Constrained Constructive Optimization implementation
Reproducing Rudolph Karch paper

CLARA JAQUET
Paris-Est University
June 15, 2016

Abstract

Implement CCO in 2D, then 3D based on Karch's work [1]. In another step consider implementation for convex volume. Combination of CFD laws, geometry, and optimization. Encapsulated articles : requires summary in one paper.

Keywords: constrained constructive optimization, implementation

Contents

Introduction

Constrained Constructive Optimization (CCO) consists of growing a tree governed by minimizing a target function.

In Karch's method the tree is constrained into a given convex perfusion volume, and the target function minimizes the total tree volume during growth. Segment are added one by one and fulfill both local optimization (single bifurcation scale) and global optimization (tree scale). The local optimization is based on Kamiya's work [2], whereas the global optimization has been implemented first by Schreiner in 2D [3].

1 Global optimization

Initialization of the method requires some physiological parameters as input, and a randomized starting point.

Then Karch's protocol consists of a complete loop for each added segment. A random location is picked under some constraints (geometry and physiology), to use it as a candidate for segment extremity. Its connection is tested with neighbor segments, producing a bifurcation under topological, structural and functional constraints. In view of this new branch impact on the whole tree (induced by fluid mechanics laws), the optimal connection is selected by minimizing a target function (the minimal volume of the total tree).

1.1 Assumptions and boundary conditions

The vascular tree is grown under specific assumptions and boundary conditions.

The perfused volume is convex and supposed homogeneously filled. The terminal segments correspond to pre-arteriole level, feeding a non modeled micro-vasculature. The blood is an incompressible, homgeneous Newtonian fluid, studied in a steady state and in laminar flow conditions.

The resistance and the pressure drop of a segment j are defined by:

$$R_j = \frac{8\mu}{\pi} \frac{l_j}{r_j^4} \text{ with } \mu \text{ the viscosity} \tag{1}$$

$$\Delta P_j = R_j Q_j \tag{2}$$

The total resistance of the tree is calculated recursively by tree decomposition, considering parallel and serial arrangements.

The physiological parameters are defined such as in the following table:

Parameter	Meaning	Value
V_{perf}	perfusion volume	$100\,\mathrm{cm}^3$
P_{perf}	perfusion pressure	100 mmHg
P_{term}	terminal pressure	60 mmHg
Q_{perf}	perfusion flow	500 mL/ min
Q_{term}	terminal flow	0.125 mL/ min
N_{term}	number of terminals	4000
μ	viscosity of blood	3.6 cp
γ	Murray bifurcation exponent	3

The pressure at distal end of terminal segment,P_{term}, are equal and correspond to the inflow pressure to the micro-circulation. The terminal flows $Q_{term,j}$ are equal, and delivered into the micro-circulation agains P_{term}. Because of flow conservation their sum correspond to the perfusion flow at the root Q_{perf}. The laminar flow resistance of the whole tree induces a given total Q_{perf} accross ΔP. The perfusion flow Q_{perf} is the same for each step of the tree generation.

The tree grown is dichotomic, so that the total number of segments is ~~calculated from:~~

$$N_{tot} = 2N_{term} - 1 \tag{3}$$

This tree follows Murray's law, with a power coefficient equal to 3.

1.2 Initialization step

Inputs:

- convex perfusion surface or volume definition: position and shape
- number of terminal segments, N_{term}
- location of the root (in our case on the border of the perfusion territory)
- a random location inside the perfusion territory for the first segment end

1.3 Loop to add new segment

We are provided a new location, n_{loc}, and want to find its optimal connection to the existing tree. For this purpose we select the N_{con} closest existing segments to this location, compute a local optimization for each of them, then evaluate the connection impact on the whole tree, and as a global optimization process, we determine the one minimizing best the total tree volume.

