Transparent boundary conditions for wave propagation in fractal trees

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Mathematical Model and Motivation

Wave propagation in lungs

Used in **medical diagnostics**.

Modelled by the **3D wave equation in a thin fractal network** (see works by B. Maury and co-workers)

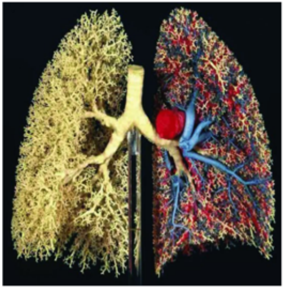
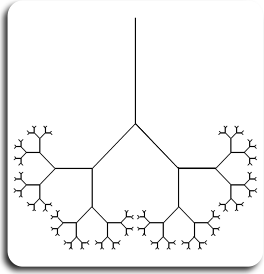


Figure: Cast of human lungs (photo by Ewald Weibel, University of Bern)

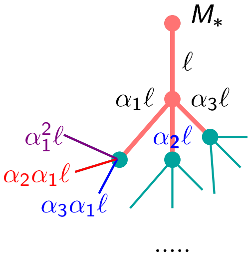


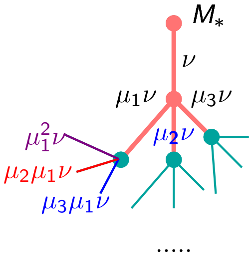
- fractal **infinite 1D** tree $\mathcal{T}$
- asymptotic analysis of [Joly, Semin, 2008] when the branch width $\to 0$

$$\mu \partial_t^2 u - \partial_s(\mu \partial_s u) = 0$$

Self-Similarity: Example (p-adic tree with $p = 3$)

$\alpha_1, \alpha_2, \alpha_3 < 1$ length ratios μ_1, μ_2, μ_3 weight ratios





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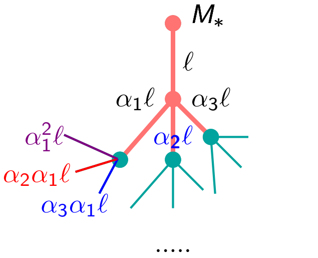

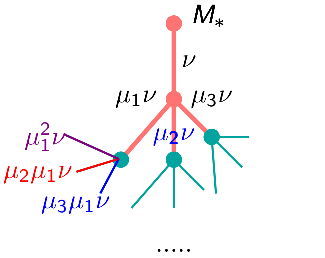

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Lung: $p = 2$, $\alpha_1 \approx \alpha_2 \approx 0.84$, $\mu_1 \approx \mu_2 \approx 0.75$ (Weibel '63)

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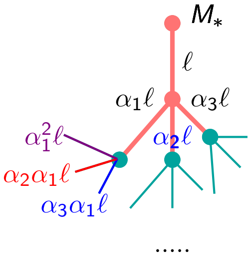

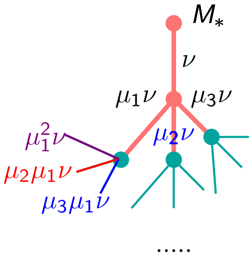

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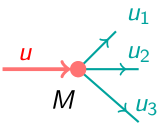
1D PDE : $\partial_s^2 u - \partial_t^2 u = 0$ **on each branch** coupled with



Continuity: $u(M) = u_j(M)$, $j = 1, 2, 3$ in all vertices M

Kirchoff: $\partial_s u(M) = \sum_j \mu_j \partial_s u_j(M)$, in all vertices M

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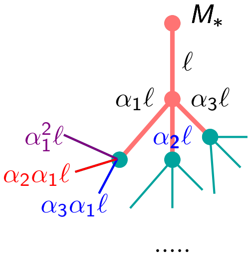

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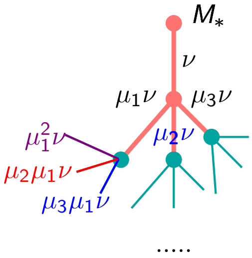

