# Continuum Modeling of Transportation Networks with Differential Equations

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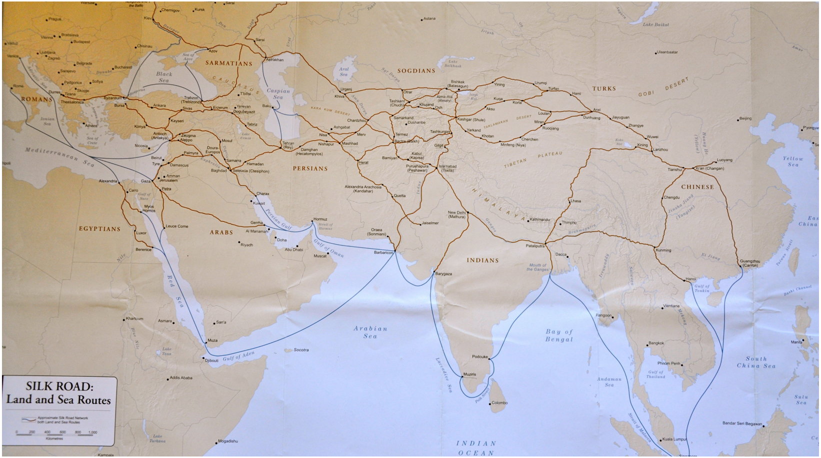
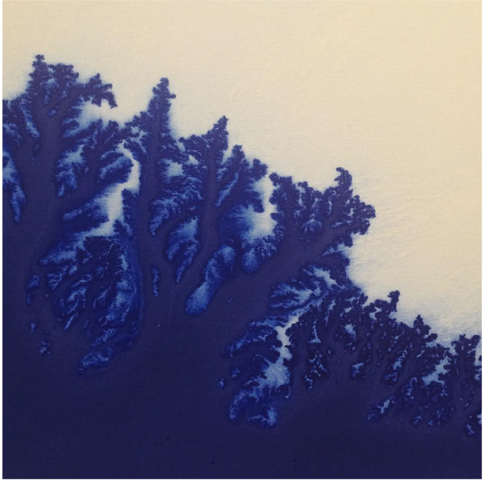
# Examples of transportation networks



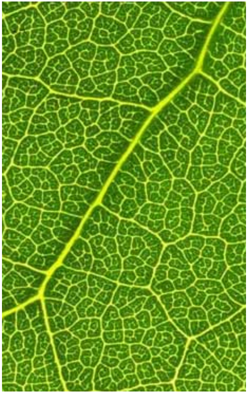

The Silk Road

# Examples of transportation networks

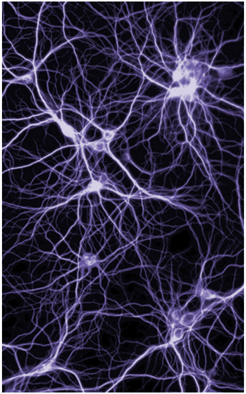


Painting by Latifa Echakhch (detail)

# Examples of transportation networks



Leaf venation

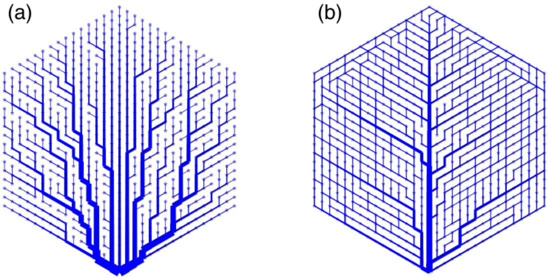


Neural network

Blood capillaries

# Discrete network models

- Static and dynamic discrete graph-based models, deterministic and (geometric) random graphs.
  Topological and geometric properties - loops, trees, connectivity, scale-free graphs [Barabasi&Albert'1999, Newman'2003, Watts&Strogatz'1998, ...]



