Numerical Simulation of Transport and Diffusion in Drainage Media

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Outline

- introduction, medical problem
- generate appropriate geometry
- advection through blood vessels
- diffusion in tissue
- coupling

Introduction

- RF ablation of tumors:
- numerical simulation of thermal processes
- heat diffusion in tissue
- transport of heat by blood flow through vessel system
- develop tools in 2D to keep things simpler

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2D Vessel Trees
- Geometric Structure
- Flow Velocities

Advection Problem
- Single Segments
- ELLAM
- Unknowns at Bifurcations
- Basis and Test Functions at Bifurcations
- Terminal Segments

Coupling to Diffusion Problem
- Exchange of Energy
- Heat Conduction in Tissue

Difference to 3D Case

3D vs 2D — what are the differences?

Blood vessels in 3D organs:

- can use "real" data obtained by medical imaging
- arterial and venous tree can "wind around each other"

In contrast, for 2D:

- no real-world data available for pairs of vessel trees
- need to generate appropriate system artificially
- individual segments have codimension 1

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Geometric Structure

- For simplicity: straight line segments & bifurcations
- Method by Schreiner et al. 1994 (for single tree): Constrained Constructive Optimization (CCO).
  - add nodes at random positions one-by-one
  - "optimize" connection to existing tree
- extended to pair of trees:
  - avoid mutual intersections
  - ensure minimum distance (in some sense)

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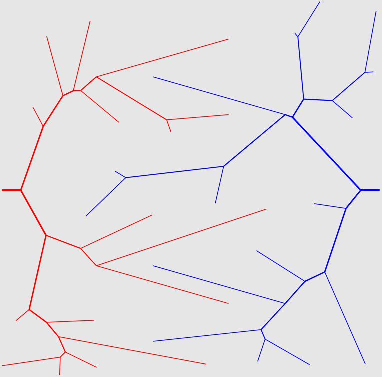
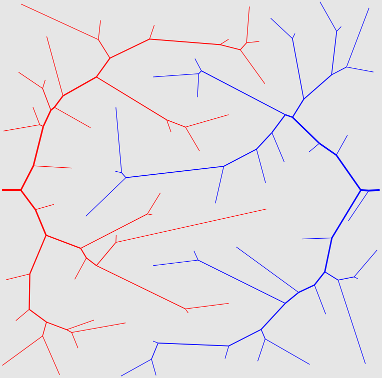
Pairs of Vessel Trees (geometric structure)





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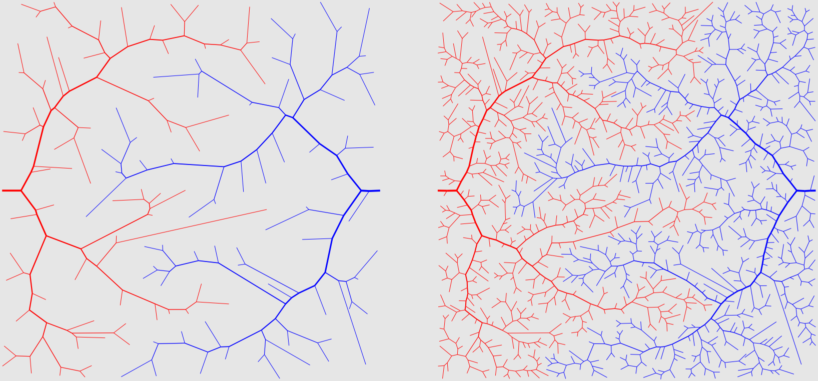

But what about flow velocities?

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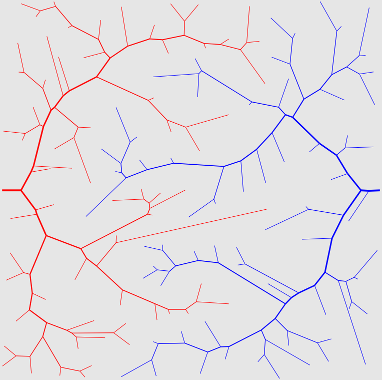

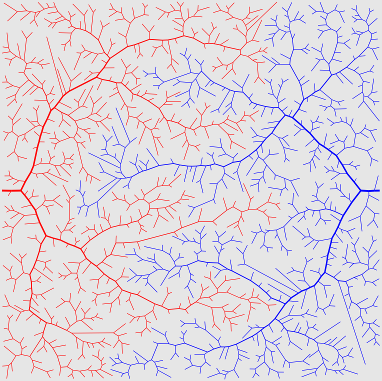

But what about flow velocities?

