 2022, **L**
Physical Review Letters 2022, Nikhaktar, Sheth, **L**, Mohahayee
Physical Review D, 2023, Nikhaktar, Padmanabhan, **L**, Sheth, Mohayaee
Physical Review D, 2024, Nikhaktar, Padmanabhan, **L**, Sheth, Mohayaee
Physical Review D, 2024, **L,** Brenier, Mohayaee
Journal of Computational Physics, **L** (pending major revision)
submitted, Dapogny, **L**, Oudet

Acknowledgements
This is joint work with :

Yann Brenier
Charles Dapogny
Sebastian von Hausegger
Hugo Leclerc,
Quentin Merigot
Roya Mohayaee
Farnik Nikhaktar,
Edouard Oudet,
Nikhik Padmanhaban
Nicolas Ray,
Ravi Sheth

COSMOGRAM-Launchpad Action Exploratoire Inria