1.3.1 Constrained new location n_{loc}

A random position is picked, that has to fulfill two constraints: belonging to the perfusion territory and respecting a distance criterion. This criterion is defined based on the final and current size of the tree:

$$d_{thresh} = (\pi r_{supp}^2 / k_{term})^{\frac{1}{2}} \tag{4}$$

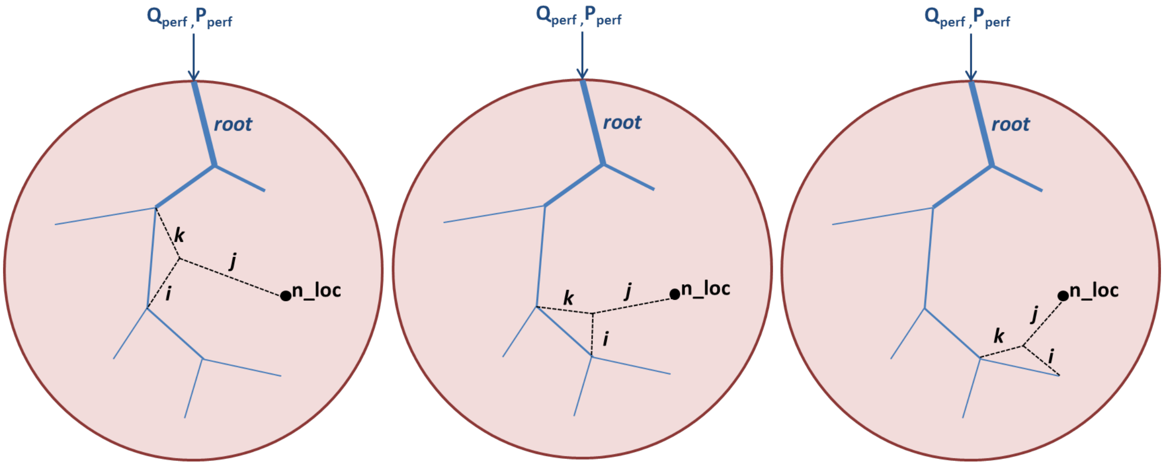


Figure 1: To add a new segment: test connection with neighbors of the new location n_{loc} and select the one minimizing total tree volume

with k_{term} the number of terminal segment at the current step, and r_{supp} defined from the estimated size of a micro-circulatory black-box area, knowing the total perfused area A_{perf}:

$$\pi r_{supp}^2 = A_{perf} / N_{term} \tag{5}$$

In 3D this criterion is defined as:

$$d_{thresh} = (\frac{4}{3}\pi r_{supp}^3 / k_{term})^{\frac{1}{3}} \tag{6}$$

with

$$\frac{4}{3}\pi r_{supp}^3 = V_{perf} / N_{term} \tag{7}$$

This distance criteron is updated after each new segment is added, so that it decreases during tree growth. If no location is found that respect this distance to existing segments within the perfusion territory, then the distance criterion is multiplied by 0.9 and the process repeated until a new position is found that fulfills both constraints.

1.3.2 Test local connection

For each neighbor segment of n_{loc} we calculate what would be the optimal connection to n_{loc} based on a single bifurcation optimization procedure established by Kamyia [2], and is fully detailed in section 2. If this local optimization process is successful, we apply two additional checks:

- We control that the resulting segments are not degenerate, which means all three segments of the new bifurcations respect the following constraint between length and radius: $2r_i \leq l_i$
- We control that none of the three resulting segments overlap any other existing tree segment.

With this step we ensure the connection to be locally optimal and plausible for the tree.

1.3.3 Propagate impact on whole tree

By adding a new terminal segments, inducing a new generated bifurcation, we perturb the distribution of segmental flows. In order to reestablish the correct terminal flows, the hydrodynamic resistance of the tree must be adjusted. As the lengths of the segments as well as the terminal and perfusion pressures are fixed, this can only be accomplished by proper rescaling of the segment's radii.

If we define the reduced hydrodynamic resistance R^* as $R_i^* = R_i r_i^4$ we can calculate the reduced hydrodynamic resistance of a segment including its left and right subtrees by recursively traversing the subtrees:

$$R^*_{sub,j} = \frac{8\mu}{\pi} l_j + \left(\frac{(r_{left,j}/r_j)^4}{R^*_{left,j}} + \frac{(r_{right,j}/r_j)^4}{R^*_{right,j}} \right)^{-1} \tag{8}$$

Considering the assumptions 2 and 1, we can then calculate the radius ratio of two children segments from resistance and flow:

$$\frac{r_i}{r_j} = \left(\frac{Q_i R^*_{sub,i}}{Q_j R^*_{sub,j}} \right)^{\frac{1}{4}} \tag{9}$$

with Q_i and Q_j the respective flow of segments i and j.