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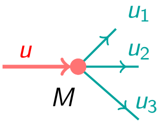

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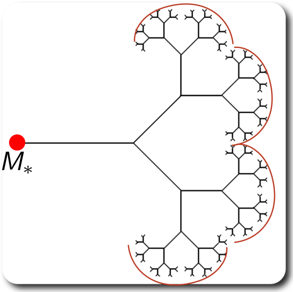
A trivial example: $p = 1$, $\mu_1 = 1$, $\alpha_1 < 1$: a 1D wave equation on an interval

Boundary Conditions



Types of boundary conditions at 'infinity'

We will consider **Neumann BCs**
The BCs will be expressed **variationally** $\Longrightarrow$ associated Sobolev spaces

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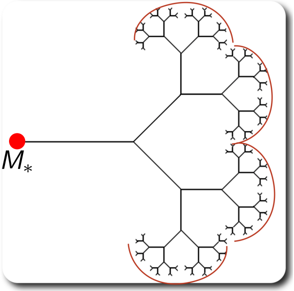

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Variational Framework

- Square-integrable functions L^2_μ on the tree $\mathcal{T}$:

$$\|u\|^2_{L^2_\mu} = \|u\|^2 = \int_{\mathcal{T}} \mu |u|^2 = \sum_{\Sigma \in \mathcal{T}} \int_{\Sigma} \mu_\Sigma |u(s)|^2 ds < \infty.$$

- Sobolev space H^1_μ: $u \in C(\mathcal{T})$, s.t.

$$\|u\|^2_{H^1_\mu} = \|u\|^2_{L^2_\mu} + \int_{\mathcal{T}} \mu |\partial_s u|^2 < \infty.$$

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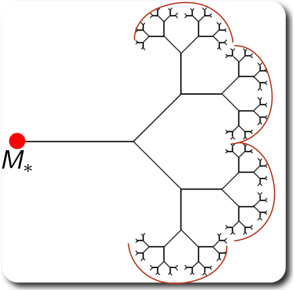

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Neumann (mixed) problem

$V := \{v \in H^1_\mu(\mathcal{T}) : \; v(M_*) = 0\}$

$$u \in C^2((0,\ T]; V) : \int_{\mathcal{T}} \mu \partial_s u \partial_s v + \int_{\mathcal{T}} \mu \partial_t^2 u v = \int_{\mathcal{T}} \mu f v, \qquad \text{for all } \; v \in V$$

$+$ zero i.c.

Difficulties and Objectives

The main objective

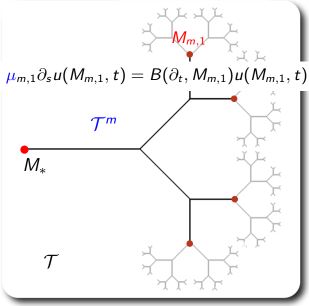
The tree is infinite $\implies$ restrict computations to a structurally finite domain

Outline:

1. transparent boundary conditions for the infinite tree and reference DtN (PhD of A. Semin (2010), P. Joly, MK, A. Semin, Netw. and Heter. Media 2019)
2. two methods for their approximation
   - convolution quadrature
   - local transparent BCs

Dirichlet-to-Neumann operators

- truncate the tree up to a level $m \implies$ truncated tree $\mathcal{T}^m$
- impose a transparent BC $\mu\partial_s u = B(\partial_t)u$ at the boundary of $\mathcal{T}^m$ (excl. M_*)



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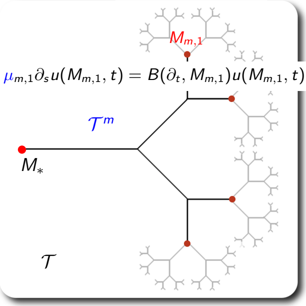

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Coupled formulation:

Find $u \in C^2(0, T; H^1_\mu(\mathcal{T}^m))$, s.t. $u(M_*) = 0$ and

$$\int_{\mathcal{T}^m} \mu\partial_t^2 u v + \int_{\mathcal{T}^m} \mu\partial_s u\partial_s v - \sum_{j=1}^{p^m} B(\partial_t, M_{m,j})u(M_{m,j}, t)v(M_{m,j}) = \int_{\mathcal{T}^m} \mu f v,$$

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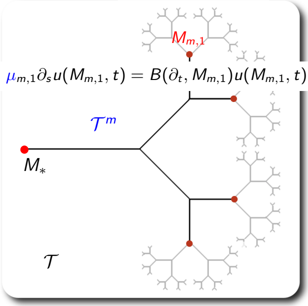

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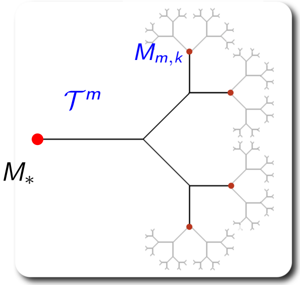
Main issues

- the operators $B(\partial_t)$ are **convolution** operators, **non-local** in time
- no closed form for their kernels or Fourier-Laplace transforms for the kernels

The reference DtN operator



Reference DtN:

$\Lambda(\partial_t)g(t)$: $g \to -\partial_s u(M_*, t)$, where

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$$u(M_*, t) = g(t),$$
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$$\Lambda(\partial_t)g(t) \equiv \int_0^t \lambda(t-\tau)g(\tau)d\tau$$

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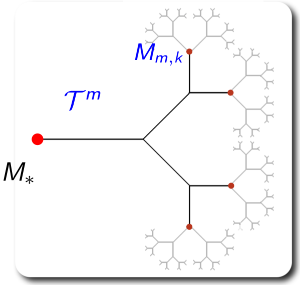

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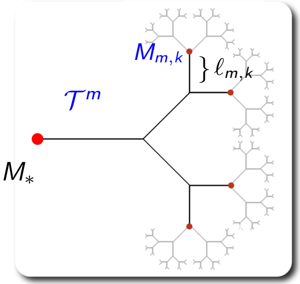

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Using the scaling argument+Kirchoff conditions (see Joly, MK, Semin '19)

$$\boldsymbol{B}(\omega, M_{m,k}) = -\sum_{k=1}^{p} \frac{\mu_k \mu_{m,k}}{\alpha_k \ell_{m,k}} \boldsymbol{\Lambda}(\alpha_k \ell_{m,k}\omega).$$

Conclusion: it suffices to be able to approximate the reference DtN operator.

The reference DtN operator: Characterization 1

Compact embedding

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Eigenvalues: $0 < \omega_1^2 \leq \omega_2^2 \leq \ldots \to +\infty,$

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Corollary

The reference DtN operator $\mathbf{\Lambda}(\omega)$ is a meromorphic function in $\mathbb{C}$ analytic in $\mathcal{B}_\varepsilon(0)$. Moreover,

$$\mathbf{\Lambda}(\omega) = \mathbf{\Lambda}(0) - \sum_{n=0}^{\infty} \frac{(\partial_s\phi_n(0))^2}{\omega_n^2} \frac{\omega^2}{{\omega_n}^2 - \omega^2}.$$

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Problem: computing the eigenvalues and eigenfunctions is expensive!

