An introduction to Quantum Graphs theory

Mario Arioli

STFC Rutherford Appleton Laboratory

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Overview of talk

- Motivations and Modelling
- Graphs, metric graphs, and quantum graphs
- Self-adjoint Hamiltonians and boundary conditions
- Modelling again
- Waves and eigenvalues problems
- Numerical issues and domain decomposition
- Open problems i.e.

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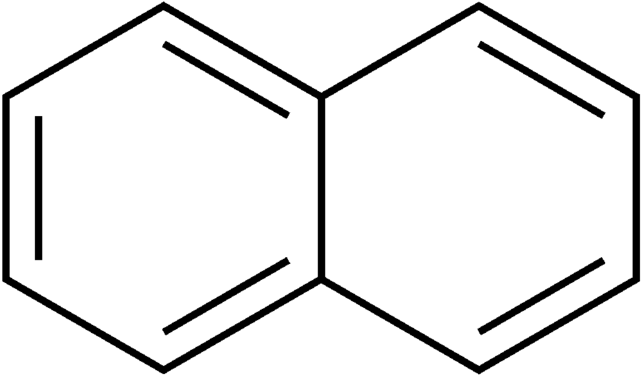
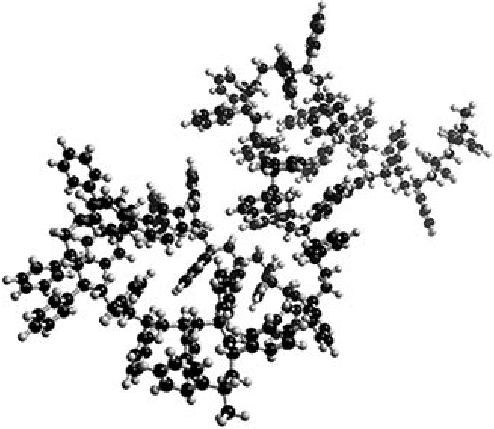
- Graphs, metric graphs, and quantum graphs
- Self-adjoint Hamiltonians and boundary conditions
- Modelling again
- Waves and eigenvalues problems
- Numerical issues and domain decomposition
- Open problems i.e. The things I have not understood yet!!!

