

The melting Rubik cube: From Fluids to Combinatorics and vice versa

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THE BIG BANG THEORY!



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Featuring Sheldon Cooper and the melting Rubik's cube...



FROM COMBINATORICS TO FLUIDS AND VICE VERSA

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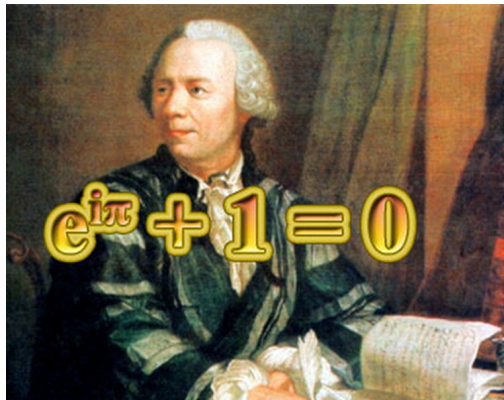
**Optimal transport theory:
convexity and combinatorics.**

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Euler: portrait, bank note and stamp...

XXI. Nous n'avons donc qu'à égaliser ces forces accélératrices avec les accélérations actuelles que nous venons de trouver, & nous obtiendrons les trois équations suivantes :

$$P - \frac{1}{q} \left(\frac{dp}{dx} \right) = \left(\frac{du}{dt} \right) + u \left(\frac{du}{dx} \right) + v \left(\frac{du}{dy} \right) + w \left(\frac{du}{dz} \right)$$

$$Q - \frac{1}{q} \left(\frac{dp}{dy} \right) = \left(\frac{dv}{dt} \right) + u \left(\frac{dv}{dx} \right) + v \left(\frac{dv}{dy} \right) + w \left(\frac{dv}{dz} \right)$$

$$R - \frac{1}{q} \left(\frac{dp}{dz} \right) = \left(\frac{dw}{dt} \right) + u \left(\frac{dw}{dx} \right) + v \left(\frac{dw}{dy} \right) + w \left(\frac{dw}{dz} \right)$$

Si nous ajoutons à ces trois équations premièrement celle, que nous a fournie la considération de la continuité du fluide :

$$\left(\frac{dq}{dt}\right) + \left(\frac{d \cdot q u}{dx}\right) + \left(\frac{d \cdot q v}{dy}\right) + \left(\frac{d \cdot q w}{dz}\right) = 0.$$

Si le fluide n'étoit pas compressible, la densité q seroit la même en Z , & en Z' , & pour ce cas on auroit cette équation :

$$\left(\frac{du}{dx}\right) + \left(\frac{dv}{dy}\right) + \left(\frac{dw}{dz}\right) = 0.$$

qui est aussi celle sur laquelle j'ai établi mon Mémoire latin allégué ci-dessus.

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(Of course, the "source terms" P-Q-R in the Euler equations are usually very difficult to model in numerical codes: they rely on complex thermal exchanges between sun, earth, air and water.)

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In addition, the Euler equations and the companion Navier-Stokes equation are deeply linked to one of the most outstanding open questions in physics:

The understanding of fluid turbulence.

tombent dans la surface même. Or nous voyons par là suffisamment, combien nous sommes encore éloignés de la connoissance complète du mouvement des fluides, & que ce que je viens d'expliquer, n'en contient qu'un foible commencement. Cependant tout ce que la Théorie des fluides renferme, est contenu dans les deux équations rapportées cy-dessus (§. XXXIV.), de sorte que ce ne sont pas les principes de Méchanique qui nous manquent dans la poursuite de ces recherches, mais uniquement l'Analyse, qui n'est pas encore assez cultivée, pour ce dessein : & partant on voit clairement, quelles découvertes nous restent encore à faire dans cette Science, avant que nous puissions arriver à une Théorie plus parfaite du mouvement des fluides.

Euler's conclusion: a mathematical challenge for the future

GEOMETRY OF THE EULER MODEL OF INCOMPRESSIBLE FLOWS.

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According to Arnold, an incompressible fluid, confined in a domain denoted by D and moving according to the Euler equations, just follows a (constant speed) geodesic curve along the manifold of all possible incompressible maps of D .

