# A Continuum Model of Biological Transport Networks

On a PDE based modeling of biological transportation networks

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# Previous Review

## Symbols and Notations

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- The flow rate of an oriented flux in $i \to j$ is denoted by $Q_{ij} := \dfrac{C_{ij}(\Delta P)_{ij}}{L_{ij}}$.
- The strength of $i$, denoted by $S_i$, is defined as the negative summation of $Q_{ij}$ for all $j \in N(i)$.

# Formulæ

## Kirchhoff first law

- Kirchhoff's first law is that the algebraic sum of currents in a network of conductors meeting at a point (or node) is zero.

$$S_i = \sum_{j \in N(i)} C_{ij} \frac{(\Delta P)_{ji}}{L_{ij}} = - \sum_{j \in N(i)} C_{ij} \frac{(\Delta P)_{ij}}{L_{ij}}$$

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## Global mass conservation

- The global mass conservation reveals that the algebratic sum of strength over all nodes is zero, that is, there are many sinks for many sources.

$$\sum_{i \in V} S_i = 0$$

# Formulæ

## Joule's law

- The kinetic energy is in proportion to both pressure drop and flow rate.

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## Metabolic consumption (in energy form)

- The metabolic consumption is in proportion to its length and a power of its conductivity.

$$\mathcal{E}_2[C_{ij}] := \frac{\nu}{\gamma} C_{ij}^{\gamma} L_{ij}$$

# Formulæ

## The entire energy consumption

- The entire energy consumption functional is given by

$$\tilde{\mathcal{E}}[C] := \sum_{(i,j)\in E} \frac{Q_{ij}^2}{C_{ij}} L_{ij} + \sum_{(i,j)\in E} \frac{\nu}{\gamma} C_{ij}^{\gamma} L_{ij}$$

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- Here $\nu > 0$ is so-called metabolic coefficient, $\gamma$ is the effective value.

# The discussion of gradient flow

## The gradient flow

- The general formulation of a gradient flow of the functional $\tilde{\mathcal{E}} \circ C(t)$ is of the form

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\mathcal{H}[C] \cdot \nabla \tilde{\mathcal{E}}[C]$$

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- The gradient of $\tilde{\mathcal{E}}$ on $C$ is

$$\nabla \tilde{\mathcal{E}}[C] = \left( \cdots, \nu C_{ij}^{\gamma-1} L_{ij} - \frac{Q_{ij}^2}{C_{ij}^2} L_{ij}, \cdots \right)$$

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- Moreover, we have the dissipation of the energy since

$$\frac{\mathrm{d}\tilde{\mathcal{E}}[C]}{\mathrm{d}t} = \nabla \tilde{\mathcal{E}}[C] \cdot \frac{\mathrm{d}C}{\mathrm{d}t} = \left\langle \nabla \tilde{\mathcal{E}}[C], \nabla \tilde{\mathcal{E}}[C] \right\rangle_{\mathcal{H}[C]} < 0$$

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## The duality map $\mathcal{H}[C]$

- We denote the space of tanent and cotangent vectors at $C \in \mathcal{C}$ by $\mathcal{T}_C\mathcal{C}$ and$\mathcal{T}_C^*\mathcal{C}$ respectively. Therefore $\mathcal{H}[C]$ can be regarded as a duality map

$$\mathcal{H}[C] : \mathcal{T}_C^*\mathcal{C} \to \mathcal{T}_C\mathcal{C}$$

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- Since the effect of $\mathcal{H}$ on the system is local $\mathcal{H}[C] = \mathcal{H}_1[C] \otimes \cdots \otimes \mathcal{H}_{|E|}[C]$ Here

$$\mathcal{H}_{ij}[C] : \partial_{C_{ij}}|_C \mapsto \varphi_{ij}(C_{ij}) \cdot dC_{ij}$$

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$$\mathcal{H}_{ij}[C] : \partial_{C_{ij}}|_C \mapsto \varphi_{ij}(C_{ij}) \cdot dC_{ij}$$

- We usually choose $\varphi_{ij}(C_{ij}) = C_{ij}^{\alpha}$. Here $1 - \gamma \leq \alpha \leq 2$ is designate with respect to a weighted Euclidean distance.

# On the ODE based modeling

## The global existence of $C(t)$

- Consider the ODE system

$$
\begin{cases}
\dfrac{\mathrm{d}C_{ij}}{\mathrm{d}t} = \left( \dfrac{Q_{ij}}{C_{ij}^2} L_{ij} - \nu C_{ij}^{\gamma} L_{ij} \right) C_{ij}^{\alpha-1} L_{ij} \\
\text{coupled with } S_i = -\displaystyle\sum_{j \in N(i)} C_{ij} \dfrac{(\Delta P)_{ij}}{L_{ij}}
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- Edges with initial positive conductivity are non-vanishing (in finite time) and bounded.

$$|\nabla \tilde{\mathcal{E}}|^2 = \sum_{(i,j) \in E} \left(\frac{Q_{ij}}{C_{ij}^2} L_{ij} - \nu C_{ij}^{\gamma} L_{ij}\right)^2 C_{ij}^{\alpha-1}$$

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The goal of this section is to

- derive the formal macroscopic limit of the discrete model as the number of nodes and edges tends to infinity,
- establish the PDE model,
- take a glance at the weak solutions of the corresponding gradient flow.