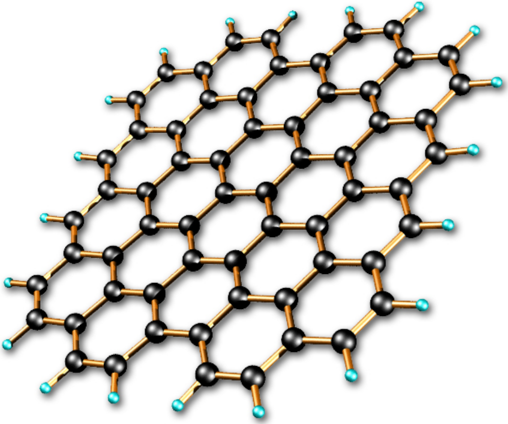
Example: Naphthalene



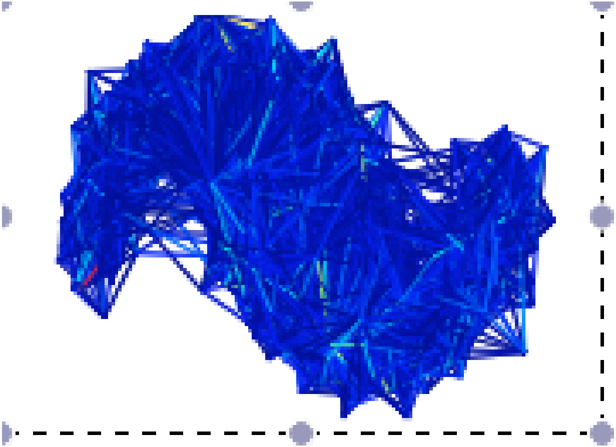
Example: Polystyrene



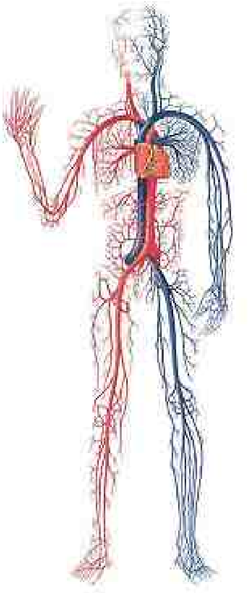
Example: Graphene



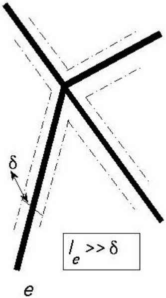
Example: spectral clustering



Example: Human body

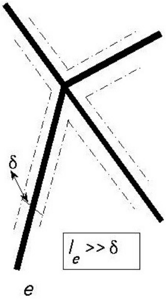


Modelling (examples)



A fat graph (l_e length of edge e)

Modelling (examples)



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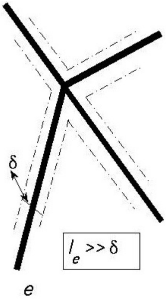

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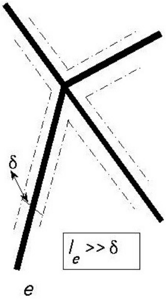

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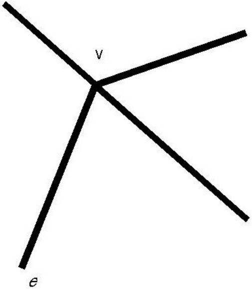

Graph (*e* edge and *v* vertex)

- Difficult to have a decent triangulation of the fat domain!
- Irregular solution (corners)
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Combinatorial and metric Graphs

- A Combinatorial Graph Γ is defined by a set $\mathcal{V} = \{v_j\}$ of vertices and a set $\mathcal{E} = \{e_k\}$ of edges connecting the vertices that can be finite or countably infinite. Each edge e can be identified by the couple of vertices that it connects ($e = (v_{j_1}, v_{j_2})$).

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- A graph Γ is a "*Metric Graph*" if at each edge e is assigned a length $l_e \in (0, \infty)$ and a measure (normally the Lebesgue one). Each edge can be assimilated to a finite or infinite segment of the real line $(0, l_e) \in \mathbb{R}$, with the natural coordinate s_e.

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- Γ is provided with a global metric and the distance between two points (not necessarily vertices) is the length of the shortest path between them. Thus, the points on Γ are the vertices and all the points on the edges. The Lebesgue's measure is well defined on all of Γ for finite graphs.

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- Γ is NOT necessarily embedded in a Euclidean space ($\mathbb{R}^n$)

Conditions on infinite graphs

Condition A An edge of infinite length has only one vertex. It is a ray starting from a vertex.

Condition B For any positive number r and any vertex v there is only a finite number of vertices w at a distance less than r from v.

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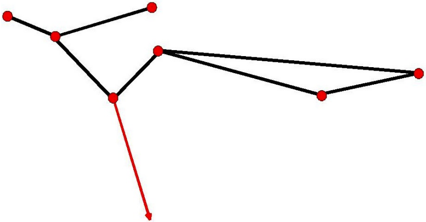

Hilbert spaces

Definition-$L^2(\Gamma)$:

$$L^2(\Gamma) = \bigoplus_{e\in\mathcal{E}} L^2(e)$$

$$f(s) \in L^2(\Gamma) \qquad \text{iff} \qquad ||f||^2_{L^2(\Gamma)} = \sum_{e\in\mathcal{E}} ||f||^2_{L^2(e)} < \infty$$

Definition-$H^1(\Gamma)$ (Sobolev space) :

$$H^1(\Gamma) = \Big(\bigoplus_{e\in\mathcal{E}} H^1(e)\Big) \cap C^0(\Gamma)$$

$$f(s) \in H^1(\Gamma) \qquad \text{iff} \qquad ||f||^2_{H^1(\Gamma)} = \sum_{e\in\mathcal{E}} ||f||^2_{H^1(e)} < \infty$$

$C^0(\Gamma)$ space of continuous functions on Γ.