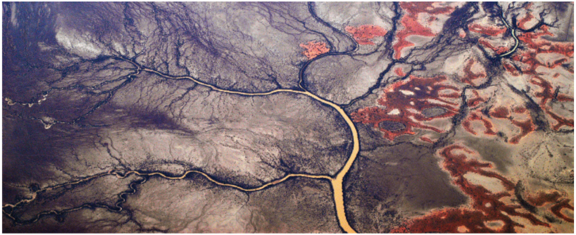

- Solutions obtained by global energy minimization; combinatorial approach with NP-completness issues.

# Optimal mass transportation network modeling

- Based on a transportation cost law and Monge-Kantorovich theory [Bernot&Caselles&Morel'2009, Villani'2003&'2008, ...]
- $c(x, y)$ - cost of transport of a unit mass from $x$ to $y$
- Find a measure $\gamma(x, y)$ which minimizes the total transportation cost

$$C_\gamma := \int_{\Omega\times\Omega} c(x, y)\gamma(\mathrm{d}x, \mathrm{d}y)$$

where the marginals of $\gamma$ are given.



River Branching

# Discrete modeling - adaptive dynamics

- Flow of a material through the network-graph $(\mathcal{V}, \mathcal{E})$

Pressures $P_j$ on vertices $j \in \mathcal{V}$

Conductivities $C_{ij}$ on edges $(i, j) \in \mathcal{E}$

- Assume low Reynolds number (Poiseuille flow), then

$$\text{Poiseuille fluxes} \quad Q_{ij} = -C_{ij} \frac{P_i - P_j}{L_{ij}}$$

- Conservation of mass - Kirchhoff law with sources $S_j$,

$$\sum_i Q_{ij} = -\sum_i C_{ij} \frac{P_i - P_j}{L_{ij}} = S_j \qquad \text{for each } j \in \mathcal{V}$$

# Discrete model of [Hu&Cai'2014]

Energy cost functional

$$E := \frac{1}{2} \sum_{(i,j)\in\mathcal{E}} \left( \frac{Q_{ij}^2}{C_{ij}} + \nu C_{ij}^{\gamma} \right) L_{ij}$$

consisting of

- pumping power (Joule's law: power = potential $\times$ current)

$$(P_i - P_j)Q_{ij} = \frac{Q_{ij}^2}{C_{ij}} L_{ij}$$

- metabolic cost $\sim C_{ij}^{\gamma} L_{ij}$
  - $\gamma = 1/2$ for blood flow
  - $1/2 \leq \gamma \leq 1$ for leaf venation

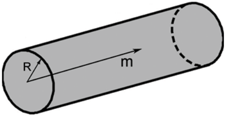
ODE system = gradient flow of $E$, constrained by the Kirchhoff law:

$$\frac{\mathrm{d}C_{ij}}{\mathrm{d}t} = \left( \frac{Q_{ij}^2}{C_{ij}^2} - \nu\gamma C_{ij}^{\gamma-1} \right) L_{ij}$$

# Transition to continuum description

Modelling of the permeability tensor in a porous medium:

- Principal directions of network flow ($m$ = conductance vector)
  - $m/|m|$ with principal permeability $\kappa > 0$
  - $m^\perp$ with principal permeability $0$




- Carmen–Kozeny equation: $\kappa \sim R^2$
- Therefore:

$$|m| := R \qquad \text{and} \qquad \mathbb{P}[m] = m \otimes m$$

- Identify the discrete and continuum variables:

$$C_{ij} \cong |m(x)|^2, \qquad P_{ij} \cong p(x), \qquad Q_{ij} \cong q(x)$$

- Darcy's law:

$$q(x) = -\mathbb{P}[m]\nabla p$$

- Continuum analogue of the discrete energy

$$E[m] = \frac{1}{2}\int c^2(m\cdot\nabla p)^2 + \frac{|m|^{2\gamma}}{\gamma}\,\mathrm{d}x$$

# Transition to continuum description

- Kirchhoff law $\rightsquigarrow$ Poisson equation

$$-\nabla\cdot(\mathbb{P}[m]\nabla p) = S \qquad \text{with } S = S(x) \text{ given}$$

Formal $L^2$-gradient flow of the continuum energy constrained by the (highly degenerate) Poisson equation

$$\partial_t m = c^2(m\cdot\nabla p)\nabla p - |m|^{2(\gamma-1)}m$$
$$-\nabla\cdot[(m\otimes m)\nabla p] = S$$

The discrete model of [Hu&Cai'2014] is a finite difference discretization of the PDE system for $(m,p)$ on an equidistant rectangular mesh.