# The modeling of continuum case

## The energy consumption functional on $\mathbb{R}^d$

- Let $(i-1)_k$ and $(i+1)_k$ denote the left and right neighbours of vertex $i$ on the $k$-th spatial dimension respectively. Thus the Kirchhoff law is then written as

$$-\sum_{k=1}^{d} C_{(i-1)_k,i}\frac{(\Delta P)_{(i-1)_k,i}}{L_{(i-1)_k,i}} - C_{i,(i+1)_k}\frac{(\Delta P)_{i,(i+1)_k}}{L_{i,(i+1)_k}} = S_i$$

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- Equal $c_k(x_{(i\pm 1/2)_k})$ with $C_{i,i\pm1}$, $S_i$ with $S(x_i)$, $P_i$ with $p(x_i)$ and $P_{i\pm1}$ with $p(x_{i\pm1})$. Here $c = \text{diag}\,(c_1, c_2, \cdots, c_d)$ is a diagonal permeability tensor field with scalar non-negative functions $c_k \in C(\Omega)$.

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- The rescaled Kirchhoff's law is concluded to be the discrete approximation of the Poisson function.

# The modeling of continuum case

## Discrete approximation of the Poisson equation

- Proof of the approximation

$$
\begin{aligned}
S = &- \nabla \cdot (c \nabla p) \\
= &- \sum_{k=1}^{d} \partial_{x_k} (c_k \partial_{x_k} p) \\
= &- \sum_{k=1}^{d} \frac{c_k(x_{(i+1/2)_k}) \partial_{x_k} p(x_{(i+1/2)_k}) - c_k(x_{(i-1/2)_k}) \partial_{x_k} p(x_{(i-1/2)_k})}{h_k^{(d)}} + O(h_k^{(d)}) \\
= &- \sum_{k=1}^{d} \frac{c_k(x_{(i+1/2)_k}) \cdot \frac{p(x_{(i+1)_k}) - p(x_{(i_k)})}{h_k^{(d)}} - c_k(x_{(i-1/2)_k}) \cdot \frac{p(x_{(i)_k}) - p(x_{(i-1)_k})}{h_k^{(d)}}}{h_k^{(d)}} + O \\
= &\cdots \\
= &- \sum_{k=1}^{d} C_{(i-1)_k, i} \frac{(\Delta P)_{(i-1)_k, i}}{L_{(i-1)_k, i}} - C_{i,(i+1)_k} \frac{(\Delta P)_{i,(i+1)_k}}{L_{i,(i+1)_k}} + O(h_k^{(d)})
\end{aligned}
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## Discrete approximation of the other formulæ

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- The metabolic term in continuum case:

$$\int_{\Omega} \frac{\nu}{\gamma}|c_k|^{\gamma}\mathrm{d}x = \frac{\nu}{\gamma}W^{(d)} \sum_{i \in V} |c_k(X_{(i+1/2)_k})|^{\gamma} + O(h_k^{(d)})$$

Here $W^{(d)} := \prod_{k=1}^{d} h_k^{(d)}$ is the unit cube.

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- The pumping power term in continuum case:

$$\int_{\Omega} c_k(\partial_{x_k} p)^2\mathrm{d}x = W^{(d)} \sum_{i \in V} c_k(X_{(i+1/2)_k}) \left( \frac{p(X_{(i+1)_k}) - p(X_i)}{h_k^{(d)}} \right)^2 +$$

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## Discrete approximation of the other formulæ

- Thus the energy functional can be written as

$$\tilde{\mathcal{E}}[C] = \frac{1}{2} \sum_{k=1}^{d} \sum_{i \in V} \sum_{j \in N(i;k)} \left( \frac{Q_{ij}^2[C]}{C_{ij}} + \frac{\nu}{\gamma} C_{ij}^{\gamma} \right) h_k^{(d)}$$

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- Here $N(i;k)$ denotes $N(i) \cap \{(i \pm 1)_k\}$, that is, the neighbour in the $k$th spatial dimension.
- Via the discrete approximation, we deduce the energy functional

$$\mathcal{E}[c] := \int_{\Omega} \nabla p \cdot c \nabla p + \frac{\nu}{\gamma} |c|^{\gamma} \mathrm{d}x = \tilde{\mathcal{E}}[C] + O(W^{(d)})$$

# The modeling of continuum case

## The formal $L^2$ -gradient flow of the energy

- In retrospect to how we have deducted $\frac{\mathrm{d}C}{\mathrm{d}t}$, we shall estimate the the formal $L^2$-gradient flow of the continuum energy functional coupled with the Poisson equation. The relation between the discrete and continuum model is presented below.

$$\begin{array}{ccccc} \tilde{\mathcal{E}}[C] & + & \text{Kirchhoff law} & \Rightarrow & \text{gradient flow (discrete)} \\ \updownarrow & & \updownarrow & & \updownarrow \\ \mathcal{E}[c] & + & \text{Poisson equation} & \Rightarrow & L^2 \text{ -gradient flow (continuous)} \end{array}$$

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- The energy functional $\mathcal{E}[c] = \int_\Omega \nabla p \cdot c \nabla p + \frac{\nu}{\gamma}|c|^\gamma \mathrm{d}x$
- How shall we deduce $\frac{\partial c_k}{\partial t}$?