Quantum Graphs

Let $\mathcal{H}$ an operator (Hamiltonian) defined on $H^1(\Gamma)$.

A Quantum Graph is a metric graph where an Hamiltonian $\mathcal{H}$ and boundary conditions that assure $\mathcal{H}$ is self-adjoint are defined.

Hamiltonian

Operators (s denotes the coordinate on an edge)

Second derivative $f \to -\dfrac{d^2 f}{ds^2}$

A natural condition is to assume that $f(e) \in H^2(e), \ \forall e \in \mathcal{E}$.

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Others: pseudo-differential, higher order derivative, etc...

A natural condition is to assume that $f(e) \in H^2(e), \ \forall e \in \mathcal{E}$.

Hamiltonian

Operators (s denotes the coordinate on an edge)

Second derivative We will focus on $f \to -\dfrac{d^2 f}{ds^2}$

A natural condition is to assume that $f(e) \in H^2(e)$, $\forall e \in \mathcal{E}$.

Boundary conditions

We are interested in local conditions at the vertices. Let d be the degree of vertex v. For functions $f_j \in H^2(e_v)$ on the edges connected at v, we expect boundary conditions involving the values of the functions and their directional derivative taken in the outgoing directions at the vertex v:

$$A_v F + B_v F' = 0$$

where $A \in \mathbb{R}^{d \times d}$ and $B \in \mathbb{R}^{d \times d}$, $F = (f_1(v), \ldots, f_d(v)$ and $F' = (f_1'(v), \ldots, f_d'(v)$.

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The rank of the matrices $[A_v, B_v] \in \mathbb{R}^{d\times 2d}$ must be equal to d.

Finite graphs

Theorem

Let Γ be a metric graph with finitely many edges. Consider the operator $\mathcal{H}$ acting as $-\dfrac{d^2}{ds^2}$ on each edge $e \in \mathcal{E}$, with the domain consisting of the functions $f \in H^2(e)$ on e and satisfying the conditions

$$A_v F + B_v F' = 0$$

at each vertex $v \in \mathcal{V}$.

Let $\left\{A_v \in \mathbb{R}^{d_v \times d_v}, B_v \in \mathbb{R}^{d_v \times d_v} | v \in \mathcal{V}\right\}$ a collection of matrices such that $Rank(A_v, B_v) = d_v$ for all v.

$$\mathcal{H} \text{ is self-adjoint iff } \forall v \in \mathcal{V}, A_v B_v^T = B_v A_v^T$$

(Kostrykin Schrader, 1999) (Kuchment, 2004)

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A linear algebra bit (1)

We drop the subscript v for a moment

$$B \quad = \quad W\Sigma V^T = (W_1, W_2)\begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} \qquad \text{(SVD)}$$

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$$W^T(A, B)\begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & \Sigma_1 & 0 \\ 0 & R_{22} & 0 & 0 \end{pmatrix}$$

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A linear algebra bit (2)

$$W^T(A,B)\begin{pmatrix} V^TF \\ V^TF' \end{pmatrix} = 0 \Longleftrightarrow \begin{pmatrix} R_{11} & R_{12} & \Sigma_1 & 0 \\ 0 & R_{22} & 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^TF \\ V_2^TF \\ V_1^TF' \\ V_2^TF' \end{pmatrix} = 0$$

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$$\begin{aligned} &\Longrightarrow \quad R_{11}V_1^TF + \Sigma_1V_1^TF' = 0 \Longrightarrow V_1^TF' = -\Sigma_1^{-1}R_{11}V_1^TF \\ &\Longrightarrow \quad F' = -V_1\Sigma_1^{-1}R_{11}V_1^T \iff F' = LF \quad \big(\text{min norm solution}\big) \\ &\qquad\quad \Big((AB^T = BA^T\Big) \Longrightarrow L = L^T \end{aligned}$$

A linear algebra bit (3)

Let $P_v = I - V_1 V_1^T$ and $Q_v = I - P_v$ be the orthogonal projectors relative to node v then

$$A_v F + B_v F' = 0 \Longleftrightarrow \begin{cases} P_v F = 0 \\ Q_v F' + L_v F = 0 \end{cases} \quad (*)$$

