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Geometrical and topological optimization and their relation to the bifurcation laws in optimized arterial tree models

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Abstract

In generating models of vascular trees, the method of Constrained Constructive Optimization (CCO) draws on the assumption that optimization criterions can be utilized to derive the geometrical and structural features of the tree models, without using informations from topographic anatomy. The boundary conditions imposed describe pressures and flows at the inlet and outlets of the binary branching model tree as well as the ratios of radii at a bifurcation ("power-law" for bifurcations).

During phylogenesis of species, bifurcation laws, tree geometry and tree topology have most likely been simultaneously optimized. In contrast, a supposed optimum form of bifurcation law is prescribed in the CCO-simulation, and geometry together with structure are optimized "within" that frame.

It is shown that CCO trees optimized under different bifurcation laws initially show slightly different geometries but identical topological structures. At a certain stage of development, however, accumulated geometric deviations lead to changes in topology as a result of optimization. From there on we observe different "evolutionary paths" of tree development.

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Finally we demonstrate that each fully developed tree can be rescaled to any given bifurcation law in order to be compared to another model tree actually optimized under the respective form of bifurcation law. Quantitative differences are evaluated and discussed.

Introduction

Vascular trees fulfill the crucial task of carrying blood to the tissue and removing metabolic endproducts therefrom. Many efforts have been made to gain a thorough understanding of the hemodynamic details of blood transport for both improved diagnosis and therapy. Over the last decade computer simulation has emerged as a potent tool to model blood flow, based on mechanical models of the respective arterial trees.

The first and most simple approach was a compartmental representation, where properties (resistances, compliances) of whole classes of vessel segments are lumped into several compartments (Bruinsma [1]). Evidently such models cannot represent details in structure and lend themselves only for obtaining global results. A second approach is the "anatomical" modeling (Rooz [2]) of small portions of arterial trees, where topographic information is directly represented by corresponding models of arterial segments. These models are "accurate" in detail, they cannot represent the complete vascular system of an organ, however. A third approach, namely self similar arterial tree models offer detailed structures which also reproduce the features of real arterial trees in a statistical sense (West [3], Pelosi [4], Dawant [5], Levin [6]). However, the geometrical arrangement of vessel segments in these "fractal" models follows *ab initio* rules rather than being adapted to the physiological needs of blood supply.

We therefore established a new method of generating dichotomously branching models for arterial trees combining the benefits of the approaches discussed above. This method, called **C**onstrained **C**onstructive **O**ptimization (CCO), starts from first principles:

- Blood should be distributed as evenly as possible over the whole part of tissue to be perfused.
- A given pressure (p_{term}) should be available to perfuse the microcirculation distal to the CCO-model.
- At each bifurcation the radii of vessel segments should fulfill a "bifurcation law" adapted to results found in real arterial trees (Arts [7], Zamir [8], Sherman [9], Zamir [10]). We choose $\gamma = 2.55$ for the so called "bifurcation exponent" (Zamir [11], Zamir [12]).
- Structure and geometry of the CCO-model tree should be designed such that a given optimization target function, being calculated from the model tree as

a whole, is minimized (Thompson [13], Cohn [14], Cohn [15], Zamir [16], Lefevre [17], In the present work we select total intravascular volume as optimization target (Sherman [9], Kamiya [18]).

In principle, CCO generates the model tree by successively adding new terminal segments while preserving all constraints throughout the process of model growth. Each step of growth is governed by geometrical optimization nested within structural optimization, both types of optimization being performed according to the same target function. Details of the method and the algorithm have been reported in previous papers (Schreiner [19], Schreiner [20]).

Method of CCO

The model itself consists of straight cylindrical tubes, rooting at the boundary of the perfusion area and bifurcating so as to spread all over the perfusion area. The entrance to the network (root segment) is perfused by a pressure p_{perf} with the flow Q_{perf} whereas each terminal segment yields the same flow ($Q_{\text{term}} = Q_{\text{perf}} / N_{\text{term}}$) (CCO-boundary conditions). Segment radii are chosen to have resistances according to POISEUILLE'S law (Fung [21]) which entail exactly the flow distribution described above.