Flow Velocities

Balance flow velocities to avoid artificial wide-range components.

- Model: vector $S \in \mathbb{R}^{\approx 1000}$
  - outflow out of arterial terminal segments
  - inflow into venous terminal segments
  - both are assumed constant on each segment
  - mass conservation at bifurcations and in domain
- pressure p in domain depends on S via PDE
- minimize dissipation of kinetic energy by friction: $E(p) = \int_\Omega \nabla p \cdot \nabla p$
- discretize and optimize subject to "nasty" constraints

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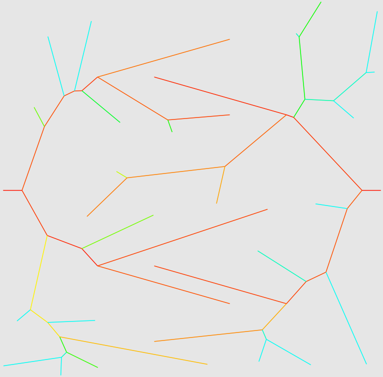
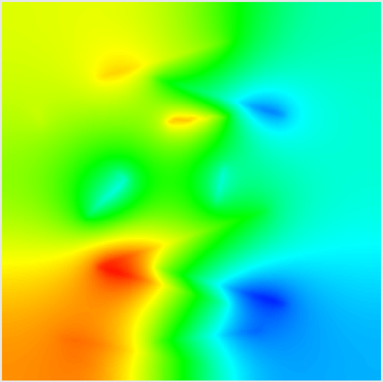
Flow velocities and pressure profile





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Advection Problem

Single Segments

ELLAM

Unknowns at Bifurcations

Basis and Test Functions at Bifurcations

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Advection in Vessel Trees: Overview

- single segments
- $\prec$ and $\succ$ bifurcations
- terminal segments
- trees

1D Advection

First consider 1D advection with constant velocity:

$$\partial_t u(t,x) + v\partial_x u(t,x) = f(t,x) \tag{1}$$

$u(t,x)$ is energy content (energy per length = energy density times cross section area).
To solve initial-boundary value problem numerically, use ELLAM (Eulerian-Lagrangian Locally Adjoint Method) by Celia et al. (1990)

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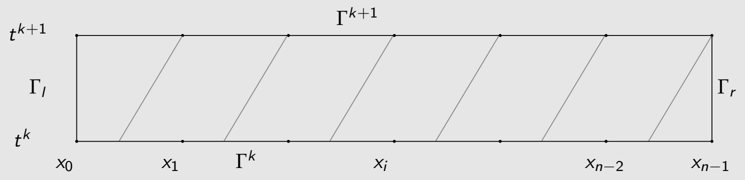
ELLAM

Obtain weak formulation by integrating over space-time rectangle



$$\int_0^\ell \int_{t^k}^{t^{k+1}} (\partial_t + v \cdot \partial_x)\, u \cdot w = \int_0^\ell \int_{t^k}^{t^{k+1}} f \cdot w \qquad (2)$$

ELLAM: for test functions w constant along characteristic curves.