All self-adjoint realizations of $\mathcal{H}$ (the negative second derivative) on Γ with the vertex boundary conditions satisfy the following:

$$\forall v \in \mathcal{V} \; \exists P_v \text{ and } Q_v = I_{d_v} - P_v$$

(orthogonal projections) and

$$\forall v \in \mathcal{V} \; \exists L_v \text{ in } Q_v \mathbb{C}^{d_v}.$$

All $f \in \mathcal{D}(\mathcal{H}) \subset \bigoplus H^2(e)$ are described by (*) at each finite vertex.

Quadratic form

The Quadratic form h of $\mathcal{H}$ is

$$\begin{aligned} h[f,f] &= \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds - \sum_{v\in\mathcal{V}} \sum_{e\in\mathcal{E}} (L_v)_{jk}\, f_j(v)\overline{f_k(v)} \\ &= \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds - \sum_{v\in\mathcal{V}} \langle L_v F, F\rangle, \end{aligned}$$

where $\langle\cdot,\cdot\rangle$ is the standard Hermitian inner product in $\mathbb{C}^{d_v}$. The domain of h consists of all $f \in \bigoplus_{e\in\mathcal{E}} H^1(e)$ such that $P_v F = 0$.

Examples of b.c.

δ*-type conditions*

$$\begin{cases} f(s) \quad \text{is continuous on } \Gamma \\ \forall v \in \Gamma \qquad \sum_{e \in \mathcal{E}_v} \dfrac{df}{ds_e}(v) = \alpha_v f(v) \end{cases}$$

$\mathcal{E}_v$ is the subset of the edges having v as a boundary point.
α_v are real fixed numbers
We describe the case for a node v of degree 3 (generalization is easy)

Examples of b.c.

$$A_v = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -\alpha_v & 0 & 0 \end{pmatrix} \qquad B_v = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

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$$L_v = \frac{-\alpha_v}{d_v} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

Examples of b.c.

The Hamiltonian of the problem has the following h

$$\begin{aligned} h[f,f] &= \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds - \sum_{v\in\mathcal{V}} \langle L_v F, F\rangle \\ &= \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds + \sum_{v\in\mathcal{V}} \alpha_v \left|f(v)\right|^2 . \end{aligned}$$

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The case $\alpha_v \equiv 0$ corresponds to the **Neumann-Kirchhoff** conditions

$$\begin{cases} f(s) \quad \text{is continuous on} \;\; \Gamma \\ \forall v \in \Gamma \qquad \sum_{e\in\mathcal{E}_v} \dfrac{df}{ds_e}(v) = 0 \end{cases}$$

$$h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds.$$

Examples of b.c.

δ'-type conditions

$$\begin{cases} \forall v \in \Gamma \\ \text{The value of the derivative } \dfrac{df_e}{ds_e}(s) \text{ is the same } \forall e \in \mathcal{E}_v \\ \sum_{e\in\mathcal{E}_v} f_e(v) = \alpha \dfrac{df}{ds_e}(v) \end{cases}$$

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The self-adjoint condition is satisfied iff $\alpha \in \mathbb{R}$
If $\alpha_v = 0$ for some v then $L_v = 0$.

$$L_v = 0 \quad \forall v \Longrightarrow h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds.$$

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The self-adjoint condition is satisfied iff $\alpha \in \mathbb{R}$
If $\alpha_v \neq 0$ then B_v is invertible and $P_v = 0$ and $Q_v = I$.
$(L_v)_{i,j} = -\dfrac{1}{\alpha d_v} \quad \forall\, i,j$

Examples of b.c.

The Hamiltonian of the problem has the following h

$$h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds + \sum_{\{v\in\mathcal{V}|\alpha_v\neq 0\}} \frac{1}{\alpha_v} \left|\sum_{e\in\mathcal{E}_v} f(v)\right|^2 .$$

The domain consists of all $f(s) \in \bigoplus_e H^1(e)$ that have at each vertex where $\alpha_v = 0$ the sum of the vertex values along all the incident edges is equal to 0.