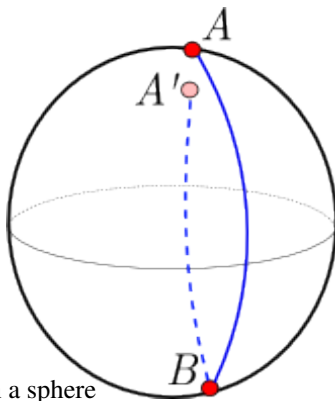
Geometric interpretation of the Euler equations by Arnold, 1966.

VLADIMIR ARNOLD

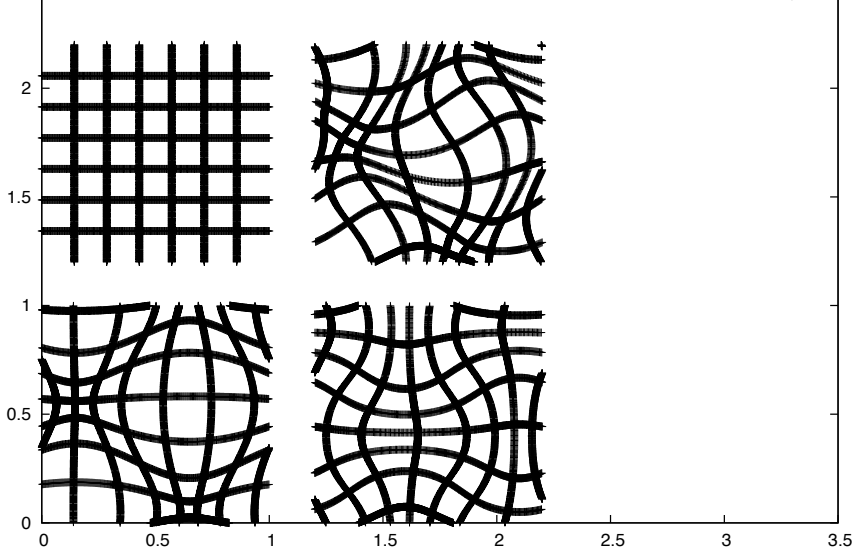
**Sur la géométrie différentielle des groupes de
Lie de dimension infinie et ses applications à
l'hydrodynamique des fluides parfaits**

Annales de l'institut Fourier, tome 16, n° 1 (1966), p. 319-361.

http://www.numdam.org/item?id=AIF_1966__16_1_319_0



Two geodesic curves on a sphere



Three maps of the (periodized) square: only one is incompressible.

From a more concrete and computational viewpoint, it is worth considering the discrete version of an incompressible motion inside D

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FROM COMBINATORICS TO FLUIDS AND VICE VERSA

Example of a discrete incompressible motion with 7 time steps and 12 sub-cells (in line)



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|---|---|---|---|---|---|---|---|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
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7 time steps have been performed.

Time is on vertical axis and space on horizontal axis.

The trajectories of 2 selected sub-cells (4 and 5) are drawn in red.

"transportation cost" to reach the final permutation

| | | | | | | | | | | | |
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The "cost" is obtained by adding up the squares of all displacements at all steps. Here: $12+10+12+42+10+12+10=108$.

"transportation cost" to reach the final permutation

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The "cost" is obtained by adding up the squares of all displacements at all steps. Here: $12+10+12+4+10+12+10=108$. This is the "cost" to reach the final permutation in 7 steps. Notice that step 4 costs a lot!

Obviously, there is at least a solution leading to the final permutation at the lowest possible cost, among the... $(12!)^6 \sim 10^{52}$ possible candidates!

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This is the discrete version of a minimizing geodesic along the semi-group of all volume preserving maps.

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This is what we will do in the second part of the lecture, combining probability and convexity tools.

Exercise: let us try to find a discrete geodesic leading to permutation 12-11-10-9-8-7-6-5-4-3-2-1 using twelve steps

| | | | | | | | | | | | |
|----|----|----|---|---|---|---|---|---|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
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| | | | | | | | | | | | |
| | | | | | | | | | | | |
| 12 | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 |

LET US TRY TO MOVE BY EXCHANGING NEIGHBORS...

| | | | | | | | | | | | |
|----|----|----|---|---|---|---|----|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
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| | | | | | | | | | | | |
| 12 | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 |