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- (Calculus of variations) Let $\phi = \text{diag}\ (\phi_1, \phi_2, \ldots, \phi_n)$ be a diagonal matrix, and $\varepsilon$ is arbitrarily small. We have the expansion

$$p[c + \varepsilon\phi] = p_0 + \varepsilon p_1 + O(\varepsilon^2)$$

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- Consider the derivation at $\varepsilon = 0$, e.g. $\left.\dfrac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{E}[c + \varepsilon\phi]\right|_{\varepsilon=0}$

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- (Calculus of variations) Let $\phi = \text{diag}\ (\phi_1, \phi_2, \ldots, \phi_n)$ be a diagonal matrix, and $\varepsilon$ is arbitrarily small. We have the expansion
$$p[c + \varepsilon\phi] = p_0 + \varepsilon p_1 + O(\varepsilon^2)$$
- Consider the derivation at $\varepsilon = 0$, e.g. $\left.\dfrac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{E}[c + \varepsilon\phi]\right|_{\varepsilon=0}$
- Estimate the $L^2$ -gradient flow with the identities one deduces.

# The modeling of continuum case

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- (Proof to the next page)

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Steps for the proof.

1. The expansion $p[c+\varepsilon\phi] = p_0 + \varepsilon p_1 + O(\varepsilon^2)$.
2. $\left.\dfrac{\mathrm{d}\mathcal{E}[c+\varepsilon\phi]}{\mathrm{d}t}\right|_{\varepsilon=0} = \displaystyle\sum_{k=1}^{d}\int_\Omega (\partial_{x_k}p_0)^2\phi_k + 2c_k(\partial_{x_k}p_0)(\partial_{x_k}p_1) + \nu|c_k|^{\gamma-2}c_k\phi_k \mathrm{d}x.$
3. Let $\mathcal{M}[c+\varepsilon\phi] = \displaystyle\sum_{k=1}^{n}\int_\Omega p[c+\varepsilon\phi]\cdot\partial_{x_k}(c_k\partial_{x_k}p[c+\varepsilon\phi])\mathrm{d}x$, we have
$$\sum_{k=1}^{d}\int_\Omega (c_k+\varepsilon\phi_k)\left(\partial_{x_k}p_0\right)^2 + \varepsilon c_k\left(\partial_{x_k}p_0\right)\left(\partial_{x_k}p_1\right)\mathrm{d}x = \int_\Omega Sp_0 \,\mathrm{d}x + \mathcal{O}\left(\varepsilon^2\right).$$
4. Substracting the identity
$$\sum_{k=1}^{d}\int_\Omega c_k(\partial_{x_k}p_0)^2 \,\mathrm{d}x = \int_\Omega Sp_0 \,\mathrm{d}x$$
5. Plugging into 1. to obtain
$$\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{E}[c+\varepsilon\phi]\right|_{\varepsilon=0} = \sum_{k=1}^{d}\int_\Omega \left[-(\partial_{x_k}p_0)^2 + \nu|c_k|^{\gamma-2}c_k\right]\phi_k \,\mathrm{d}x$$
6. Hence $\partial_t c_k = (\partial_{x_k}p)^2 - \nu|c_k|^{\gamma-2}c_k$.

# The establishment of full PDE system

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- The amended Poisson equation

$$\nabla \cdot (c'\nabla p) = \nabla \cdot (c + r\mathbb{I}\nabla p) = s$$

is uniformly elliptic as long as the eigenvalues of $c'$ are non-negative.

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- A linear diffusive term $D^2 \nabla^2 c_k$ is introduced to model the random fluctuations in the medium.
- Hence we obtain

$$\partial_t c_k = D^2 \nabla^2 c_k + (\partial_{x_k} p)^2 - \nu |c_k|^{\gamma-2} c_k$$

# The establishment of full PDE system

## The solution

- The solution of the PDE system

$$\begin{aligned} \partial_t c_k &= D^2 \nabla^2 c_k + |\nabla p|^2 - \nu |c_k|^{\gamma-2} c_k \\ S &= -\nabla \cdot ( + r\mathbb{I}\nabla p) \end{aligned}$$

$$c(t,x) \equiv 0, \quad \partial_n p(t,x) \equiv 0, \quad \text{for all } x \in \partial\Omega \text{ and } t > 0$$

is

$$\mathcal{E}'[c(t)] = \mathcal{E}'[c_0] + \sum_{k=1}^{d} \int_0^t \int_\Omega \left(\partial_t c_k(s,x)\right)^2 \mathrm{d}x\mathrm{d}s$$

Thanks for listening.