The reference DtN operator: Characterization 2

The non-linear equation defining the DtN

$$\mathbf{\Lambda}(\omega) = \frac{\sum_{k=1}^{p} \frac{\mu_k}{\alpha_k} \mathbf{\Lambda}(\alpha_k \omega) - \omega \tan \omega}{1 + \omega^{-1} \tan \omega \sum_{k=1}^{p} \frac{\mu_k}{\alpha_k} \mathbf{\Lambda}(\alpha_k \omega)} \qquad \text{(E)}$$

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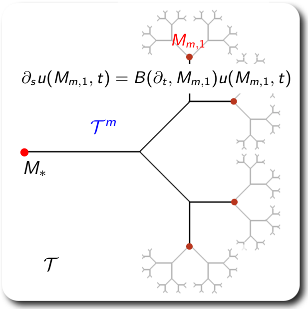
- knowing $\boldsymbol{\Lambda}(\alpha_k \omega)$, $\alpha_k < 1 \implies \boldsymbol{\Lambda}(\omega)$
- $\boldsymbol{\Lambda}$ for $|\omega| < r$ can be found from the truncated **Laurent** series (computable)

Coupled formulation



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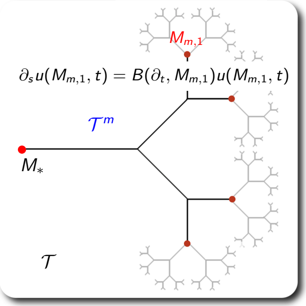

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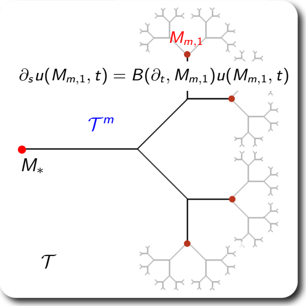
- convolution quadrature (Ch. Lubich '88)
- local transparent BCs



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Trapezoid CQ applied to the construction of transparent BCs

- semi-discretize the original problem in time with the θ-scheme ($\theta = \frac{1}{4}$)

$$\begin{aligned} &\mu \frac{u^{n+1} - 2u^n + u^{n-1}}{(\Delta t)^2} - \partial_s(\mu \partial_s \{u^n\}_{1/4}) = \mu f^n, \\ &u^n(M_*) = 0, \qquad u^0 = u^1 = 0, \ (+\text{b.c.}). \end{aligned} \tag{D}$$

Here $u^n \sim u(., n\Delta t)$,

$\{u^n\}_{1/4} = \frac{1}{4}\left(u^{n+1} + 2u^n + u^{n-1}\right)$

Convolution quadrature (CQ)

Ch. Lubich, 1988: discretize $\int_0^t \mathcal{K}(t-\tau)u(\tau)d\tau$ with multistep (RK) solvers

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- construct exact reference DtN $\mathbf{\Lambda}_{\Delta t}$, and the DtNs $\mathcal{B}_j^{\Delta t}$ for the semi-discrete (D).

Computing $\mathbf{\Lambda}_{\Delta t}$

Continuous problem	Semi-discrete problem	
$-i\omega \; (\sim \partial_t)$	$\underbrace{\frac{2}{\Delta t}\frac{1-z}{1+z}}_{-i\omega+O((\Delta t)^2)}$	$z = \mathrm{e}^{i\omega\Delta t}$ Fourier of a shift

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From frequency domain to time domain

Step 1. Define convolution weights $\lambda_k^{\Delta t}$ ($\mathbf{\Lambda}_{\Delta t}(z)$ is analytic for $|z| < 1$):

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Coupled formulation

Implicit form

$$\int_{\mathcal{T}^m} \mu (\partial_t^{\Delta t})^2 u^n v + \int_{\mathcal{T}^m} \mu \partial_s \{u^n\}_{1/4} \partial_s v - \sum_j \{\mathcal{B}_j^{\Delta t} u^n (M_{m,j})\}_{1/4} v(M_{m,j}) = \int_{\mathcal{T}^m} \mu f \, v.$$

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Stability of the coupled formulation

For the continuous formulation the stability is ensured by $\int_0^t \mathbf{\Lambda}(\partial_t) u \partial_t u \geq 0$.