At each bifurcation the radii of the parent segment (r_0) and the radii of the larger (r_1) and smaller (r_2) daughter fulfill a „bifurcation law“

$$r_0^{\gamma} = r_1^{\gamma} + r_2^{\gamma} \qquad \textbf{eq. 1}$$

The bifurcation exponent is chosen as $\gamma = 3$ according to morphometrical measurements in human coronary arteries (Zamir [8]). Note that the method of CCO is feasible for any choice of $\gamma > 0$, with reasonable values lying in the range $2.5 \leq \gamma \leq 3$. It can be shown that the boundary conditions together with the bifurcation law can be implemented in any dichotomously branching tree, regardless of its connective structure and geometry.

A second prerequisite - besides the possibility of implementing the boundary conditions - is the selection of an optimization target function characterizing the degree of optimality of the model. The most well-known candidate is the total intravascular volume which will be used throughout the present work. In more general terms (and disregarding constant factors irrelevant for optimization) we may define

$$T(\lambda) = \sum_{i=1}^{N_{tot}} l_i \cdot r_i^{\lambda} \qquad \textbf{eq. 2}$$

For $\lambda = 2$ this target is proportional to the intravasal volume (except for a factor π), for $\lambda = 1$ the target is proportional to the vascular surface (except for a factor $2 \cdot \pi$), for $\lambda = 0$ eq. 2 represents the total sum of segment lengths. $\lambda = 3$ and $\lambda = 4$ represent "hypervolumes" which have no direct interpretation but can easily be constructed as extensions of the concept. The differences in morphometric properties of the respective CCO trees have extensively been discussed before (Schreiner [22]).

Minimizing the total volume has been motivated by theoretical arguments (Sherman [9]) and will be used in generating the „reference tree“ for the present work. For a given connective structure and geometrical location of the segments the target function has a precisely defined value, provided the boundary conditions and the bifurcation law have been implemented. Any geometrical displacement of a bifurcation, even if all other segments tree remain at their positions, changes the value of the target function. This is easily seen by considering the fact that (in general) the three segments of the displaced bifurcation change in lengths. In order to reimplement boundary conditions and the bifurcation law, radii have to be rescaled in all segments along the path towards the root. This adjustment of radii together with changes in lengths of course changes the target function, cf. eq. 2.

Based on the above described prerequisites, the constructive element of CCO can be implemented as follows. Given a tree of k segments, which fulfills the boundary conditions and the bifurcation law, the next terminal segment is added as follows: The location of its distal end is drawn from a pseudo random number sequence and the segment is tentatively connected to its nearest neighbour. The new bifurcation is then optimized geometrically by a gradient method, the boundary conditions and bifurcation law being reimplemented after each incremental step of optimization. Then the new connection is desolved. In the same way the new terminal is testwise connected to each of its neighbours and the value of the target function for the optimized positions are compared. Finally that connection which yields the lowest minimum is made permanent.

This process of geometrical optimization, nested within a „search where to connect the new segment“, grows the model tree by two new segments. Repetition of this procedure is capable of growing very realistic models of arterial trees even on medium size computing facilities.

3 Results

3.1 Small Geometrical Differences Devide further Growth

The bifurcation exponent γ exerts a large influence on relative segment radii and, as a consequence, also determines the value of the optimization target function for a given geometry and topology. Hence the coordinates to which geometrical optimization converges for a particular bifurcation depend (slightly) on γ (even for identical locations of the distal ends of the terminal segments). In order to evaluate the consequences of this effect we generated two CCO trees with parameters totally identical except for the value of γ. In Figure 1 the small differences in segment locations can be noticed at careful inspection even by the naked eye in a tree with only seven terminal segments (upper panels). Yet the topologies (i.e. the connective structure) of both trees is still identical. Adding the 8^{th} terminal segment, however, shifts a switch: The optimum connection sites are found at different segments (shown in dark grey tone in the upper panels of Figure 1,) in the two trees with different γ, thereby initiating diverging future developments of both trees. In fact, the topological difference is much more striking than differences in geometric location. It is evident that totally different evolutionary paths are the consequence. The fully developed trees (with N_{term} = 2000) are shown in Figure 2.