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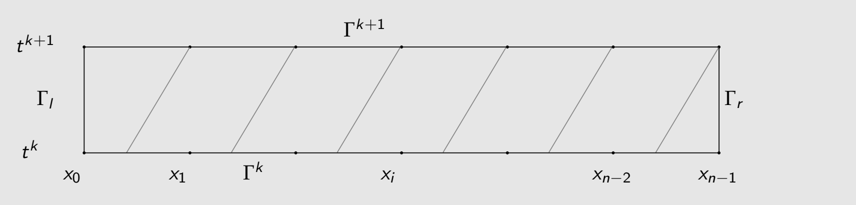

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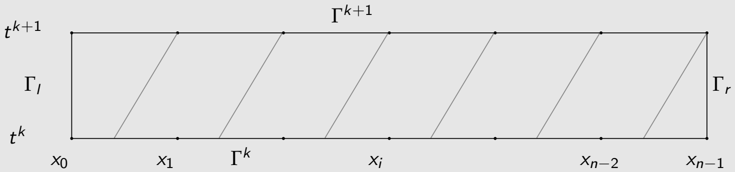

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Integrate by parts in space and time:

$$\begin{aligned}
&\int_{\Gamma^{k+1}} u(t^{k+1},x)\cdot w(t^{k+1},x)\,\mathrm{d}x - \int_{\Gamma^k} u(t^k,x)\cdot w(t^k,x)\,\mathrm{d}x \\
&+ \int_0^\ell \int_{t^k}^{t^{k+1}} u(t,x)\underbrace{(-\partial_t - v\cdot\partial_x)\,w(t,x)}_{=0 \text{ (ELLAM test function)}}\,\mathrm{d}t\,\mathrm{d}x \qquad (3)\\
&+ v\cdot\int_{\Gamma_r} u(t,\ell)w(t,\ell)\,\mathrm{d}t - v\cdot\int_{\Gamma_l} u(t,0)w(t,0)\,\mathrm{d}t \\
=&\int_0^\ell \int_{t^k}^{t^{k+1}} f(t,x)\cdot w(t,x)\,\mathrm{d}x\,\mathrm{d}t
\end{aligned}$$

Discretization

Basis functions:

- Nodal basis functions: piecewise linear hat functions,
- height = cross section area of segment
- discrete values are proportional to temperature

Test functions:

- At "new" time level: same shape as basis function,
- height = 1 (partition of unity)
- constant along characteristic curves
- roof-shaped in space-time

Restriction for time step: $v \leq 1 \frac{\text{grid cell}}{\text{time step}}$

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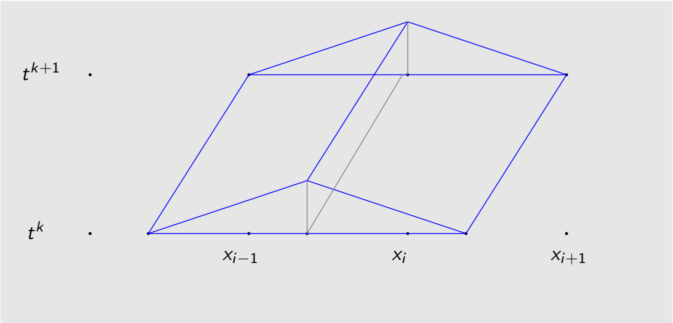
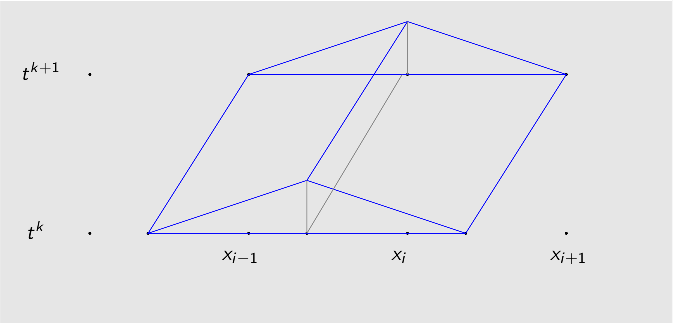


Evaluate products of base functions and test functions.

Test Functions



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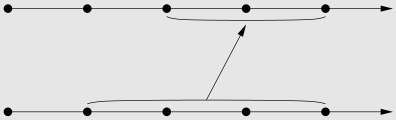
ELLAM

which leads to a scheme:



$$\begin{bmatrix} * & * & & & & \\ * & * & * & & & \\ & * & * & * & & \\ & & \ddots & \ddots & \ddots & \\ & & & * & * & * \\ & & & & * & * \end{bmatrix} \begin{bmatrix} \vdots \\ n \\ e \\ w \\ \vdots \end{bmatrix} = \begin{bmatrix} * & * & & & & & \\ * & * & * & & & & \\ * & * & * & * & & & \\ & \ddots & \ddots & \ddots & \ddots & & \\ & & & * & * & * & * \\ & & & & * & * & * \end{bmatrix} \begin{bmatrix} \vdots \\ o \\ l \\ d \\ \vdots \end{bmatrix}$$

Gaußian elimination?

