Numerical Simulation of Transport and Diffusion in Drainage Media

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Outline

- medical background
- generate appropriate geometry
- advection problem
- coupling to
- diffusion problem
- results

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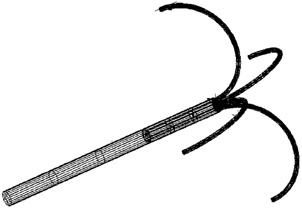
Medical Background

- liver carcinoma
- minimally invasive treatment: RF ablation



- destroy tumor by heating, preserve surrounding tissue
- heat conduction (diffusion) and blood flow (advection)
- body responds by increasing blood flow

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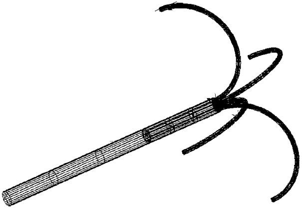

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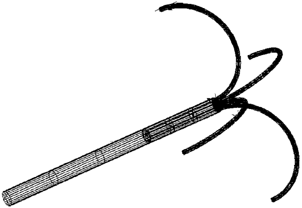

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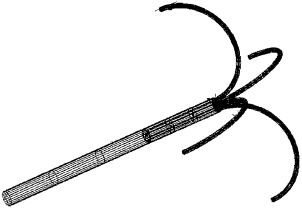

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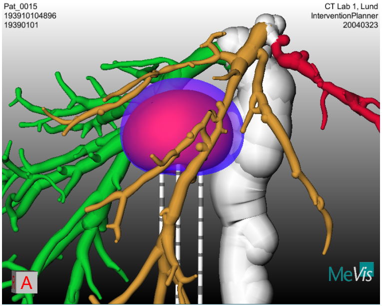
Modelling: State of the Art

- joint project with MeVis and others
- 3D heat conduction with stationary blood vessels



Our Model Problem

aim:

- develop method for 1D advection through vessels systems
- coupling with heat conduction in surrounding tissue

Model: reduce to 2D

- blood vessels: 1D straight line segments (pipes, ∅-area)
- arteries form binary tree: bifurcations
- same for veins
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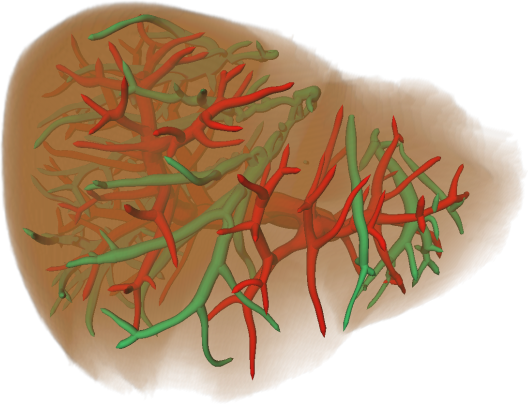
Blood Vessels in 3D Liver



Vessel Trees in 2D

- pairs of arterial and venous vessel tree do not appear in nature
- fundamentally different from 3D
- need to generate artificially

Generating Geometric Structure of 2D Vessel Trees

Method originally for 1 binary tree [Schreiner et al.], uniform blood supply for given domain.

- start with initial tree configuration
- add new terminal nodes one-by-one to each tree in turn
- random position
- find optimal connection
- verify feasibility
- adapt radii

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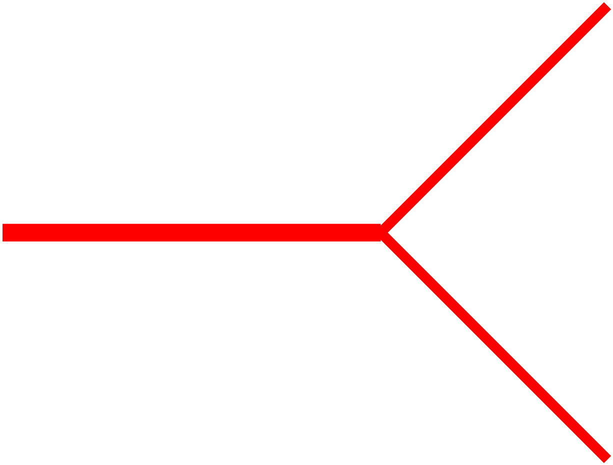