Discrete formulation: $\Delta t \sum_{k=0}^{n} \left\{\mathbf{\Lambda}_{\Delta t} u^k\right\}_{1/4} \frac{u^{k+1} - u^{k-1}}{2\Delta t} \geq 0$

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After the space discretization:

Explicit form

$$\int_{\mathcal{T}^m} \mu(\partial_t^{\Delta t})^2 u^n v_h + \int_{\mathcal{T}^m} \mu \partial_s^h u_h^n \partial_s^h v_h - \sum_j \{\mathcal{B}_j^{\Delta t} u_h^n(M_{m,j})\}_{1/4} v_h(M_{m,j}) = \int_{\mathcal{T}^m} \mu f \, v_h.$$

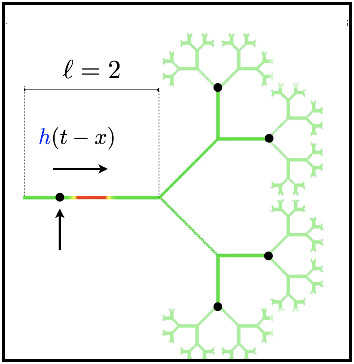
The stability is ensured under the classical CFL condition.

Complexity: evaluating $\{\mathcal{B}_m^{\Delta t} u^n\}_{1/4} v$ is of $O(n) \implies O(N^2)$ for $O(N)$ time steps

Numerical experiments

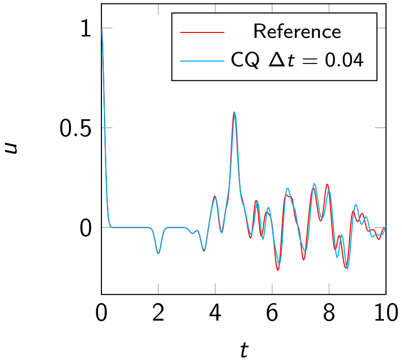
Tree parameters

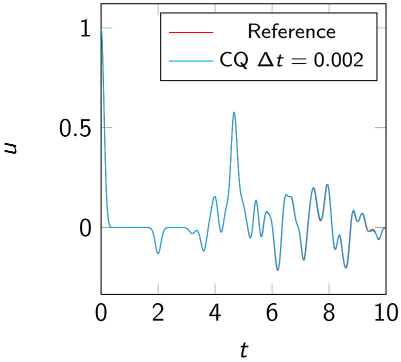
$\alpha_1 = 0.4$, $\alpha_2 = 0.3$, $\mu_1 = 1$ and $\mu_2 = 0.3$. Neumann case.



Dirichlet data: $u(M_*, t) = h(t) = \mathrm{e}^{-50(t-1)^2}$. Cutoff after 3 generations.
Reference solution: on $\mathcal{T}^m$ with m large

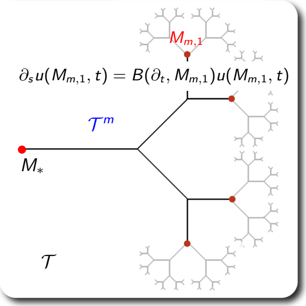
Convolution Quadrature





Remark: Computational times (including pre-computations): $\sim 1-2$ mins for truncated problems; $\sim 10h$ for reference

Coupled formulation



$B(\partial_t, M_{m,1}) := B_1(\partial_t)$ is a **full-tree** DtN operator

$$\boldsymbol{B}(\omega, M_{m,k}) = -\sum_{k=1}^{p} \frac{\mu_k \mu_{m,k}}{\alpha_k \ell_{m,k}} \boldsymbol{\Lambda}(\alpha_k \ell_{m,k}\omega).$$

Coupled formulation:

Find $u \in C^2(0,T; H^1_\mu(\mathcal{T}^m))$, s.t. $u(M_*) = 0$ and

$$\int_{\mathcal{T}^m} \mu \partial_t^2 u v + \int_{\mathcal{T}^m} \mu \partial_s u \partial_s v - \sum_{j=1}^{p^m} B(\partial_t, M_{m,j}) u(M_{m,j},t) v(M_{m,j}) = \int_{\mathcal{T}^m} \mu f v,$$

$\forall v \in H^1_\mu(\mathcal{T}^m)$, with $v(M_*) = 0$.