Examples of b.c.

Dirichlet and Neumann conditions.

Dirichlet vertex conditions require that at each vertex the boundary conditions impose $f(v) = 0$

The operator is decoupled in the sum of the negative second derivative and

$$h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left| \frac{df}{ds} \right|^2 ds$$

$f \in H^1(\Gamma)$.

The spectrum $\sigma(\mathcal{H})$

$$\sigma(\mathcal{H}) = \left\{ \frac{n^2\pi^2}{l_2^2} \,|e \in (E),\ n \in \mathbb{Z} - 0 \right\}$$

Examples of b.c.

Dirichlet and Neumann conditions.

Under *Neumann vertex conditions* no restriction on the value of the function at vertices are required. The derivative at the vertices are instead required to be zero. The operator is decoupled in the sum of the negative second derivative and

$$h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{ds}\right|^2 ds$$

$f \in H^1(\Gamma)$, as for the Dirichlet case, but on a larger domain

Symmetric vertex conditions: a classification

We want to classify the cases for which the conditions

$$\left\{ \begin{array}{l} PF = 0 \\ QF' + LF = 0 \end{array} \right. \quad (*)$$

are invariant under the action of the symmetric group of the coordinate permutations. (again we drop the subscript v)

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We want to classify the cases for which the conditions

$$\begin{cases} PF = 0 \\ QF' + LF = 0 \end{cases} \quad (*)$$

are invariant under the action of the symmetric group of the coordinate permutations. (again we drop the subscript v) The invariant space of the permutation group is the one dimensional space generated by the vector of entries equal to one

$$\vec{\psi} = \frac{1}{\sqrt{d}}(1, \cdots, 1)^T \in \mathbb{C}^d.$$

Then (*) are invariant under the action of this group iff P, Q, and L are. We have 4 possible cases.

Symmetric vertex conditions: a classification

1. $P = 0, \quad Q = I, \quad L = \alpha \vec{\psi} \vec{\psi}^T + \beta I$
    - $\beta = 0$ δ'-conditions
    - $\alpha = \beta = 0$ Neumann-conditions

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Symmetric vertex conditions: a classification

2. $P = I, \quad Q = 0$ (L irrelevant) Dirichlet-conditions

Symmetric vertex conditions: a classification

3. $P = I - \vec{\psi}\vec{\psi}^T, \;\; Q = \vec{\psi}\vec{\psi}^T, \;\; L = \alpha Q$ δ-conditions

Symmetric vertex conditions: a classification

4. $P = \vec{\psi}\vec{\psi}^T, \quad Q = I - \vec{\psi}\vec{\psi}^T, \quad L = \alpha P$????

Are these all the possible cases?

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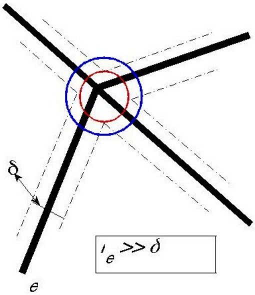
NO!!

Modelling (Neumann Schrödinger example)



Ω_d fat graph (l_e length of edge e)

Let Ω_d denote the fat graph and $\delta = d \times p(s)$ where $p(s) > 0$ is a function of the arc length that can be discontinuous at the vertices. Each vertex neighbouring is contained in a ball of radius $\sim d$ and star-shaped with respect to a smaller ball of diameter $\sim d$.

Modelling (Neumann Schrödinger example)

On Ω_d we define the Schrödinger operator

$$H_d(\mathbf{A}, q) = \left(\frac{1}{i} \nabla - \mathbf{A}(s) \right)^2 + q(s)$$

with Neumann conditions on $\partial\Omega_d$ (q scalar electric and $\mathbf{A}$ vector magnetic potentials

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$$H(\mathbf{A}, q)f(s_e) = -\frac{1}{p}\left(\frac{d}{ds_e} - iA_e^t(s)\right)p\left(\frac{d}{ds_e} - iA_e^t(s)\right)f + q_e(s)f$$

where A_e^t is the tangential component of **A** and q_e is the restriction of q to the graph.