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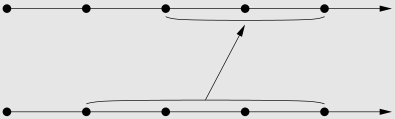

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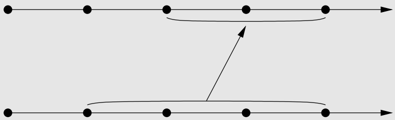

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Gaußian elimination?

Arterial Bifurcations

- Flow is split $\frac{A_d v_d}{A_p v_p} : \frac{A_e v_e}{A_p v_p}$.
- Temperature is split continuously
- temperature content is split $\frac{A_d}{A_p} : \frac{A_e}{A_p}$.

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Venous Bifurcations

- Flow is combined $\frac{A_d v_d}{A_p v_p} + \frac{A_e v_e}{A_p v_p}$.
- Temperature is combined discontinuously (weighted average of inflowing temperatures)
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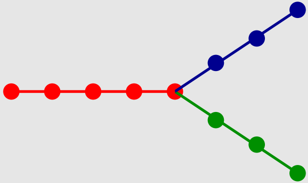
Location of Unknowns



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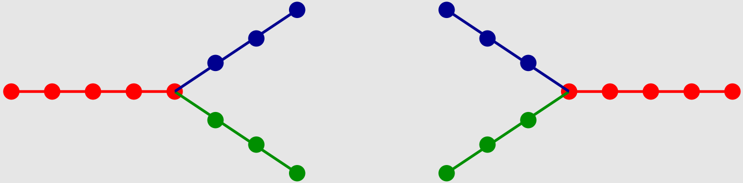
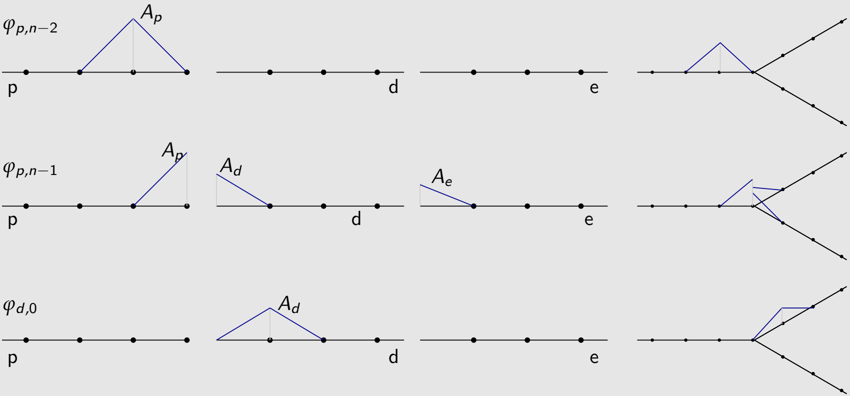
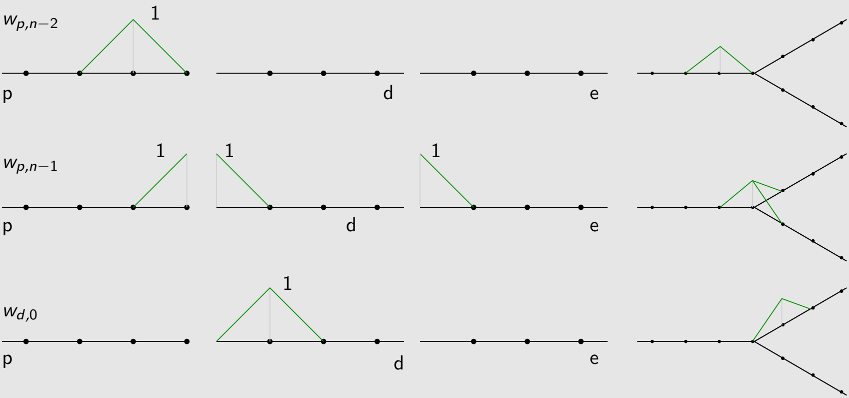