Computing time-domain convolutions $B(\partial_t)u$

- convolution quadrature (Ch. Lubich '88)
- local transparent BCs

Local transparent BCs

$$\boldsymbol{\Lambda}(\omega) = \boldsymbol{\Lambda}(0) - \sum_{n=0}^{\infty} a_n \frac{\omega^2}{{\omega_n}^2 - \omega^2}, \quad a_n = \frac{(\partial_s \phi_n(0))^2}{\omega_n^2}.$$

Time-domain realization of the reference DtN operator

$$\Lambda(\partial_t) v = \boldsymbol{\Lambda}(0) v + \sum_{n=0}^{\infty} a_n \frac{d\lambda_n}{dt},$$

$$\frac{d^2}{dt^2}\lambda_n + \omega_n^2 \lambda_n = \frac{d}{dt} v, \qquad \lambda_n(0) = \frac{d}{dt}\lambda_n(0) = 0, \quad 0 \leq n < \infty.$$

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Approximation of the reference DtN operator

$$\Lambda_N(\partial_t) v = \boldsymbol{\Lambda}(0) v + \sum_{n=0}^{N-1} a_n \frac{d\lambda_n}{dt},$$

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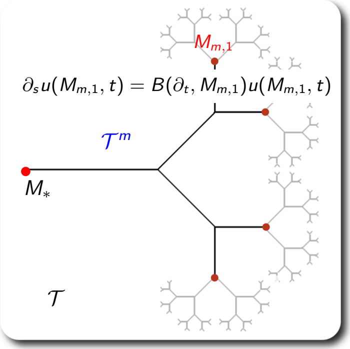
Implementation: a_n and ω_n^2 via the residue theorem+contour integration

Approximating transparent boundary conditions



The 'outer' boundary of $\mathcal{T}^m$:
$\{M_{m,j},\ j = 1, \ldots, p^m\}$.

Transparent boundary conditions

$$B(\partial_t, M) = -\sum_{k=1}^{p} \frac{\mu_k \mu_{m,k}}{\alpha_k \ell_{m,k}} \Lambda(\alpha_k \ell_{m,k} \partial_t) \implies$$

$$B_N(\partial_t, M) = -\sum_{k=1}^{p} \frac{\mu_k \mu_{m,k}}{\alpha_k \ell_{m,k}} \Lambda_N(\alpha_k \ell_{m,k} \partial_t)$$

For brevity: $B_j(\partial_t) := B(\partial_t, M_{m,j})$.

Stability

Uniform in N stability: energy analysis ($a_n \geq 0$ in $\mathbf{\Lambda}(\omega) = \mathbf{\Lambda}(0) - \sum_{n=0}^{\infty} a_n \frac{\omega^2}{\omega_n{}^2 - \omega^2}$)

Error

Error analysis

u_N solution with B_N on $\mathcal{T}^m$, u exact. For $e_N := u_N - u$:

$$\|\partial_t e_N(.,t)\|_{\mathcal{T}^m} + \|\partial_s e_N(.,t)\|_{\mathcal{T}^m} \leq Ct\|\partial_s u\|_{W^{4,1}(0,t;L^2_\mu)} \sum_{n=N}^{\infty} (\partial_s \phi_n(0))^2 {\omega_n}^{-4}.$$

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Goal

Find N s.t. $\sum_{n=N}^{\infty} (\partial_s \phi_n(0))^2 \omega_n^{-4} < \varepsilon$

Reminder

${\omega_n}^2$ are eigenvalues of $-\mu^{-1}\partial_s(\mu\partial_s)$ on $V := \{v \in H^1_\mu : v(0) = 0\}$,
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What does not work