# Corrections of the PDE model

- **P1.** The Poisson equation $-\nabla \cdot [(m \otimes m)\nabla p] = S$ is degenerate in directions $m^\perp$ and, in general, unsolvable.
  **Fix:** Introduce isotropic background permeability of the medium $r(x) \geq r_0 > 0$,

$$\mathbb{P}[m] := r(x)I + m \otimes m, \qquad -\nabla \cdot (\mathbb{P}[m]\nabla p) = S$$

- **P2.** The $m$-equation is local in $x$ (no network growth).
  **Fix:** Introduce a linear diffusive term $D^2 \Delta m$,

$$\partial_t m = D^2 \Delta m + c^2 (m \cdot \nabla p)\nabla p - |m|^{2(\gamma-1)} m$$

The energy functional has to be updated as

$$E = \frac{1}{2} \int D^2 |\nabla m|^2 + c^2 r(x) |\nabla p|^2 + c^2 (m \cdot \nabla p)^2 + \frac{|m|^{2\gamma}}{\gamma} \, \mathrm{d}x$$

Poisson equation for the pressure $p$

$$-\nabla \cdot [(r(x)I + m \otimes m)\nabla p] = S$$

coupled to the reaction-diffusion system for the conductance $m$

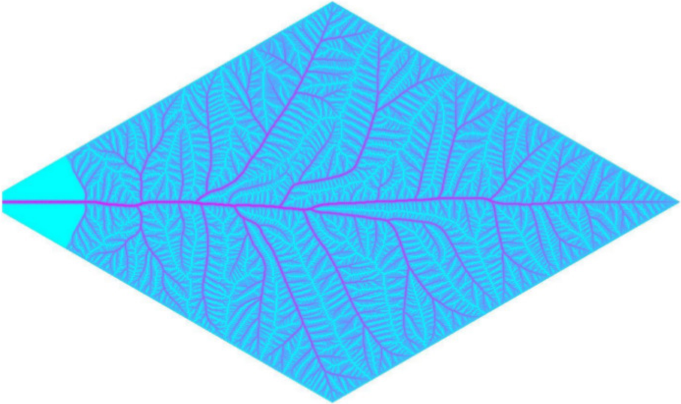
$$\frac{\partial m}{\partial t} = \underbrace{D^2 \Delta m}_{\substack{\text{random effects}\\ \text{in the porous medium}}} + \underbrace{c^2 (m \cdot \nabla p)\nabla p}_{\substack{\text{activation (force)}\\ \text{term}}} - \underbrace{|m|^{2(\gamma-1)} m}_{\text{relaxation term}}$$

- $c > 0$ - activation parameter, $D \geq 0$ - diffusivity
- $\gamma \geq 1/2$ - relaxation exponent
- Homogeneous Dirichlet BC for $m$ and $p$,

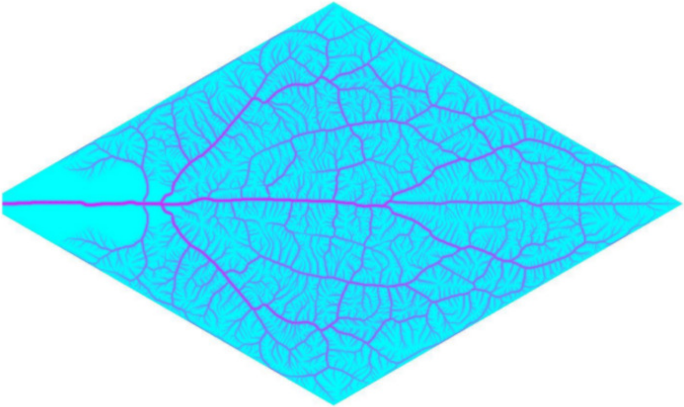
$$m|_{\partial\Omega} = 0, \qquad p|_{\partial\Omega} = 0 \qquad \forall t > 0$$