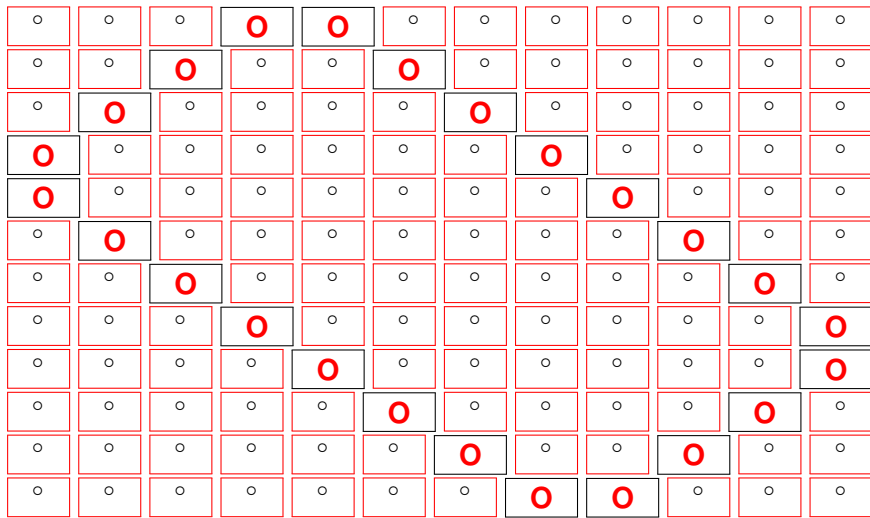
FINALLY ARRIVED...AFTER 12 STEPS.

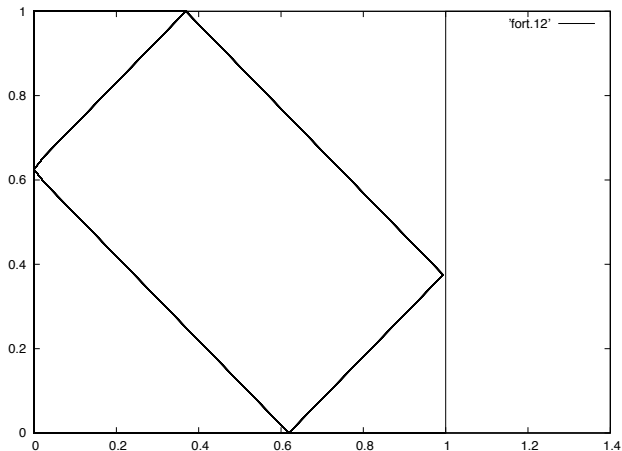
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| 10 | 8 | 12 | 6 | 11 | 4 | 9 | 2 | 7 | 1 | 5 | 3 |
| 10 | 12 | 8 | 11 | 6 | 9 | 4 | 7 | 2 | 5 | 1 | 3 |
| 12 | 10 | 11 | 8 | 9 | 6 | 7 | 4 | 5 | 2 | 3 | 1 |
| 12 | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 |

LET US FOLLOW THE TRAJECTORIES OF TWO NEIGHBOURS: 4 AND 5

| | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|
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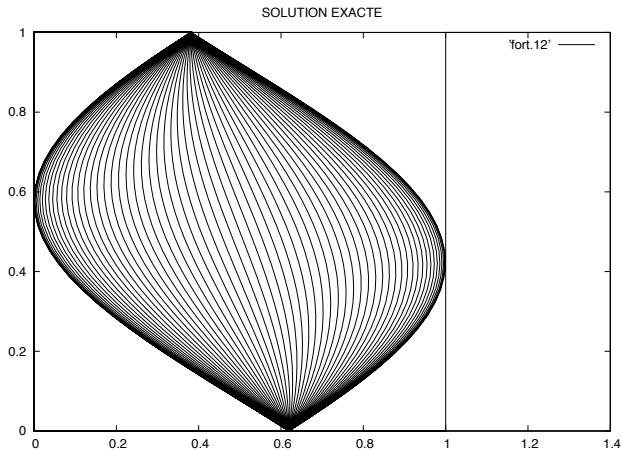
Is it really the lowest possible cost?