Instead of storing the absolute radius for each segment, we consider the ratio between parent and its children: $\beta_k^i = r_i/r_k$ and $\beta_k^j = r_j/r_k$ with i and j the children, k the parent segment. Because of the tree respects Murray's law, these ratios can actually be calculated directly from the ratio between children segments (see annexe for details):

$$\beta_k^i = \left(1 + (\frac{r_i}{r_j})^{-\gamma} \right)^{-\frac{1}{\gamma}} \text{ and } \beta_k^j = \left(1 + (\frac{r_i}{r_j})^{\gamma} \right)^{-\frac{1}{\gamma}} \tag{10}$$

Calculating the reduced resistance for each children with (8), and knowing the flow, we obtain the children radius ratio from (9), which is used to calculate the β values, stored with the parent segment properties. The subtrees distal to the new bifurcation remain constant and unaffected by the addition of the new branch, whereas upstream bifurcations are updated following this exact same process. By this method, called "balancing of bifurcation ratios", ~~the~~ radius rescaling is propagated up the tree.

1.3.4 Measure target function

Calculate the root radius from

$$r_{root} = \left(R^*_{sub,root} \frac{Q_{perf}}{P_{perf} - Q_{term}} \right)^{\frac{1}{4}} \tag{11}$$

Then for each segment we obtain the radius from:

$$r_i = r_{root} \prod_{k=i}^{root} \beta_k \tag{12}$$

So we can calculate the total tree volume, that is the target function to minimize:

$$T_i = l_i^{\mu} r_i^{\lambda} \tag{13}$$

1.3.5 Select best connection between neighbors

We store the target function result in the Connection Evaluation Table (CET), for each of the tested neighbor connection. The connection with the lowest result (minimum tree volume) is considered as the optimal one and definitely added to the tree, with the consequent flow and resistance updates.

If the CET doesn't contain at least two plausible connections among the N_{con} tested, then we extend the research to the N_{max} neighbor segments. If there is still not two plausible connections, we reject the tested location n_{loc} and start again the loop to add a new segment with a new random location. By plausible connection we mean the local optimization converges, with no degenerate segment and no crossing of any other tree segment.

1.4 Example of results

1.4.1 2D

1.4.2 3D

2 Local optimization: single bifurcation scale

Kamiya proposes a numerical solution to determine minimum volume bifurcation under restriction of physiological parameters, determinant pressure and flow, and locations of origin and terminals.

This method built in 2D assumes the flow to be laminar and vessels are composed of straight ducts lying on a plane.

Note: Karch found that the optimum positions of the bifurcations in their 3D model trees were always found to lie in the plane defined by the endpoints of the respective three neighboring segments, which is consistent with the literature [4].

Process: iterative nested loops

Defining a starting position as the convex average of origin and terminal locations, weighted by respective flows.

$$(x, y) = (\frac{f_0 x_0 + f_1 x_1 + f_2 x_2}{2 f_0}, \frac{f_0 y_0 + f_1 y_1 + f_2 y_2)}{2 f_0}) \tag{14}$$

Calculate each segment length.

$$l_i^2 = (x - x_i)^2 + (y - y_i)^2 \tag{15}$$

Numerically calculate the new radii r_0, r_1,r_2. They are expected to satisfy both Hagen-Poiseuille's law and volume minimization.

