Previous Review

Symbols and Notations

- $G(V, E)$ is a graph with vertex set V and edge set E.
- The adjacency matrix of E is denoted by $A = (a_{ij})_{n\times n}$, where $n := |V|$.
- The neighbour of node/vertex $i \in V$ is defined as $N(i) := \{j : j \sim i\}$.
- The conductivity and length of edge $i \to j$ are denoted by C_{ij} and L_{ij} correspondingly, where $C_{ij} \geq 0$ and $L_{ij} > 0$.
- The pressure of the vertex $i \in V$ is denoted by P_i. Thus we can define the pressure drop $(\Delta P)_{ij} := P_j - P_i$ by definition.
- 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.

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

Global mass conservation

- The global mass conservation reveals that the algebraic 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.

$$\mathcal{E}_1[C_{ij}] := (\Delta P)_{ij} Q_{ij} = \frac{Q_{ij}^2}{C_{ij}} L_{ij}$$

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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$$\tilde{\mathcal{E}}[C] := \underbrace{\sum_{(i,j)\in E} \frac{Q_{ij}^2}{C_{ij}} L_{ij}}_{\text{the pumping power term}} + \underbrace{\sum_{(i,j)\in E} \frac{\nu}{\gamma} C_{ij}^{\gamma} L_{ij}}_{\text{the metabolic cost term}}$$

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the pumping power term　　the metabolic cost term

- Here $\nu > 0$ is so-called metabolic coefficient, γ 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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$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\mathcal{H}[C] \cdot \nabla\tilde{\mathcal{E}}[C]$$

- 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

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

The discussion of gradient flow

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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- 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

$$\begin{cases} \dfrac{\mathrm{d}C_{ij}}{\mathrm{d}t} = \left(\dfrac{Q_{ij}}{C_{ij}^2} L_{ij} - \nu C_{ij}^{\gamma} L_{ij} \right) C_{ij}^{\alpha-1} L_{ij} \\ \text{coupled with } S_i = -\displaystyle\sum_{j \in N(i)} C_{ij} \dfrac{(\Delta P)_{ij}}{L_{ij}} \end{cases}$$

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- Edges with initial positive conductivity are non-vanishing (in finite time) and bounded.

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

Form discrete parallelotopes to a continuum

What if the step size turns to zero?

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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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- If each point has with the equal length h_k to the left or right neighbour with respect to the k-th spatial dimension, then

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

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- : First difference operation(s).

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- : First difference operation(s).
- : Second difference operation(s).

The modeling of continuum case

Discrete approximation of the Poisson equation

- Consider the solution $p(x)$ of the Poisson equation

$$-\nabla \cdot (c\nabla p) = S$$

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- Equal $c_k(x_{(i\pm 1/2)_k})$ with $C_{i,i\pm 1}$, S_i with $S(x_i)$, P_i with $p(x_i)$ and $P_{i\pm 1}$ with $p(x_{i\pm 1})$. 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 \dfrac{p(x_{(i+1)_k}) - p(x_{(i_k)})}{h_k^{(d)}} - c_k(x_{(i-1/2)_k}) \cdot \dfrac{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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The modeling of continuum case

Discrete approximation of the other formulæ

- The global mass conservation formula

$$\sum_{i \in V} S_i = 0 \Longleftrightarrow \int_{\partial\Omega} S(x)\mathrm{d}x = 0$$

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$$\sum_{i\in V} S_i = 0 \Longleftrightarrow \int_{\partial\Omega} S(x)\mathrm{d}x = 0$$

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

- The pumping power term in continuum case:

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

The modeling of continuum case

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 kth 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.

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\begin{array}{ccccc}
\tilde{\mathcal{E}}[C] & + & \text{Kirchhoff law} & \Rightarrow & \text{gradient flow (discrete)} \\
\updownarrow & & \updownarrow & & \updownarrow \\
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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 $\frac{\partial c_k}{\partial t}$?

The modeling of continuum case

The formal L^2 -gradient flow of the energy

- We shall prove that $\partial_t c_k = (\partial_{x_k} p)^2 - \nu |c_k|^{\gamma-2} c_k$.

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

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

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- Consider

$$\sum_{k=1}^{d} \int_{\Omega} (c_k + \varepsilon\phi_k)(\partial_{x_k} p_0)^2 + \varepsilon c_k (\partial_{x_k} p_0)(\partial_{x_k} p_1) \mathrm{d}x$$

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- We obtain

$$\sum_{k=1}^{d} \int_\Omega \phi_k (\partial_{x_k} p_0)^2 + c_k (\partial_{x_k} p_0)(\partial_{x_k} p_1) \mathrm{d}x = 0$$

The establishment of full PDE system

Two drawbacks of the theoretical Poisson function

- The Poisson equation $\nabla \cdot (c\nabla p) = s$ is possibly strongly degenerate since in general the eigenvalues (i.e., diagonal elements) of the permeability tensor c may vanish.

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- The diffusion constant r is introduced, i.e. $c' := r\mathbb{I} + c$ with $r(x) \geq r_0 > 0$, where $\mathbb{I}$ is the unit matrix with dimension d.
- 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

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

Thanks for listening.