Basis Functions at Arterial Bifurcations



Test Functions at Arterial Bifurcations



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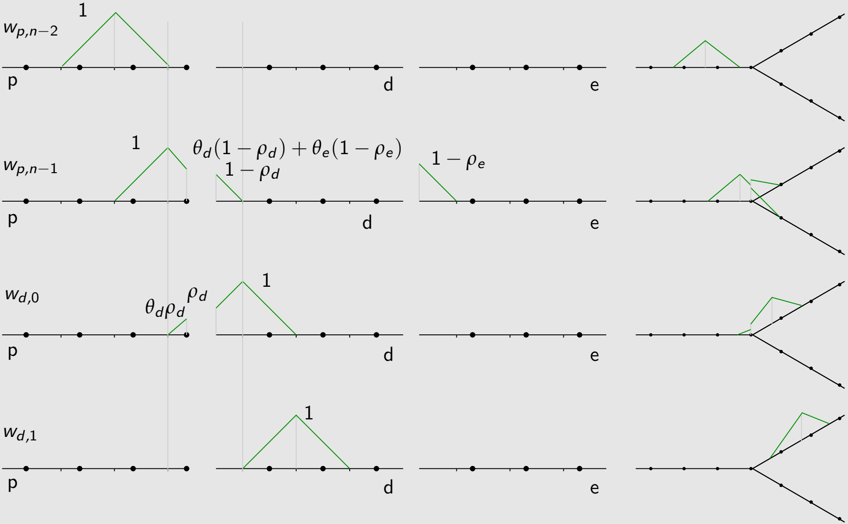

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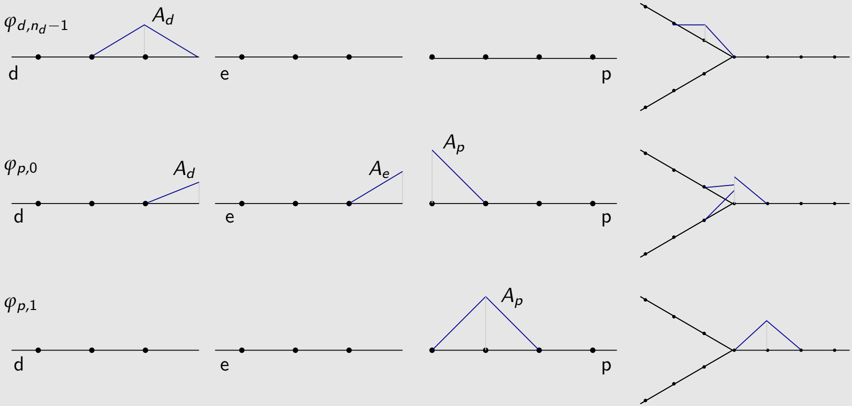

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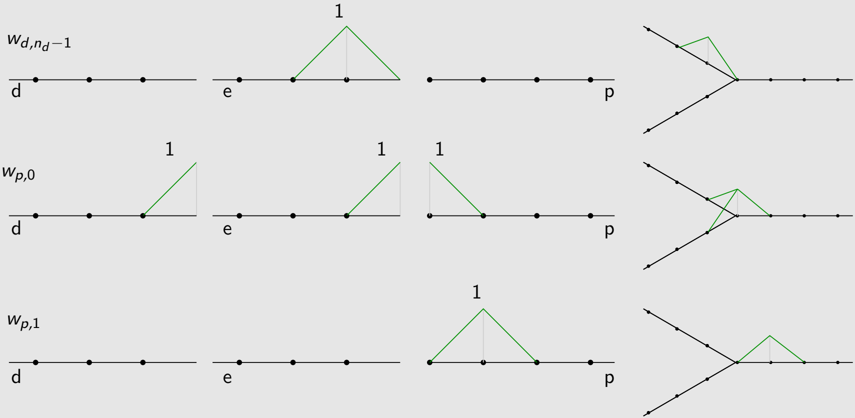