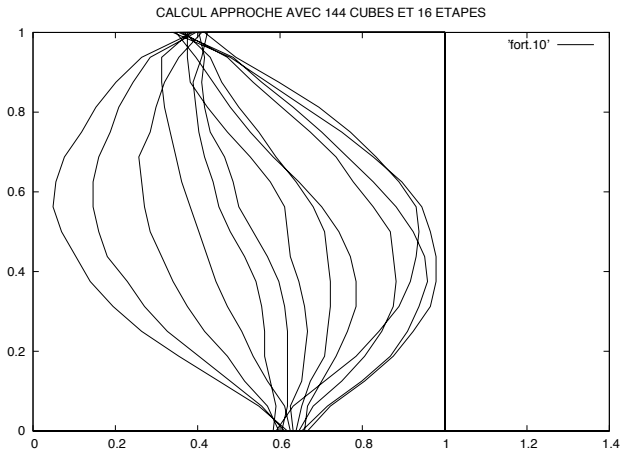


ANYWAY, IT IS EASY TO "PASS TO THE LIMIT"

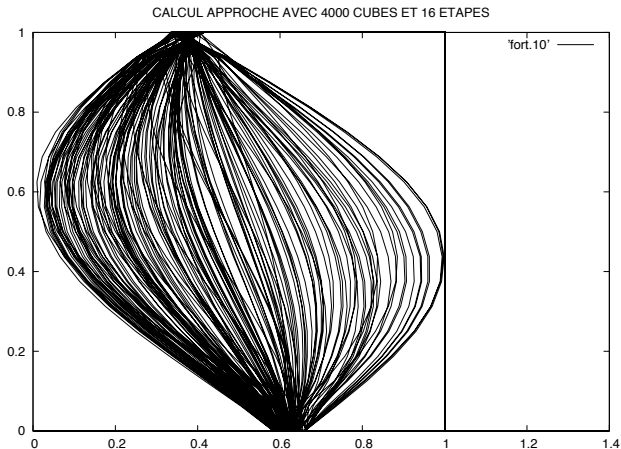
**AS A MATTER OF FACT, THIS IS NOT THE BEST
SOLUTION. THE COST CAN BE REDUCED BY
FACTOR $\pi^2/12 \sim 0.8225$**



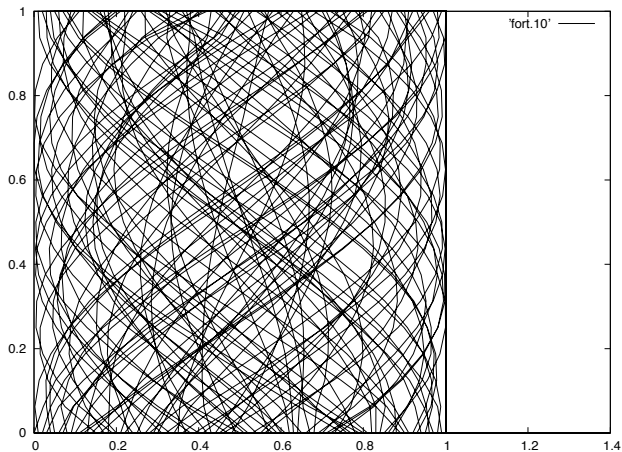
EXACT SOLUTION



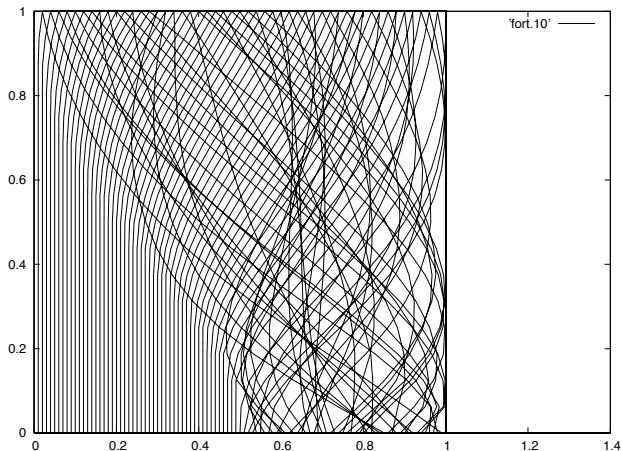
NUMERICS WITH 144 CUBES AND 16 STEPS



NUMERICS WITH 4000 CUBES AND 16 STEPS



SOME OF THE 4000 TRAJECTORIES (1 out of 40)



ANOTHER MINIMIZING GEODESIC for 1-3-5-7-9-11-12-10-8-6-4-2

Let us go back to the combinatorial setting. We define a "discrete geodesic with L steps" as a sequence of $L+1$ permutations $\sigma^0, \sigma^1, \sigma^2, \dots, \sigma^{L-1}, \sigma^L$

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$$\sum_{i=1, N} \text{dist}(A_{\sigma_i^{(0)}}, A_{\sigma_i^{(1)}})^2 + \sum_{i=1, N} \text{dist}(A_{\sigma_i^{(1)}}, A_{\sigma_i^{(2)}})^2 \\ + \dots + \sum_{i=1, N} \text{dist}(A_{\sigma_i^{(L-1)}}, A_{\sigma_i^{(L)}})^2$$

where we denote by A_1, \dots, A_N the centers of the N sub-cells and by dist the Euclidean distance.