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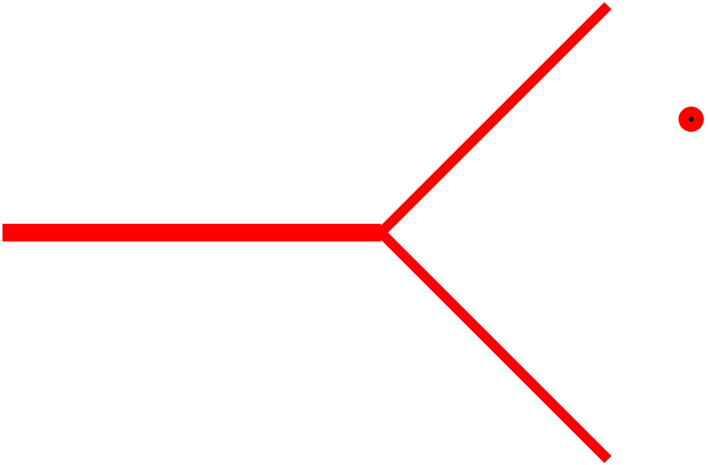
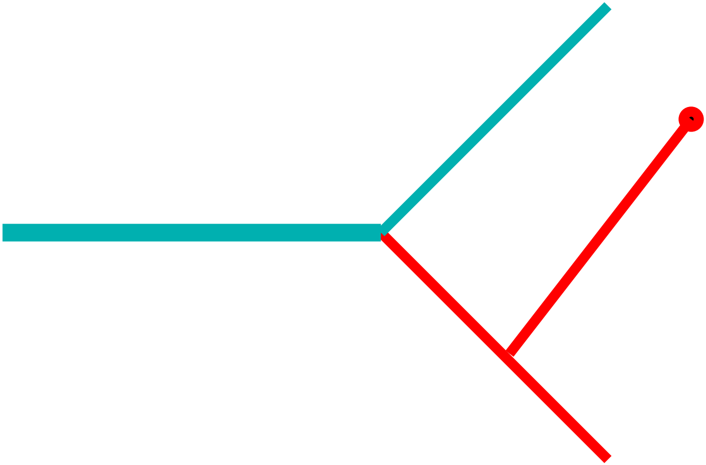


First Attempt



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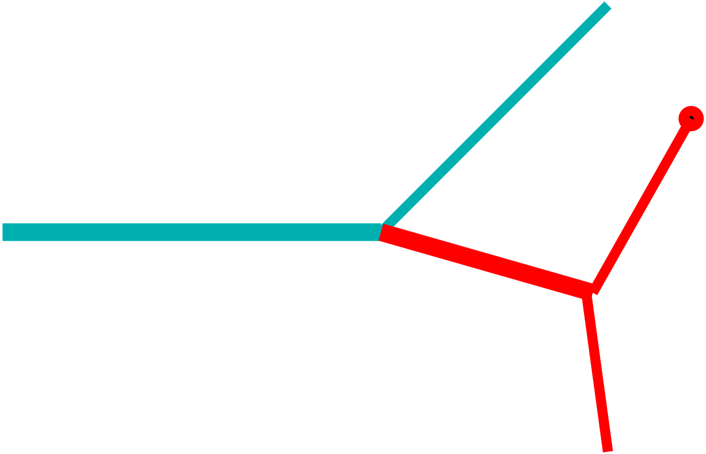

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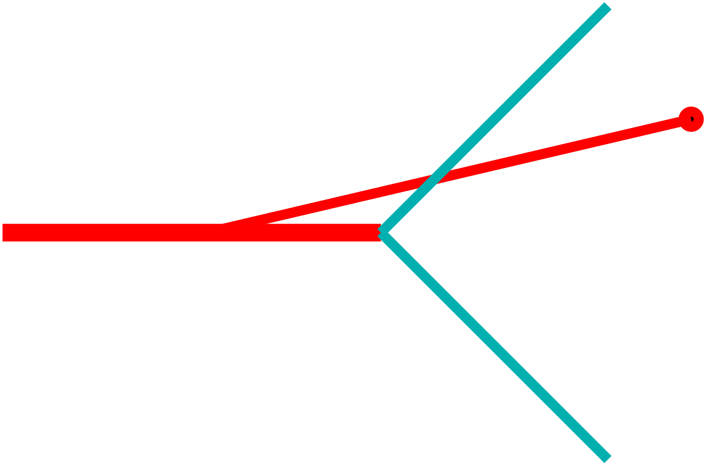

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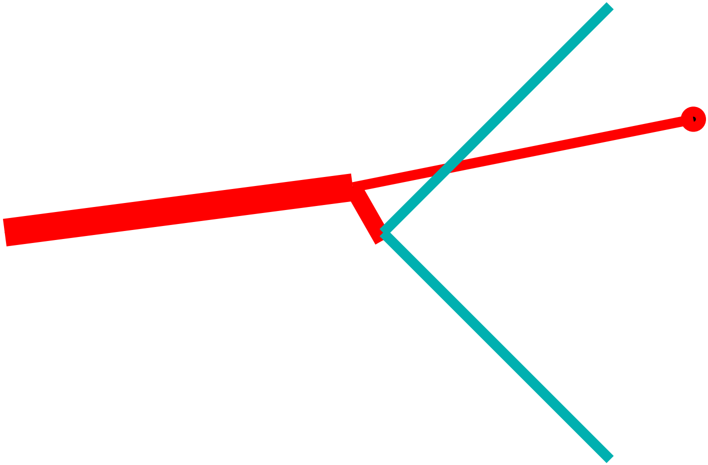