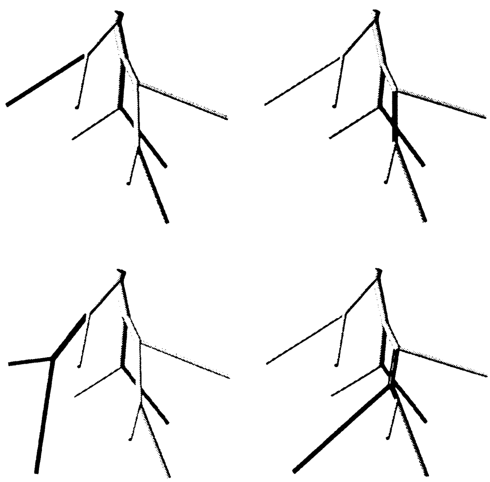

Figure 1: Early stages of development of CCO trees with different bifurcation laws. Left panels: $\gamma = 2$, right panels: $\gamma = 3$, cf. eq. 1. In both cases minimum intravasal volume is the optimization target. Up to 7 terminal segments topologies are equal (upper panels) while geometries differ slightly. When adding the 8^{th} terminal segment topologies (and as a consequence) also geometries diverge.

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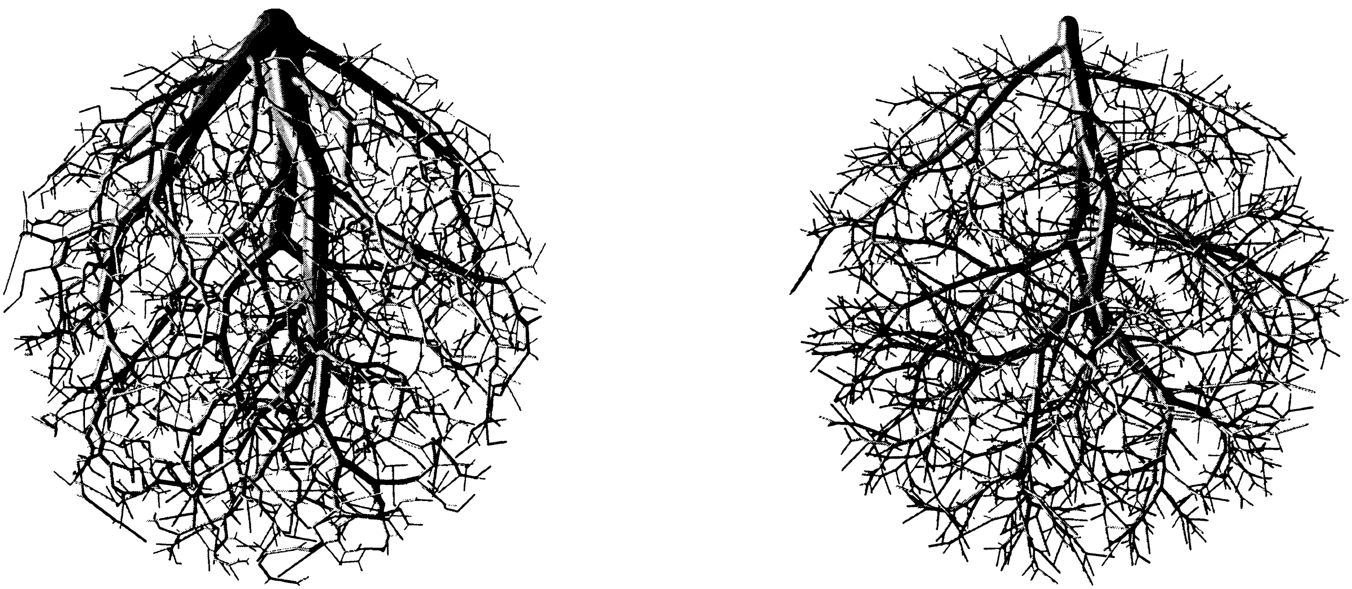

Figure 2: Fully developed CCO trees with 2000 terminal segments. Left panel: $\gamma = 2$, right panel: $\gamma = 3$. Optimization targets: Minimum intravasal volume.