By doing so, we have expressed the Euler model for incompressible flows as a "combinatorial optimization problem":

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which, up to the discretization, is fully consistent with the differential equations written by Euler!

A necessary optimality condition:
for each k fixed from 1 to L-1,
 σ^k must minimize among all permutations σ

$$\sum_{i=1,N} \text{dist}^2(A_{\sigma_i^{(k-1)}}, A_{\sigma_i}) + \sum_{i=1,N} \text{dist}^2(A_{\sigma_i}, A_{\sigma_i^{(k+1)}})$$

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or, equivalently,

$$c(1, \sigma_1) + c(2, \sigma_2) + c(3, \sigma_3) + \cdots + c(N, \sigma_N) ,$$

$$c(i, j) = \text{dist}^2(B_i, A_j), \quad B_i = (A_{\sigma_i^{(k+1)}} + A_{\sigma_i^{(k-1)}})/2$$

This exactly means that $\sigma^{(k)}$ solves the so-called "linear assignment problem" (well known in both combinatorial optimization theory and Economics): minimize, among all permutations σ ,

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where $c(i, j)$ is the "assignment cost matrix".

(Interpretation in Economics: we want to assign agents $i = 1, \dots, N$ to tasks $j = 1, \dots, N$ with cost $c(i, j)$ in an optimal way.)

The assignment problem (as well as its continuous limit) was analyzed in 1942 by Leonid KANTOROVICH (1912-1986) (who got the unique Nobel prize of Economy obtained by former Soviet Union!) and shown to be equivalent to a much simpler convex optimization problem.

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Kantorovich' method is a good example.

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(Reduction to convexity is rather simple once we observe that permutations matrices are just the extreme points of the convex set of all matrices with nonnegative coefficients such that each line and each column add up to one.)



Leonid Kantorovich (1912-1986)

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Minimize, among all permutations σ ,

$$\sum_{i,j=1,N} \lambda(i,j) \mathbf{c}(\sigma_i, \sigma_j)$$

where both $\mathbf{c}(i,j)$ and $\lambda(i,j)$ are given matrices.

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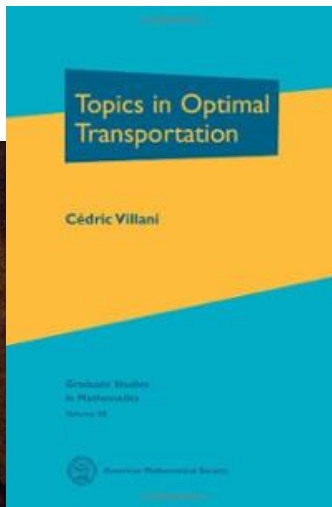
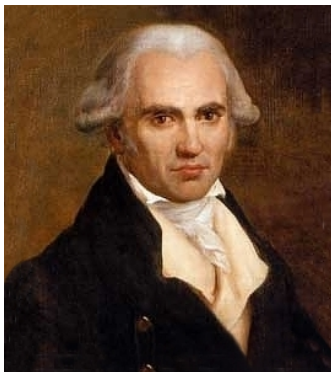
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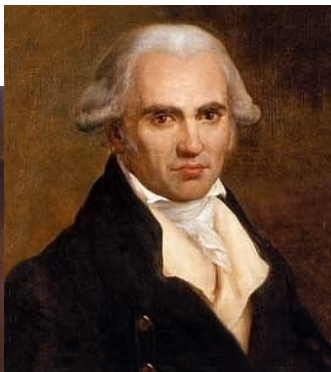
Interestingly enough, this more difficult problem appears to be a discrete version of the problem of finding *stationary* (i.e. time independent) solution to the Euler equations.

The continuous version of the linear assignment problem goes back to 1780 with Gaspard MONGE (1746-1818) and his "mémoire sur les déblais et les remblais".

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This was the prototype of what is nowadays known as "optimal transport theory", a very active field of mathematics with many connections (analysis, probability, geometry, partial differential equations) and applications (image processing, machine learning, economics, cosmology...).





The loop is now closed between Euler and Monge through Kantorovich