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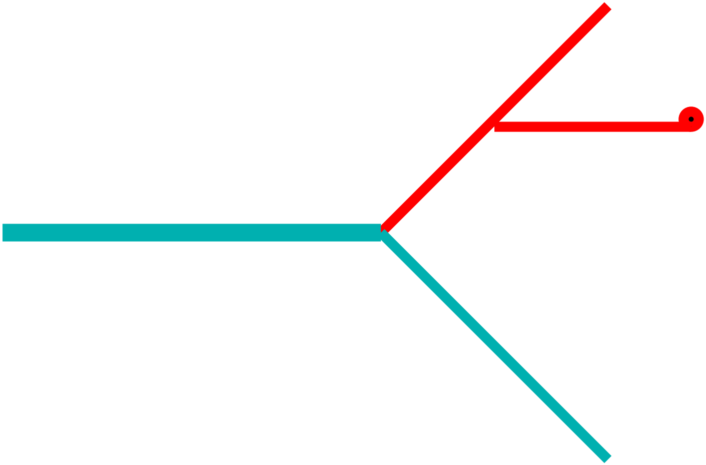

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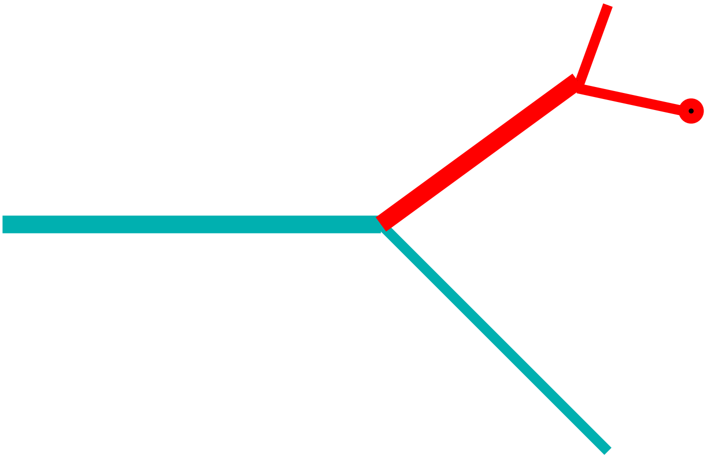
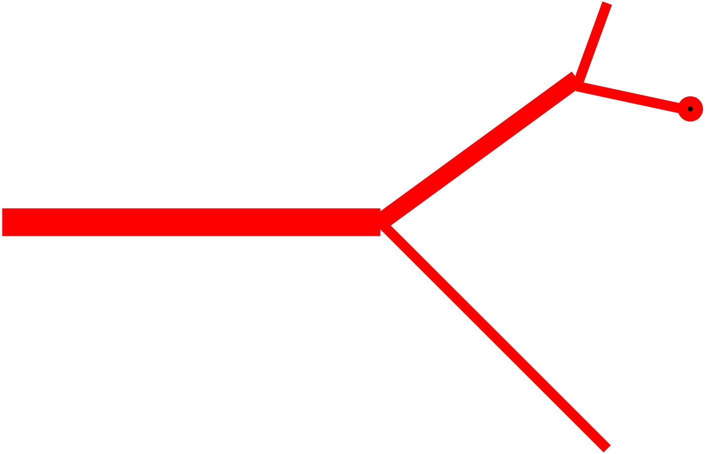
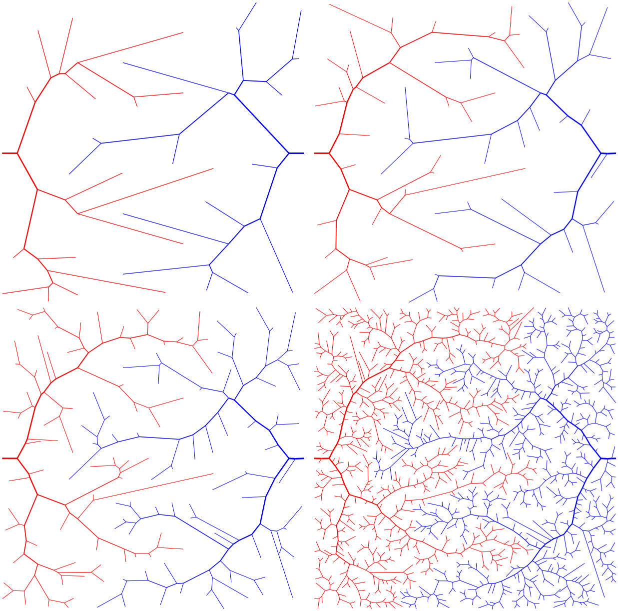


New Node Added



Generating Pairs of Trees



Flow Velocities for 2D Vessel Trees

- have geometric structure
- need flow velocities $\neq f(\text{radius})$

Idea for model:

- isotropic, incompressible flow through porous medium
- outflow out of terminal segments: S
- can express pressure $p = f(S)$ (PDE, steady state BVP)
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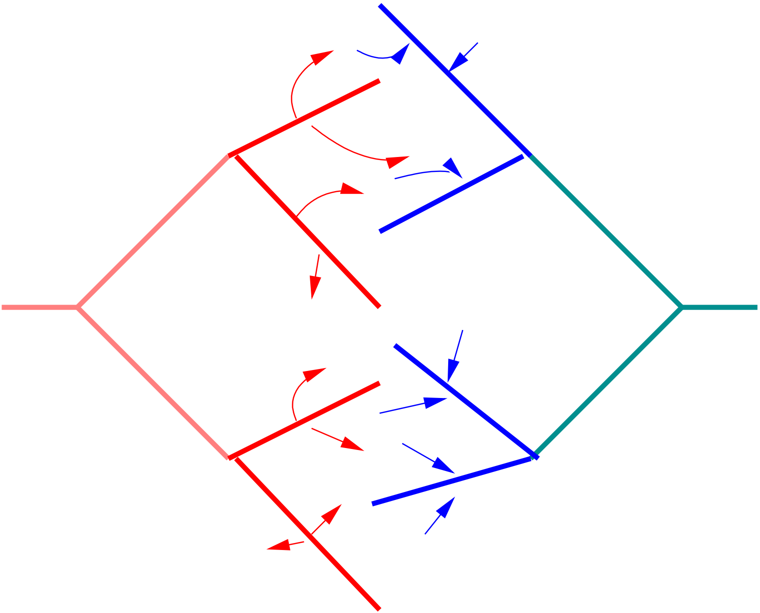
Blood Flow



Discrete Optimization Problem

Discretize tissue & obtain problem:

$$h(S) = A^T L^{-1} AS \cdot S \longrightarrow \min!$$

subject to

$$S \geq 0$$
$$\ell_a \cdot S = C = \ell_v \cdot S$$

nonnegativity and inflow = outflow = const.
Typically: tissue has 257×257 grid cells,

- $S \in \mathbb{R}^{1024}$
- $A : \mathbb{R}^{1024} \rightarrow \mathbb{R}^{66049}$
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Optimization Procedure

Quadratic optimization problem, but constraints are nasty.

- initial guess: S^0: uniform distribution
- generate sequence $S^{k+1} = S^k + \alpha^k d^k$:
  - d^k feasible descent direction:
  - i. e. $S^k + \epsilon d^k$ feasible and
  - $h(S^k + \epsilon d^k) < h(S^k)$ for small ϵ
  - α^k "good" step size

Problems:

- convergence is slow (need many steps)
- each step: many function evaluations
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Cascadic Approach

Expensive part of $A^t L^{-1} A$ is L^{-1}, complexity depends on tissue discretization.

Idea:

- solve on coarse grid
- take as initial guess for finer grid
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Compare to Multigrid.

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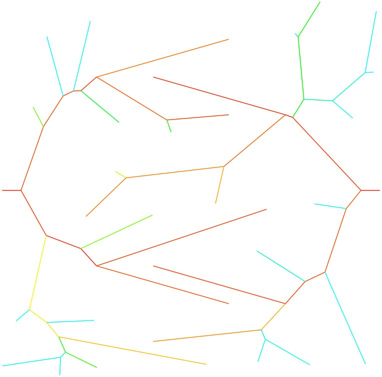
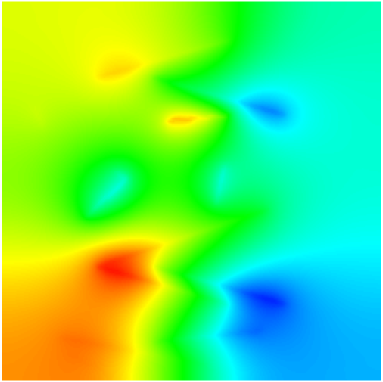
Resulting Velocities and Pressure





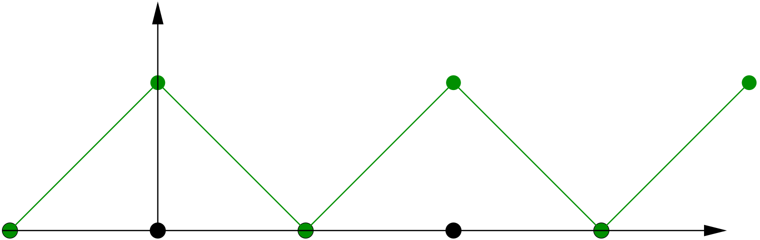
Transport Through the Vessel System

Now model transport through vessel system.
First consider single 1D segment.
Analytically, advection equation

$$\partial_t u(t,x) + v\partial_x u(t,x) = f(t,x)$$

is solved by tracking back along characteristics.

Why not Simply Trace Back along Characteristics?