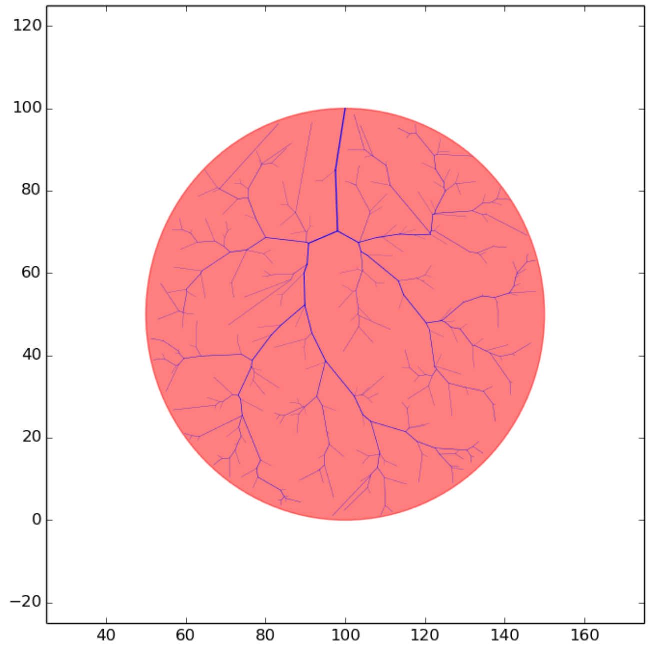


Figure 2: CCO in 2D: 250 Nterm tree generated in 9 min. Note:The terminal pressure is adapted to the number of terminal segments, P_{term}=63 mmHg

When location of origin and two terminals segments, their pressure, and their flows are given, according to Hagen - Poiseuille's law:

$$\Delta P_1 = P_1 - P_0 = \kappa(\frac{f_0 l_0}{r_0^4} + \frac{f_1 l_1}{r_1^4}), \tag{16}$$

$$\Delta P_2 = P_2 - P_0 = \kappa(\frac{f_0 l_0}{r_0^4} + \frac{f_2 l_2}{r_2^4}) \tag{17}$$

According to Kamiya, differentiating the tree volume with x, y and r_0 and equating them to zero, one obtains:

$$\frac{r_0^6}{f_0} = \frac{r_1^6}{f_1} + \frac{r_2^6}{f_2} \tag{18}$$

and

$$x = \frac{x_0 r_0^2/l_0 + x_1 r_1^2/l_1 + x_2 r_2^2/l_2}{r_0^2/l_0 + r_1^2/l_1 + r_2^2/l_2}, y = \frac{y_0 r_0^2/l_0 + y_1 r_1^2/l_1 + y_2 r_2^2/l_2}{r_0^2/l_0 + r_1^2/l_1 + r_2^2/l_2} \tag{19}$$

The details of the path to these equations is provided in appendix.

Using $R = r^2$ in (18), we can express R_0 as:

$$R_0^3 = f_0\left(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2}\right) \tag{20}$$

Substituting this inside (17), one obtains the non linear system:

$$\begin{cases} \frac{\Delta P_1}{\kappa} R_1^2 \left(f_0\left(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2}\right)\right)^{\frac{2}{3}} - f_0 l_0 R_1^2 - f_1 l_1 \left(f_0\left(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2}\right)\right)^{\frac{2}{3}} = 0 \\ \frac{\Delta P_2}{\kappa} R_2^2 \left(f_0\left(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2}\right)\right)^{\frac{2}{3}} - f_0 l_0 R_2^2 - f_2 l_2 \left(f_0\left(\frac{R_1^3}{f_1} + \frac{R_2^3}{f_2}\right)\right)^{\frac{2}{3}} = 0 \end{cases} \tag{21}$$

We are looking for the root satisfying these equations using a non linear solver. If the solution converges, we get the new radii, that are needed to calculate the new position of the branching point in (19). This locations is a new input for the loop to iterate again (calculating length (15), then new radii (21), new location (19) and so on). If this iterative loop converges and the bifurcation total volume decreases, the bifurcation is solved and provided with optimal radii and position.

Note: in CCO the pressure is not determined all along vessels (only at the root and terminal segments). In order to adapt to our situation, we use an estimated radius to calculate the pressure drops using (17). At the first iteration the estimated radii are all equal to the segment's radius on which is connected the branch: $r_0 = r_1 = r_2 = r_{ori}$. Then, we will use the previously calculated radii to update the pressure drops at each iteration.

Example of results

Example of results on different type of bifurcations. For these example we used a tolerance of 0.01 and maximum number of iteration of 100.

In the figure 3 (a), for symetric flows and child locations: the optimal bifurcation point corresponds to convex average.