Modelling (Neumann Schrödinger example)

Boundary conditions at the vertices

- f is continuous through each vertex
- $$\sum_{\{k|v\in e_k\}} p_k \left(\frac{df_k}{ds_k} - iA_k^t f_k \right)(v) = 0$$

p_k function that gives the width of the tube around e_k. The values of $p_k(v)$ at the same vertex can be different for different e_k

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Theorem *For* $n = 1, 2, \ldots$

$$\lim_{\delta \to 0} \lambda_n \left(H_d(\mathbf{A}, q) \right) = \lambda_n \left(H(\mathbf{A}, q) \right),$$

where λ_n *is the n-th eigenvalue counted in increasing order (accounting multiplicity)*

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We assume that at the vertices of degree $d = 1$ we have Dirichlet conditions. Only Neumann-Kirchhoff conditions for sake of simplicity

Differential equations

Given a function $g(s) \in L^2(\Gamma)$, we want to compute the solution of the problem

$$\min_u \{h[u,u] - \langle g, u\rangle\}$$

with $u(s) \in H^1(\Gamma)$.

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We have described an abstract Domain Decomposition approach.

Finite dimensional problem

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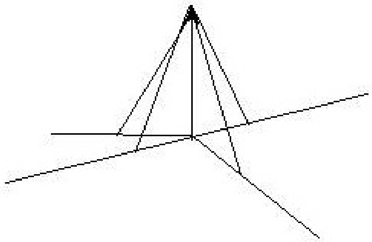


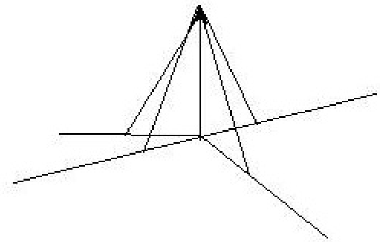
The matrix

Reordering the nodes such that the internal nodes in a edge are consecutive and the vertices are at the end we have a matrix

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{12}^T & M_{22} \end{bmatrix}$$

where M_{11} is block diagonal M_{22} is diagonal and M_{12} holds the links between the edges.

Example



$$\begin{bmatrix} M_1 & & & & c_1 \\ & M_2 & & & c_2 \\ & & M_3 & & c_3 \\ & & & M_4 & c_4 \\ c_1^T & c_2^T & c_3^T & c_4^T & b \end{bmatrix}$$

Graph (e edge and v vertex)

Eigenvalue Problem

The analysis of the spectrum of the self-adjoint operators is more subtle. Infinite quantum graphs can have Hamiltonian with continuous part of the spectrum. However, for finite quantum graphs we can have a better situation:

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Theorem

Let Γ a finite quantum graph with finite edges equipped with an Hamiltonian given by negative second derivative along the edges and vertex conditions

$$(*)\begin{cases} P_v F = 0 \\ Q_v F' + L_v F = 0 \end{cases}$$

Then the spectrum $\sigma(\mathcal{H})$ is discrete.

An interesting connection

$$\mathcal{H}f = \lambda f \qquad f \in L^2(\Gamma)$$

Let e be an edge identified by the two vertices v and w of length l_e. If $\lambda \neq n^2\pi^2 l_e^{-2}$ with $n \in \mathbb{Z} - \{0\}$ then

$$f_e = \frac{1}{\sin\sqrt{\lambda} l_e}\left(f_e(v)\sin\sqrt{\lambda}(l_e - s) + f_e(w)\sin\sqrt{\lambda}s\right)$$

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Substituting

$$f_e'(v) = \frac{l_e\sqrt{\lambda}}{\sin\sqrt{\lambda}}\left(f_e(w) - f_e(v)\cos l_e\sqrt{\lambda}\right)$$

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$$T(\lambda)F = 0$$

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Theorem
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This results connects quantum graph theory to combinatorial graph theory

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What about $\lambda = n^2\pi^2 l_e^{-2}$?
If we have only Dirichlet conditions they are the only eigenvalues, otherwise ??????

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