- Initial condition $m(t = 0, x) = m^I(x), \quad x \in \Omega$

# PDE simulation results - Trees (D. Hu, 2014)



# PDE simulation results - Loops (D. Hu, 2014)



# Gradient flow structure

$L^2(\Omega)$-gradient flow associated with the non-convex energy

$$\mathcal{E}(m) := \frac{1}{2}\int_\Omega \left( D^2|\nabla m|^2 + \frac{|m|^{2\gamma}}{\gamma} + c^2|m\cdot\nabla p[m]|^2 + c^2|\nabla p[m]|^2 \right) \mathrm{d}x$$

**Observe:** $\int_\Omega \left( D^2|\nabla m|^2 + \frac{|m|^{2\gamma}}{\gamma} \right) \mathrm{d}x$ is convex for $\gamma \geq 1/2$; non-convexity due to the coupling with the Poisson equation.

**Energy dissipation:** Along smooth solutions $m$, $p = p[m]$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(m) = -\int_\Omega \left( \frac{\partial m}{\partial t}(t,x) \right)^2 \mathrm{d}x.$$

$$-\nabla \cdot [(I + m \otimes m)\nabla p] = S$$

$$\frac{\partial m}{\partial t} = D^2 \Delta m + c^2 (m \cdot \nabla p)\nabla p - |m|^{2(\gamma-1)} m$$

- Stronger regularity results than Lax-Milgram for the Poisson equation

$$\begin{aligned} -\nabla \cdot (A(x)\nabla p) &= \nabla \cdot F \qquad \text{in } \Omega \\ p &= 0 \qquad \text{on } \partial\Omega \end{aligned}$$

  require at least $A \in L^\infty(\Omega)$.
- While the divergence part is controlled, how to control the rotational part of $(m \otimes m)\nabla p$?
- Iterating between $m$ and $p$ in the system destroys the energy dissipation equation.

- Let $S \in L^2(\Omega)$, $m^I \in L^2(\Omega)$.
- Leray-Schauder fixed point theorem for the regularized system

$$-\nabla \cdot [\nabla p + m((m \cdot \nabla p) * \eta_\varepsilon)] = S$$
$$\frac{\partial m}{\partial t} = D^2 \Delta m + c^2 [(m \cdot \nabla p) * \eta_\varepsilon] \nabla p - |m|^{2(\gamma-1)} m$$

which preserves the energy dissipation, and the choice $\eta_\varepsilon(x) := (4\pi\varepsilon)^{-d/2} \exp(-|x|^2/4\varepsilon)$ guarantees

$$\int_{\mathbb{R}^d} (m \cdot \nabla p)[(m \cdot \nabla p) * \eta_\varepsilon] \, \mathrm{d}x \geq 0$$

- Limit $\varepsilon \to 0$ based on apriori estimates in the energy space

# The case $\gamma = 1/2$

- relaxation term $|m|^{2(\gamma-1)}m := \frac{m}{|m|}$ ... singularity at $m = 0$
- but relaxation energy $R(m) := \int_\Omega |m| \,\mathrm{d}x$ convex!