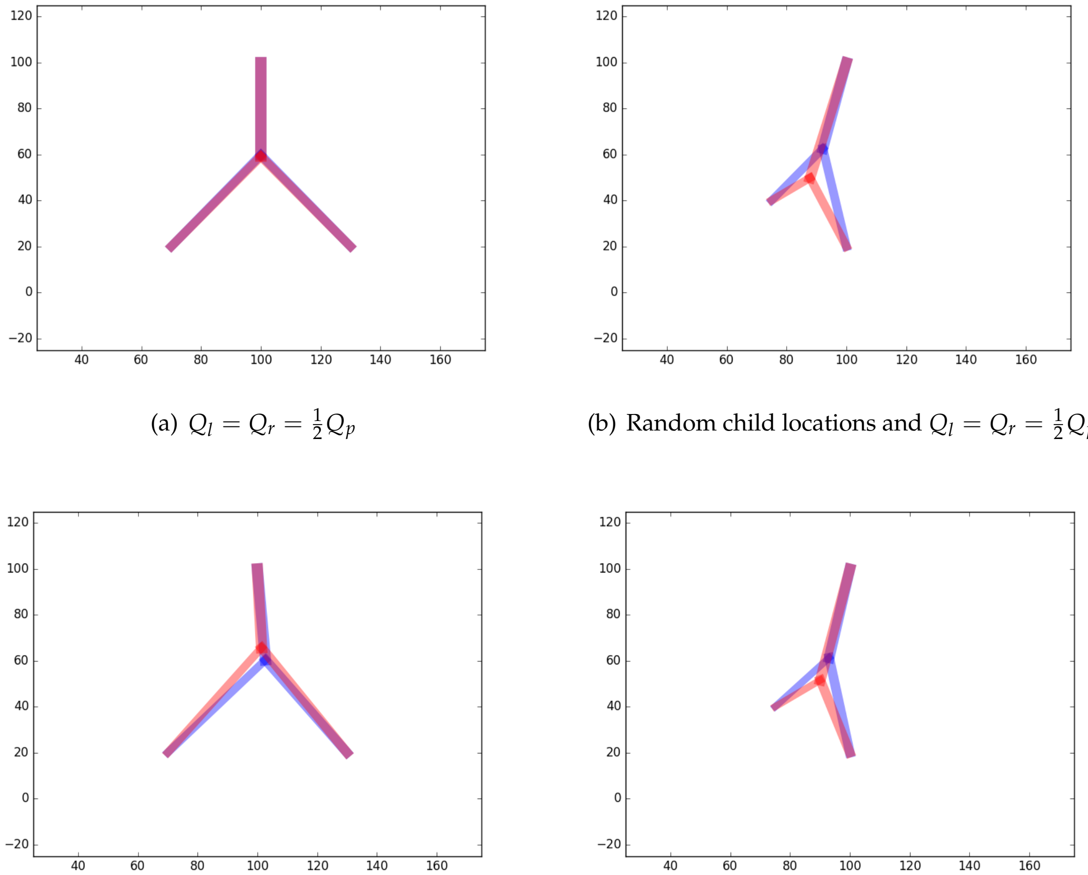
The figure 3 (b) illustrates well a Steiner solution to optimal network [5]: it is more advantageous to transport flows together by delaying bifurcation. In the fluid mechanics context, this subadditivity follows from Poiseuille's law, according to which the resistance of a tube increases when it gets thinner.

The figure 3 (c) shows influence of blood demand on the bifurcation geometry: because flow is more important on the right child, the radius is bigger and the bifurcation is dragged toward this child. Also, we note the bifurcation is less delayed than for symmetrical flows.

The figure 3 (d) shows influence of both destination and demand.

Karch implementation

Karch added lower and upper bounds to Kamiya's algorithm that ensures: (1) the bifurcation position within the perfusion volume; (2) the non degeneracy of the bifurcation to zero (by constraining segment length over segment diameter).



(a) $Q_l = Q_r = \frac{1}{2}Q_p$

(b) Random child locations and $Q_l = Q_r = \frac{1}{2}Q_p$

(c) $Q_l = \frac{1}{4}Q_p$ and $Q_l = \frac{3}{4}Q_p$

(d) Random child locations and $Q_l = \frac{1}{4}Q_p$, $Q_l = \frac{3}{4}Q_p$

Figure 3: In blue the starting bifurcation (convex average position), in red the final bifurcation after Kamiya's algorithm convergence reached (tolerance = 0.01). Convergence was reached at 15th, 24th, 31st and 21st iteration respectively in (a),(b),(c),(d). Q_p is the flow in parent branch, Q_l and Q_r are flows in left and right children.