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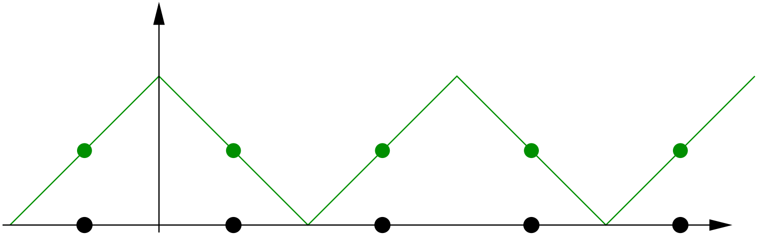

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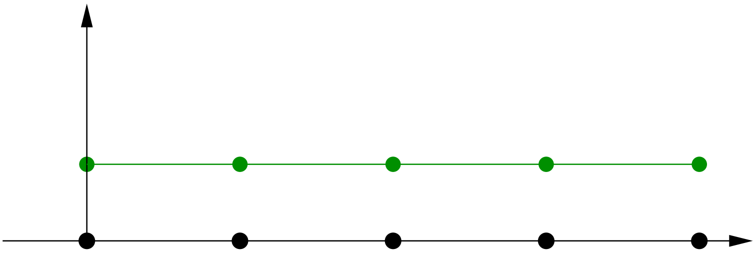

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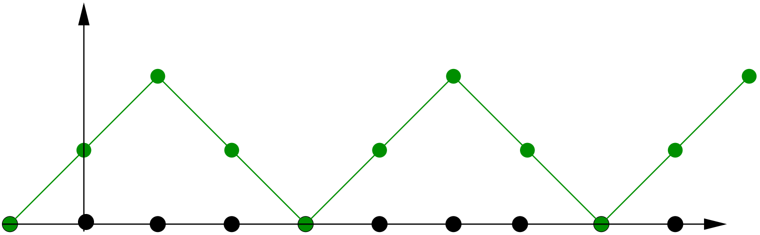

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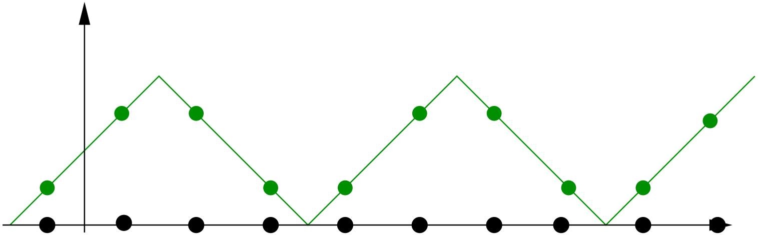

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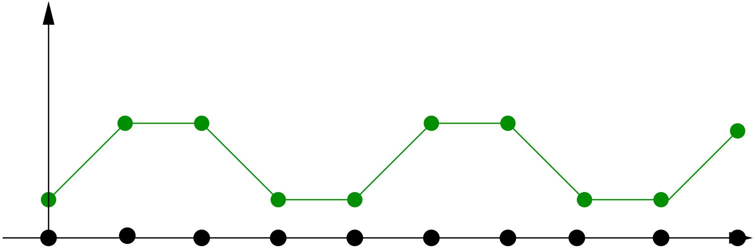
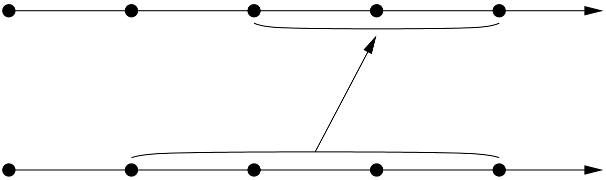


Advection on 1D segment

ELLAM [Celia et al.] scheme couples

- four values on old time level to
- three values on new time level



System of Equations

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\end{bmatrix}
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\end{bmatrix}
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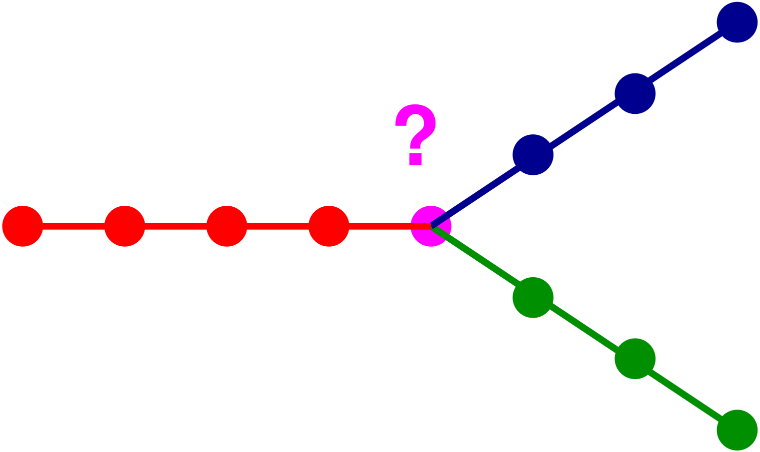
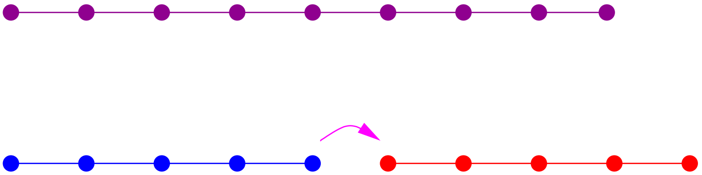
Where to Place Nodal Unknowns at Bifurcations?