Bound $|\partial_s \phi_n(0)|$ and ω_n for every n (bounding convergent series by a non-convergent one)

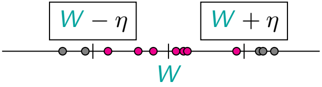
An alternative idea

Goal

Find N_ε s.t. $\sum_{n=N_\varepsilon}^{\infty} (\partial_s \phi_n(0))^2 \omega_n^{-4} < \varepsilon$

Adapting [Barnett, Hassell 2011 (Lipschitz domains)]

$$\sum_{\omega_n \colon |\omega_n - W| \leq \eta} (\partial_s \phi_n(0))^2 < C_\eta W^2.$$



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The estimate does not depend on the number of ω_n on the interval $(W - \eta, W + \eta)$

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$$\sum_{\omega_n \geq N} (\partial_s \phi_n(0))^2 \omega_n^{-4}$$

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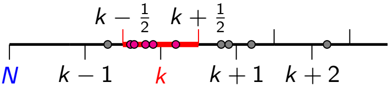

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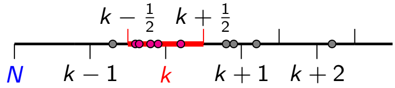

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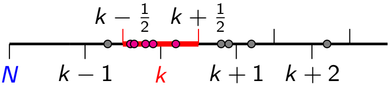

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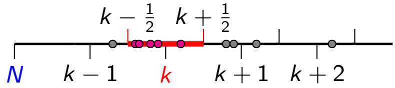

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Adapting [Barnett, Hassell 2011 (Lipschitz domains)]

$$\sum_{\omega_n :\, |\omega_n - W| \le \eta} (\partial_s \phi_n(0))^2 < C_\eta W^2.$$

Changing the point of view

$$\sum_{\omega_n \ge N} (\partial_s \phi_n(0))^2 \omega_n^{-4} \le \sum_{k=N}^{\infty} \sum_{|\omega_n - k| \le \frac{1}{2}} (\partial_s \phi_n(0))^2 \omega_n^{-4}$$

$$\le c \sum_{k=N}^{\infty} \frac{1}{k^4} \sum_{|\omega_n - k| \le \frac{1}{2}} (\partial_s \phi_n(0))^2 \le C \sum_{k=N}^{\infty} \frac{1}{k^4} k^2 \le \frac{\tilde{C}}{N}.$$

Conclusion

$$\sum_{\omega_n \ge \varepsilon^{-1}} (\partial_s \phi_n(0))^2 \omega_n^{-4} < \tilde{C} \varepsilon.$$

How is N related to ε

Goal (N plays a role in the complexity estimate)

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Bounds on N_ε

- $\sum_{k=0}^{p-1} \alpha_k < 1$ ($d_s < 1$): $N_\varepsilon = O\left(\varepsilon^{-1}\right)$

Proof: spectral analysis ideas from Kigami, Lapidus 1993 and Levitin, Vassiliev 1996

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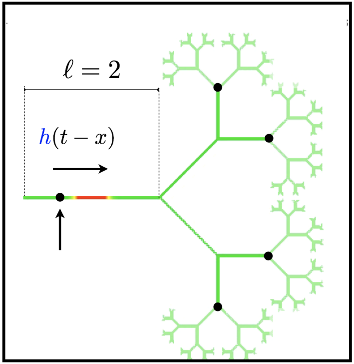
- $\sum_{k=0}^{p-1} \alpha_k > 1$ ($d_s > 1$): $N_\varepsilon = O\left(\varepsilon^{-d_s}\right)$ (Lungs: $d_s \approx 3.98$)

Proof: spectral analysis ideas from Kigami, Lapidus 1993 and Levitin, Vassiliev 1996