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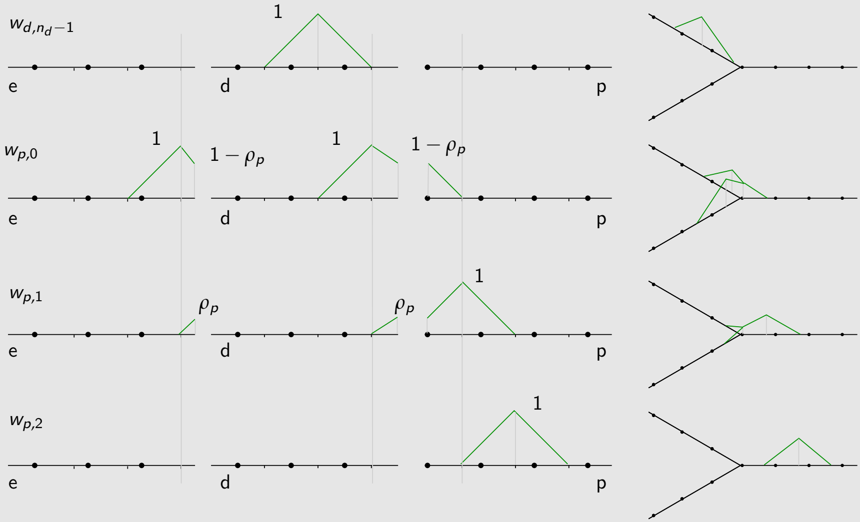

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Corresponding System of Equations

- one “big” system of equations
- block structure
- diagonal blocks almost as before
- coupling between segments $\hat{=}$ off-diagonal blocks (very few entries)
- sparse, but no longer banded system (Gaußian elimination not efficient)
- use conjugate gradient solver (no preconditioning)

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Advection at $\prec$ bifurcation

movie: splitting of a temperature profile

Advection at $\succ$ bifurcation

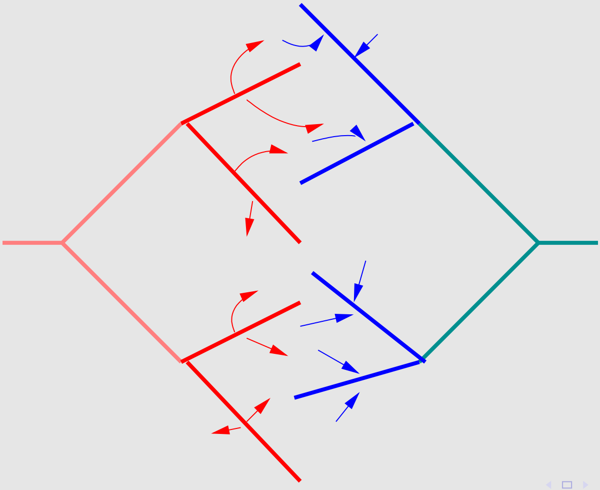
movie: continuous combination of temperature profiles

Advection at $\succ$ bifurcation

movie: discontinuous combination of temperature profiles

Terminal Segments

- Outflow of mass out of arterial terminal segments (and only these)
- Inflow of mass into venous terminal segments (and only these)



Arterial Terminal Segments

- Constant inflow temperature $\Rightarrow$ constant temperature throughout segment
- linear drop-off of temperature content towards end point (3D: quadratic?)