Consistency at Monofurcation



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- explicitely compute outflow, use as inflow

Bad b/c artificially decoupled & computation necessary

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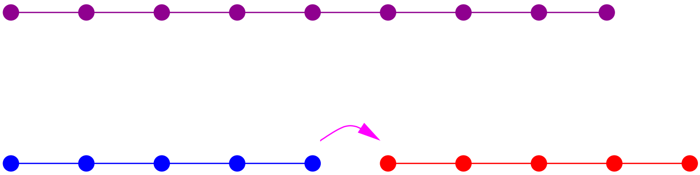

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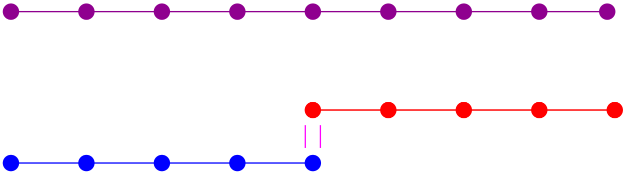

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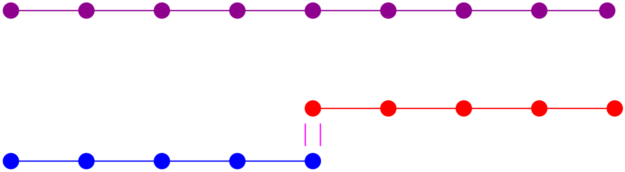

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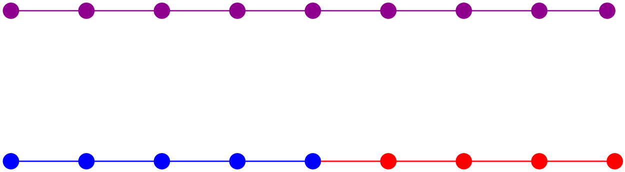

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Good: System not different from single segment case.

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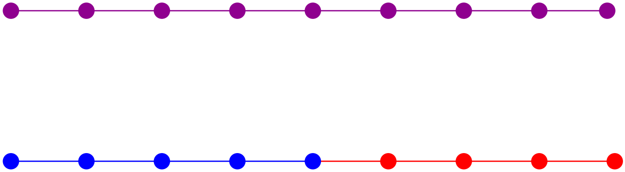

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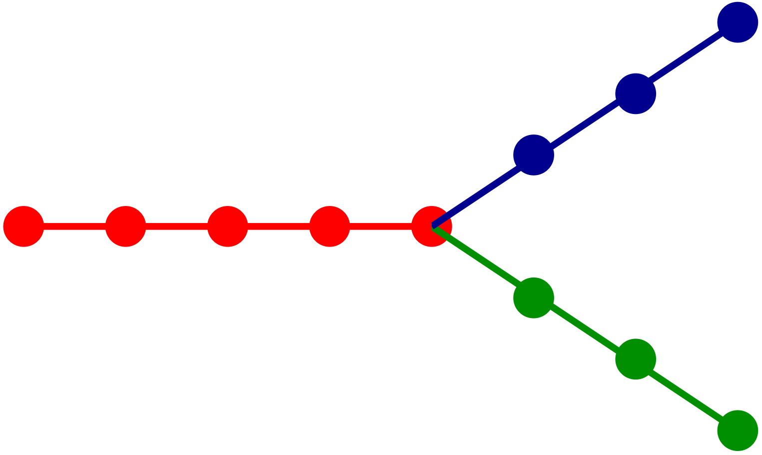
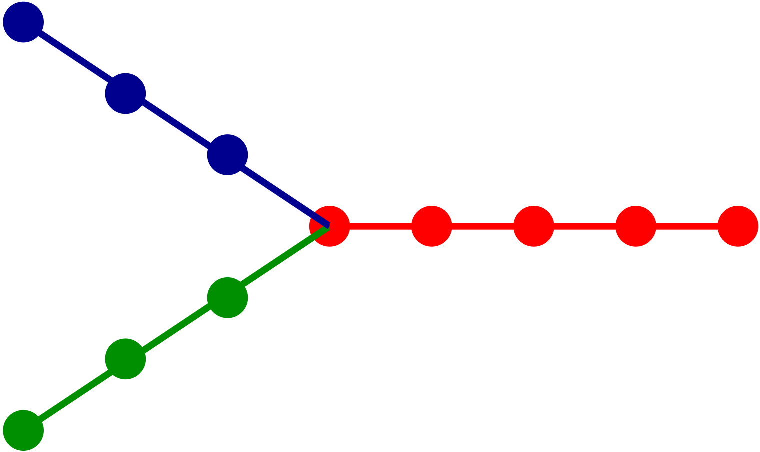