Numerical experiments

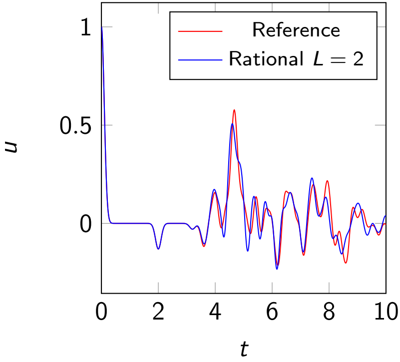
Tree parameters

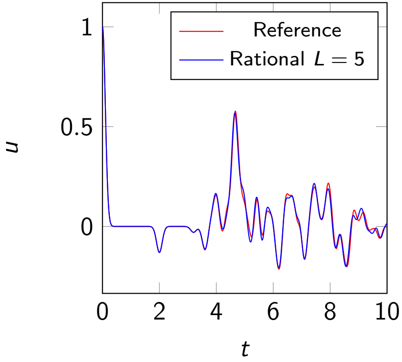
$\alpha_1 = 0.4$, $\alpha_2 = 0.3$, $\mu_1 = 1$ and $\mu_2 = 0.3$. Neumann case.



Dirichlet data: $u(M_*, t) = h(t) = \mathrm{e}^{-50(t-1)^2}$. Cutoff after 3 generations.
Reference solution: on $\mathcal{T}^m$ with m large.

Rational Function Conditions: Increasing Accuracy





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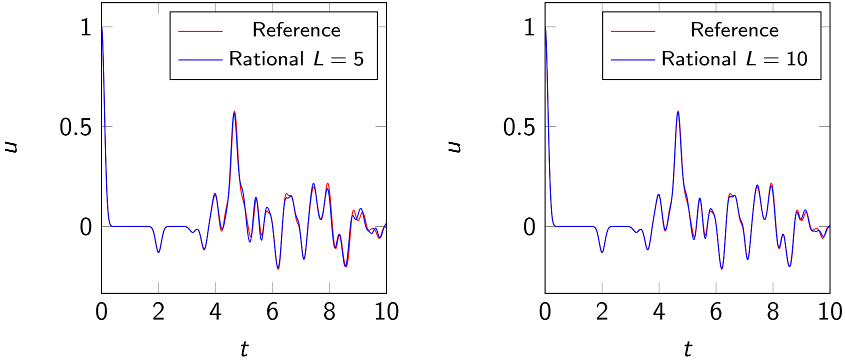

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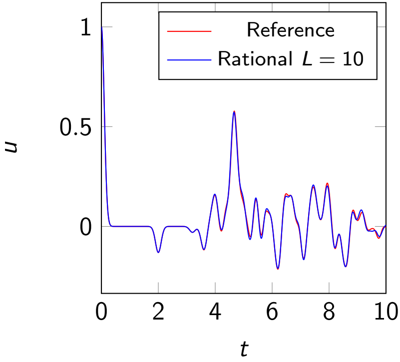

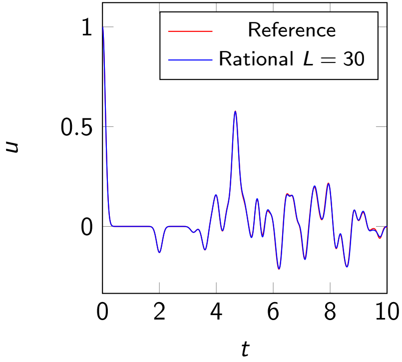

Prospectives and future work

- Improved convergence of Local Transparent BCs
- Kirchoff-like conditions accounting for angles between junctions
- BCs accounting for the interaction of the bronchioli with alveoli/lung tissue

Thank you for your attention!

References:

- theory and low-order ABC: P. Joly, MK, A. Semin, *Wave Propagation in Fractal Trees. Mathematical and Numerical Issues*, *Networks and Heterogeneous Media*
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- Convolution Quadrature: P. Joly, MK, *Transparent Boundary Conditions for Wave Propagation in Fractal Trees: Convolution quadrature*, Num. Math. 2020
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