3.2 Rescaling a CCO Tree to a Different Bifurcation Exponent

The algorithm of CCO is based on the fact that radii in any binary tree can be scaled so as to fulfill CCO boundary conditions. Even more, this can be achieved for arbitrary values of $\gamma > 0$. Besides generating CCO trees with different γ we may also change the bifurcation law *a posteriori*, as described in the following interesting investigation:

As a starting point we take a reference CCO model tree generated for $\gamma = 3$. For this particular topology and geometry we may re-calculate all radii (i.e. balance all bifurcation ratios (Schreiner [19])) in order to fulfill the very same boundary conditions regarding pressures and flows, **but for a different value of** $\gamma \neq 3$. This is always possible by starting at the terminals and in a post order traversal algorithm proceeding towards the root. In the process of tree generation, the balancing of bifurcation ratios is restricted to the respective path from the newly added segment towards the root. In the present investigation it extends over the whole tree but the method itself is (exactly) identical. CCO-trees thus offer the unique possibility to study the *net-impact* of different bifurcation exponents within trees of identical structures and segment coordinates.

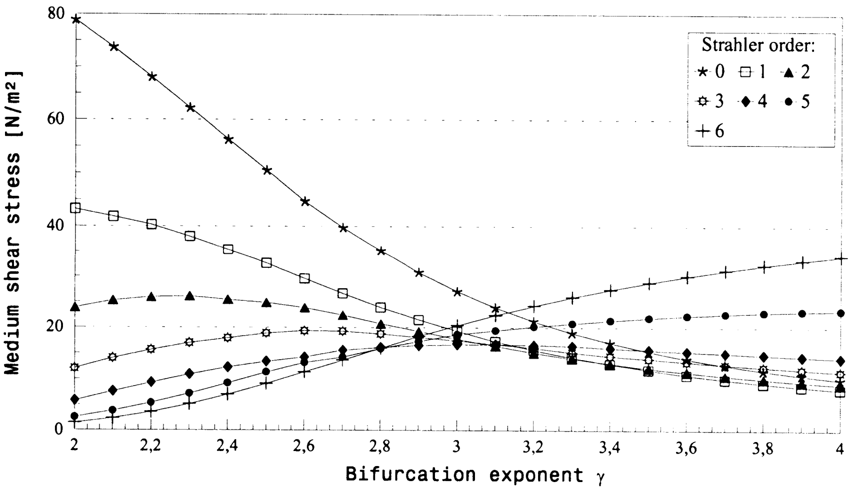

Figure 3: Shear stress under rescaling the bifurcation exponent. Within the topology and geometry of the CCO reference tree radii were rescaled to fulfill different bifurcation laws with $\gamma = 2.0$, 2.1, ... 4.0. The median shear stress [N/m²] (y-axis) is displayed separately for each STRAHLER order as a function of the bifurcation exponent γ [dimensionless] (x-axis). For symbols see the legend.

The result is displayed in Figure 3 for the shear stress between the blood and the vessel wall. Generally, rescaling radii to a different bifurcation law redistributes shear stresses drastically (roughly speaking) between large and small segments. For small segments (belonging to low STRAHLER orders) shear stress declines as γ is increased, cf. Figure 3. Conversely for large segments (belonging to high STRAHLER orders) shear stress increases with γ. The reason is simply that increasing γ makes small segments thicker on the expense of large ones, so as to keep overall resistance constant.

4 Discussion

Shear stress between blood and the arterial wall is attributed a key role in the activation of thrombocytes proceeding possible thrombus formation. Hence considerable engineering skills have been invested so as to avoid exceedingly high shear stress rates in any manmade device being implanted into the vascular system and directly exposed to the blood stream. Thus we may speculate that nature, during the evolution of species, also has optimized vascular geometry so as to reduce shear stress whenever possible, or at least to achieve a fairly homogeneous distribution.

The interest of people generating vascular models was therefore always attracted by the fact that *only a bifurcation law with* $\gamma = 3$ *is able to permit totally uniform shear stress* in the parent and daughter segments of a bifurcation. $\gamma = 3$ may be considered a kind of optimum selection. In CCO models for example, this optimum selection of the bifurcation law can be plugged in as a constraint rather than being a result of the optimization proper. However, since $\gamma = 3$ is only a *necessary* but not a *sufficient* condition for uniform shear stress, we encounter a spectrum of shear stress rather than a unique value. Thus, optimality regarding shear stress can only be judged according to the width of its spectrum, i.e. the range of values in Figure 3.

Rescaling for different values of γ shows clearly that median shear stresses in all STRAHLER orders are most close together around $\gamma = 3$. This finding indicates that the necessary condition (for uniform shear stress) is indeed also the most optimum one in terms of yielding the least possible spread of shear stress.

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