This is modelled via RHS source term:

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- can treat tree as successive bifurcations
- could use bigger time step
  - may need to trace back through multiple bifurcations
  - computation and keeping track of connectivity structure becomes arbitrarily complicated
- could treat multifurcations
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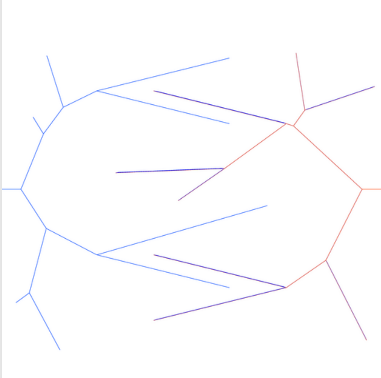
Advection: Results



Outline

2D Vessel Trees
- Geometric Structure
- Flow Velocities

Advection Problem
- Single Segments
- ELLAM
- Unknowns at Bifurcations
- Basis and Test Functions at Bifurcations
- Terminal Segments

Coupling to Diffusion Problem
- Exchange of Energy
- Heat Conduction in Tissue

Coupling to Diffusion Problem

Want to model RF ablation in tissue with blood flowing through vessels.

Goal: Couple

- heat diffusion (heat conduction) problem
- (RF probe) source in tissue to
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with appropriate mutual source terms.

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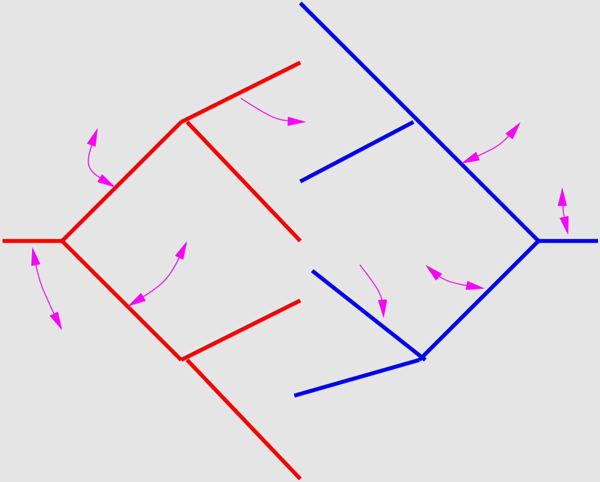
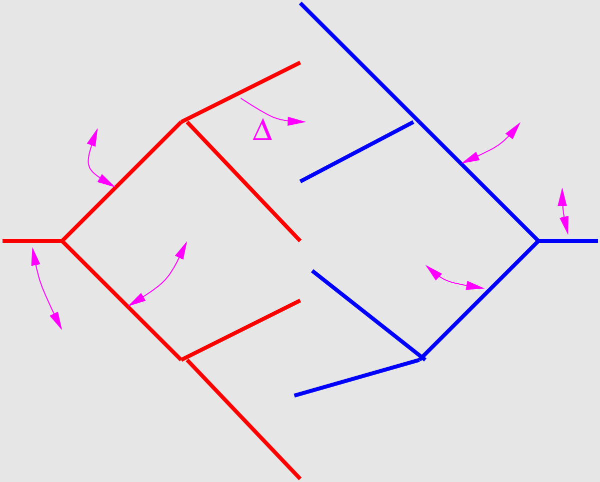


Exchange of Energy, seen by Tissue



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

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Time stepping:

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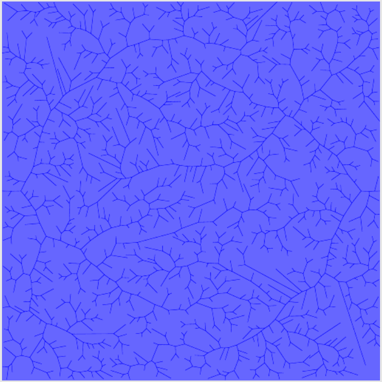
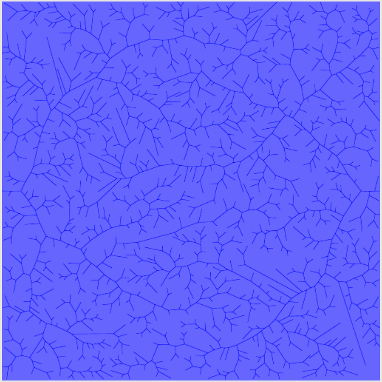
Pulses of Inflowing Warm Blood

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.



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- advection within tissue
- more detailed model of physical effects (vessel walls, non-laminar flow within vessels, thermal influence of RF probe)
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