We prove the existence of a weak solution of

$$\partial_t m \in D^2 \Delta m + c^2 (m \cdot \nabla p[m]) \nabla p[m] - \partial R(m)$$

with

$$\partial R(m) = \{ r \in L^\infty(\Omega);\ r(x) = m(x)/|m(x)| \text{ if } m(x) \neq 0, \\ |r(x)| \leq 1 \text{ if } m(x) = 0 \}$$

**Conjecture:** $m$ is a slow and very sparse solution, i.e.

$$\frac{m}{|m|} = \begin{cases} \frac{m}{|m|} & \text{for } m \neq 0 \\ 0 & \text{for } m = 0 \end{cases}$$

Compact support property of solutions (e.g., [Brezis'1974])

- Small diffusion ($D \ll 1$) creates substrate layers in $\Omega$
  BUT: $D = 0$ gives, for every fixed $x \in \Omega$, the ODE system

$$\partial_t m = \cancel{D^2 \Delta m} + c^2 (m \cdot \nabla p) \nabla p - |m|^{2(\gamma-1)} m$$

  nonlinearly coupled via $\nabla p$ as solution of the Poisson equation.
  Thus: For $D = 0$ the support of $m$ does **not** grow.

- The activation term propagates the thin substrate layers into a network if $c^2$ is large enough.

- The relaxation term makes the network stationary:
  - For $1/2 \leq \gamma \leq 1$: sparse stationary networks
  - For $\gamma > 1$: stationary network fills up $\Omega$

# Network formation and nontrivial stationary states

$$\boxed{\text{Trivial stationary state:} \qquad m_0 \equiv 0, \qquad -\Delta p_0 = S}$$

- For large $D > 0$, only the **trivial** stationary state.
- For $D > 0$ small enough, **nontrivial** stationary states are constructed as solutions of the fixed point problem

$$m = \beta L m + F(m, \beta)$$

  using the global bifurcation theorem by [Rabinowitz'71], with $\beta := c^2/D^2$ the bifurcation parameter.
- Pattern (network) formation can be seen as a consequence of (linear) instability of the trivial solution.

## Construction of stationary solutions with $D = 0$, $\gamma \geq 1$

- For $\gamma > 1$:

$$c^2(\nabla p \otimes \nabla p)m = |m|^{2(\gamma-1)} m$$

so that $m = \lambda \nabla p$ and $p$ solves

$$-\nabla \cdot \left[ \left( 1 + c^{\frac{2}{\gamma-1}} |\nabla p(x)|^{\frac{2}{\gamma-1}} \chi_{\mathcal{A}}(x) \right) \nabla p \right] = S,$$

which is the Euler-Lagrange equation of a strictly convex energy functional iff $\gamma > 1$.

- For $\gamma = 1$:

$$c^2(\nabla p \otimes \nabla p)m = m$$

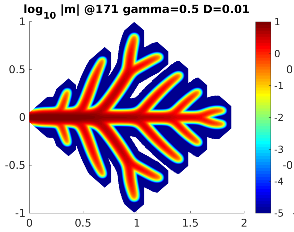
leads to the (even more) nonlinear Poisson equation

$$-\nabla \cdot \left[ \left( 1 + \frac{\lambda^2(x)}{c^2} \chi_{\{c|\nabla p|=1\}}(x) \right) \nabla p \right] = S$$

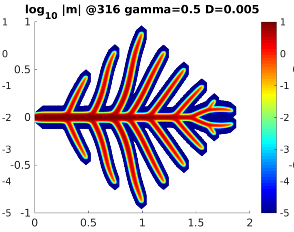
# Numerical results

# Numerical results: varying diffusivity

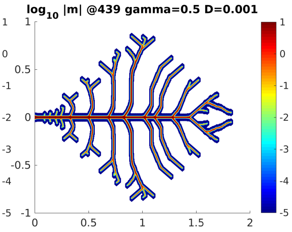
$$S \equiv -1, \quad c = 50, \quad \gamma = 1/2$$