Block System for Arterial Bifurcations

$$M^{\prec}_{\text{BLOCK}} = \left[\begin{array}{c|c|c} \begin{array}{c} M_p \\ \qquad *1 \end{array} & \begin{array}{l} \\ *2 \end{array} & \begin{array}{l} \\ *2 \end{array} \\ \hline \begin{array}{r} *3 \\ \\ \end{array} & M_d^{\dashv} & \\ \hline \begin{array}{r} *3 \\ \\ \end{array} & & M_e^{\dashv} \end{array}\right]$$

$$M^{e,\prec}_{\text{BLOCK}} = \left[\begin{array}{c|c|c} \begin{array}{c} M_p^{e} \\ \qquad *4 \quad *5 \end{array} & \begin{array}{l} \\ *6 \end{array} & \begin{array}{l} \\ *6 \end{array} \\ \hline \begin{array}{rr} *7 & *8 \\ & *9 \end{array} & M_d^{\dashv,e} & \\ \hline \begin{array}{rr} *7 & *8 \\ & *9 \end{array} & & M_e^{\dashv,e} \end{array}\right]$$

Where to Place Nodal Unknowns at Venous Bifurcations



Block System for Venous Bifurcations

$$
M_{\text{BLOCK}}^{\succ} = \left[\begin{array}{c|c|c}
\begin{matrix} *1 & & \\ & M_p^e & \\ & & \end{matrix} & \begin{matrix} & & *2 \\ & & \\ & & \end{matrix} & \begin{matrix} & & *2 \\ & & \\ & & \end{matrix} \\ \hline
\begin{matrix} & & \\ & & \\ *3 & & \end{matrix} & \begin{matrix} & & \\ & M_d^{\vdash} & \\ & & \end{matrix} & \\ \hline
\begin{matrix} & & \\ & & \\ *3 & & \end{matrix} & & \begin{matrix} & & \\ & M_e^{\vdash} & \\ & & \end{matrix}
\end{array}\right]
$$

$$
M_{\text{BLOCK}}^{e,\succ} = \left[\begin{array}{c|c|c}
\begin{matrix} *5 & & \\ *8 & M_p & \\ & & \end{matrix} & \begin{matrix} & *6 & *4 \\ & & *7 \\ & & \end{matrix} & \begin{matrix} & *6 & *4 \\ & & *7 \\ & & \end{matrix} \\ \hline
\begin{matrix} & & \\ & & \\ *9 & & \end{matrix} & \begin{matrix} & & \\ & M_d^{\vdash,e} & \\ & & \end{matrix} & \\ \hline
\begin{matrix} & & \\ & & \\ *9 & & \end{matrix} & & \begin{matrix} & & \\ & M_e^{\vdash,e} & \\ & & \end{matrix}
\end{array}\right]
$$

Different Nature of the Trees

Arterial tree:

- one inflow
- temperature split continuously
- many outflows

Venous tree:

- many inflows
- discontinuous averageing of temperature
- one outflow

Terminal Segments

- Physically: outflow along terminal segments (not at terminal nodes)
- energy content (temperature content) drops off to zero
- constant temperature & apparent cross section area drops off to zero

Arterial terminal segments:

- Sink term depends on vessel temperature
- independent of surrounding tissue

Venous terminal segments:

- Source term depends on temperature of surrounding tissue
- independent of vessel temperature

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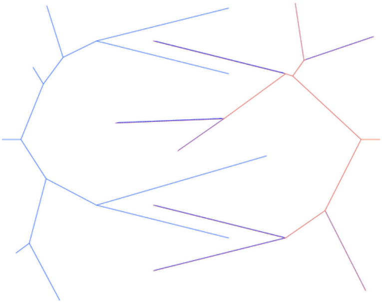
Advection on Trees

Video clip shows temperature contents:



Coupling to Heat Conduction: Exchange of Energy

Problem: Advection in tissue not modelled.

- Outflowing/Inflowing mass carries energy.
- Source / sink for tissue?

No. Steady state not modelled correctly. Instead:

- root and intermediate segments: exchange of temperature satisfying energy conservation
- arterial terminal segments: heating / cooling of tissue only if temperature difference
- venous terminal segments: no cooling effect on tissue