Conclusion

Appendices

Equation (18), from Kamiya & Togawa 1972 equation (6)

Kamiya uses Murray definition at equation (7) from Physiological principle of minimum work [6] that he calls the simplest requirement for efficiency in the circulation:

$$f = kr^3$$

With k being a constant, so that the flow of blood past any section shall everywhere bear the same relation to the cube of the radius of the vessel at that point. Using it as:

$$r_i^3 = \frac{r_i^6 k}{f_i}$$

and combining it this with Murray's law,

$$r_0^\gamma = r_1^\gamma + r_2^\gamma \text{ with } \gamma = 3$$

where r_0 is the parent radius, r_1 and r_2 are the children radii, one obtains:

$$\frac{kr_0^6}{f_0} = \frac{kr_1^6}{f_1} + \frac{kr_2^6}{f_2}$$

that can be simplified into equation (18).

Equation (19), from Kamiya & Togawa 1972 equation (7)

We have

$$V = \pi(r_0^2 l_0 + r_1^2 l_1 + r_2^2 l_2) \tag{22}$$

and

$$\begin{aligned} l_0^2 &= (x - x_0)^2 + (y - y_0)^2 \\ l_1^2 &= (x - x_1)^2 + (y - y_1)^2 \\ l_2^2 &= (x - x_2)^2 + (y - y_2)^2 \end{aligned}$$

We rewrite (22)

$$V = \pi(r_0^2\sqrt{(x - x_0)^2 + (y - y_0)^2} + r_1^2\sqrt{(x - x_1)^2 + (y - y_1)^2} + r_2^2\sqrt{(x - x_2)^2 + (y - y_2)^2})$$

We derive each term with respect to x.

$$\frac{\partial}{\partial x}\sqrt{(x - x_0)^2 + (y - y_0)^2} = \frac{x - x_0}{\sqrt{(x - x_0)^2 + (y - y_0)^2}} = \frac{x - x_0}{l_0},$$

same for the x_1 and x_2 term, so we have

$$\frac{\partial V}{\partial x} = \pi\left[\frac{r_0^2(x - x_0)}{l_0} + \frac{r_1^2(x - x_1)}{l_1} + \frac{r_2^2(x - x_2)}{l_2}\right] = 0$$

Discarding the π factor and separating the terms,

$$x\frac{r_0^2}{l_0} + x\frac{r_1^2}{l_1} + x\frac{r_2^2}{l_2} = x_0\frac{r_0^2}{l_0} + x_1\frac{r_1^2}{l_1} + x_2\frac{r_2^2}{l_2}$$
$$x(\frac{r_0^2}{l_0} + \frac{r_1^2}{l_1} + \frac{r_2^2}{l_2}) = x_0\frac{r_0^2}{l_0} + x_1\frac{r_1^2}{l_1} + x_2\frac{r_2^2}{l_2}$$

and so

$$x = \frac{x_0\frac{r_0^2}{l_0} + x_1\frac{r_1^2}{l_1} + x_2\frac{r_2^2}{l_2}}{\frac{r_0^2}{l_0} + \frac{r_1^2}{l_1} + \frac{r_2^2}{l_2}}$$

This is one half of Eq.(7) in Kamiya & Togawa. The other half is obtained by substituting x with y everywhere. This is correct but not 100% satisfying since the l_i depend on x and y.

References

1. Rudolf Karch, Friederike Neumann, Martin Neumann, and Wolfgang Schreiner. A three-dimensional model for arterial tree representation, generated by constrained constructive optimization. *Computers in biology and medicine*, 29(1):19–38, 1999.

2. Akira Kamiya and Tatsuo Togawa. Optimal branching structure of the vascular tree. *The Bulletin of mathematical biophysics*, 34(4):431–438, 1972.

3. Wolfgang Schreiner and Peter Franz Buxbaum. Computer-optimization of vascular trees. *Biomedical Engineering, IEEE Transactions on*, 40(5):482–491, 1993.

4. M Zamir and H Chee. Branching characteristics of human coronary arteries. *Canadian journal of physiology and pharmacology*, 64(6):661–668, 1986.

5. Marc Bernot, Vicent Caselles, and Jean-Michel Morel. *Optimal transportation networks: models and theory*, volume 1955. Springer Science & Business Media, 2009.

6. Cecil D Murray. The physiological principle of minimum work i. the vascular system and the cost of blood volume. *Proceedings of the National Academy of Sciences*, 12(3):207–214, 1926.