$D = 10^{-2}$

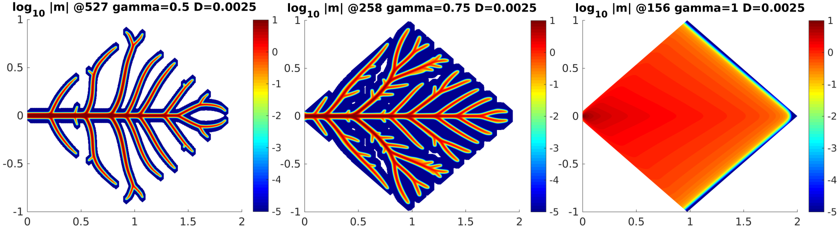



$D = 5 \times 10^{-3}$



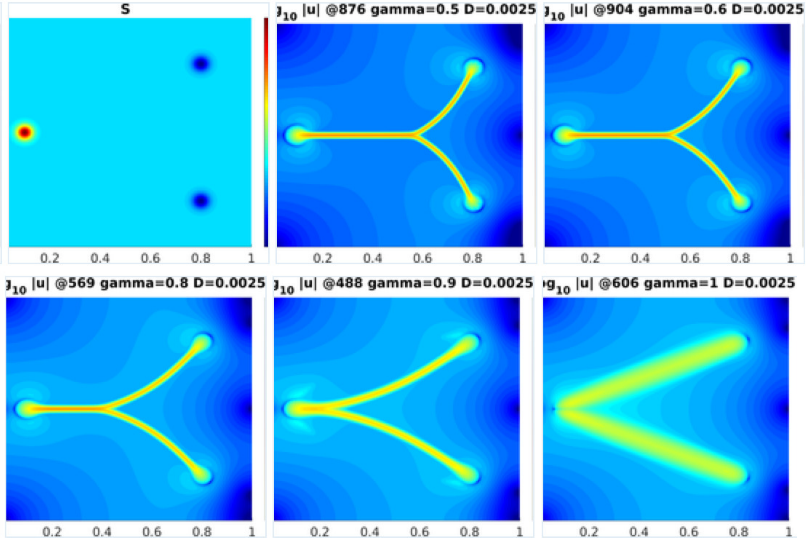

$D = 10^{-3}$

$$S \equiv -1, \quad c = 50, \quad D = 0.025$$




$\gamma = 1/2$ $\qquad$ $\gamma = 3/4$ $\qquad$ $\gamma = 1$

# One source, two sinks



# Outlook: Mesoscopic modelling

The network is described by the time-dependent probability measure $\mu_t = \mu_t(x, \theta, C)$ to have an edge of conductivity $C \geq 0$ in direction $\theta \in \mathbb{S}_+^{d-1}$ at location $x \in \Omega$. Evolution of $C$ driven by:

- Activation $\sim C|\theta \cdot \nabla p|^2$, with pressure $p$ subject to the Poisson equation

$$-\nabla \cdot (\mathbb{P}[\mu_t]\nabla p) = S, \qquad \mathbb{P}[\mu_t](x) = \int_0^\infty \int_{\mathbb{S}_+^{d-1}} C\theta \otimes \theta \, \mu_t(x, \mathrm{d}\theta, \mathrm{d}C)$$

- Relaxation $\sim -C^\gamma$

Leads to:

$$\partial_t \mu_t + \partial_C \left[ \left( c_0^2 C |\theta \cdot \nabla p|^2 - C^\gamma \right) \mu_t \right] = 0$$

**Research program:**

- Well posedness in the space of probability measures
- Connection to branched optimal transport - e.g., [Bernot, Caselles, Morel, Xia, Santambrogio, ...]
- Numerical simulations

# Open problems in network formation

- Rigorous transition from discrete to continuum modelling.
- Understanding of the branching mechanism in the PDE model.
- Is the PDE model capable of producing networks with loops?
- Does the PDE system admit fractal solutions (i.e., supported on sets of Hausdorff dimension $< d$), in scaling limits as $D \to 0$, $r \to 0$ and/or $c \to \infty$?
- Extensions of the model:
  - PIN-auxin dynamics in leaf venation
  - Angiogenesis in cancer: Brinkmann instead of Darcy for the pressure (viscous resistance in the material flow)
  - Ion transport in neural networks: Coupling with the Poisson-Nernst-Planck system

# Conclusions

Thank you for your attention!