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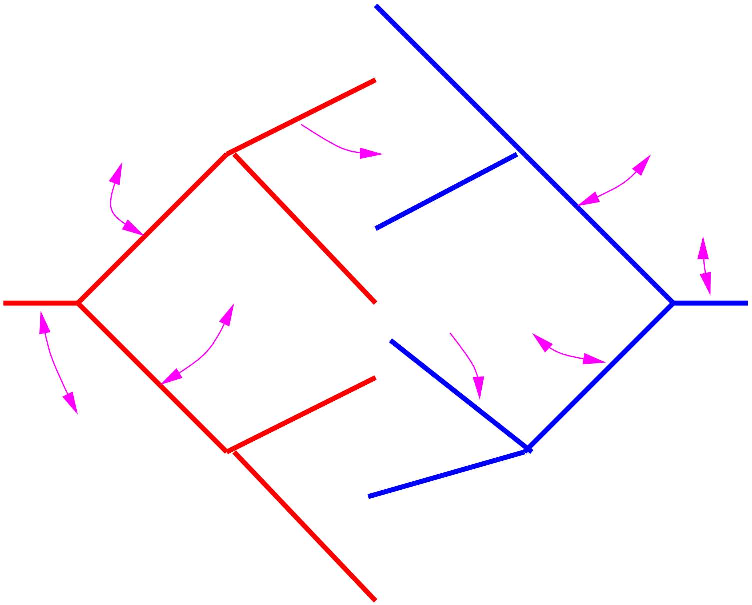
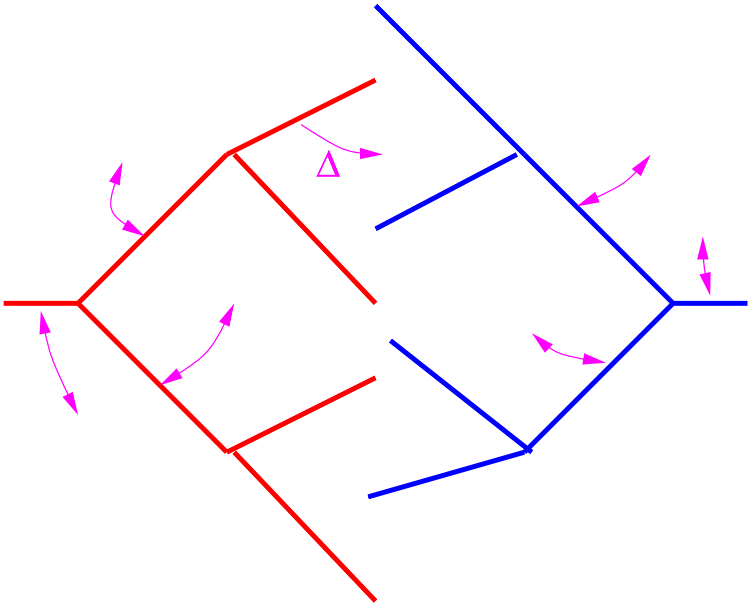
Exchange of Energy as Seen by Vessels



Exchange of Energy as Seen by Tissue



Heat conduction in Tissue

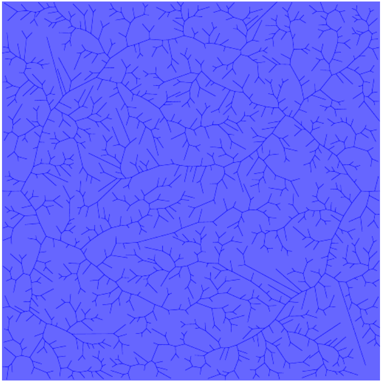
Heat conduction ($u(t,x)$ temperature, κ conductivity):

$$\partial_t u(t,x) - \kappa \Delta_x u(t,x) = f(t,x)$$

zero initial values, zero Neumann boundary values.
f on vessel trees (1D line segments) only, PDE meant in distributional sense.

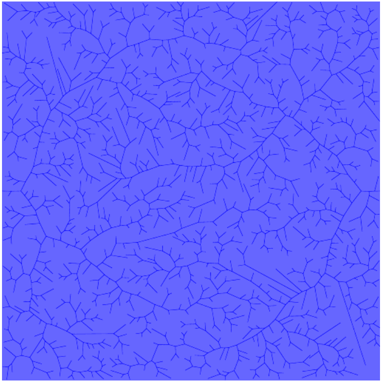
Pulses of Inflowing Warm Blood

Artificial problem: Inflowing pulses of warm blood, pulsed flow velocities.
Different color scales for tissue / vessel temperature.



Pulses of Inflowing Warm Blood

Now place RF probe near arterial vessel.
Same color scale for tissue / vessel up to opacity.



Summary

References

- M. A. Celia, T. F. Russell, I. Herrera, R. .E Ewing: An Eulerian-Lagrangian localized adjoint method for the advection-diffusion equation, Advances in Water Resouces 1990, 13(4), p 187–206
- W. Schreiner, M. Neumann et al.: The Branching Angles in Computer-Generated Models of Arterial Trees, J. Gen. Physiol., 105:979–989, 1994
- T. Preusser, H.-O. Peitgen et al.: Simulation of Radio-Frequency Ablation using Composite Finite Element Methods. Proceedings of the Scientific Workshop Medical Robotics, Navigation and Visualization, Rhein-Ahr-Campus Remagen 2004.
- L. O. Schwen: Numerical Simulation of Transport and Diffusion in Drainage Media, Diplomarbeit, Universität Duisburg-Essen, November 2005