Complex and quantum graphs and their applications

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Overview

- Motivations and Modelling (and a little bit of History)
- Complex Network
- Graphs and Random Graphs
- Metric graphs and quantum graphs
- Self-adjoint Hamiltonians and boundary conditions
- Modelling again
- Waves and eigenvalues problems
- Parabolic and time dependent problems
- Numerical issues and domain decomposition
- Open problems i.e.
Overview

- Motivations and Modelling (and a little bit of History)
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- Graphs and Random Graphs
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- Self-adjoint Hamiltonians and boundary conditions
- Modelling again
- Waves and eigenvalues problems
- Parabolic and time dependent problems
- Numerical issues and domain decomposition
- Open problems i.e. The things I have not understood yet!!!
Example: Naphthalene
Example: Polystyrene
Example: Graphene
Example: Graphene
Example: spectral clustering
Example: Human body
Complex graphs (http://www.opte.org)
MORE Complex graphs  (http://www.opte.org)
MORE Complex graphs (http://www.wikipidia)
MORE Complex graphs (http://http://www.newscientist.com)
Modelling (examples)

A fat graph \((l_e \gg \delta)\)

\(\ell\) length of edge \(e\)
Modelling (examples)

A fat graph ($l_e$ length of edge $e$)

- Difficult to have a decent triangulation of the fat domain!
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A Combinatorial Graph $\Gamma$ is defined by a set $\mathcal{V} = \{v_j\}_{j=1}^N$ of vertices and a set $\mathcal{E} = \{e_k\}_{k=1}^M$ 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 ($e = (v_{j_1}, v_{j_2})$).
Combinatorial Graphs

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Given $\Gamma$ how can I represent it using matrices?

- **Adjacency matrix:** symmetric vertex to vertex structure
  
  \[ A_{ij} = \begin{cases} 1 & \text{if there exists an edge between } v_i \text{ and } v_j \\ 0 & \text{otherwise} \end{cases} \]

- **Incidence matrix:** $E$ is a vertex to edge matrix. Each column corresponds to an edge and has two non-zero entries 1 and -1 corresponding to the first vertex and the second vertex (the sign is arbitrary and will be uninfluential for our purposes).

- There are strong relations between $A$ and $E$:
  
  \[ EE^T = L \]
  
  is the Laplacian of the graph and
  
  \[ A = \text{diag}(L) L^T \]
  
  The $\text{diag}(L)_{ii}$ entries are the number of connections that each vertex $v_i$ has, i.e. its degree.

- $E$ can be interpreted as a discrete divergence and $E^T$ as a discrete gradient. Moreover, $\ker(E^T)$ is the subset of the vectors $\mathbf{e} = (1, 1, \ldots, 1)^T$.

- $E$ is also a "Totally unimodular" matrix (discrete optimization jargon).
Combinatorial Graphs and Matrix representation

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![Adjacency Matrix](image-url)
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Complex Graph? What is it!

The concept of “complex graph” (or network) is somewhat fuzzy. We are not aware of any formal definition able to sharply distinguish within all sparse graphs what is complex from what is not. Some concrete examples, such as the Web graph, are obviously very complex even though they can be described by the deceptively simple concept of a (very sparse) adjacency matrix.
In the study of unweighted graphs, the lengths of the edges are assumed to be all equal to 1. The *diameter* of a graph is defined as the maximum length of all shortest paths between any pair of nodes in $\Gamma$. In other terms,

$$
\text{diam} (\Gamma) := \max_{u,v \in \mathcal{V}} d(u, v),
$$

where $d(u, v)$ stands for the distance between vertices $u$ and $v$. 

**Complex Graph? What is it!**
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Most real-world complex graphs are characterized by the so-called *small-world* property, that is, the diameter of the graph is a very slowly growing function of the total number $N$ of vertices. For many real graphs the diameter behaves approximately as $\log N$ or even $\log \log N$ as $N \to \infty$. For example, it is not unusual for a graph $\Gamma$ with $N \approx 10^6$ vertices to have diameter $\text{diam}(\Gamma) \approx 10$ (or even less).
Complex graphs are also usually characterized by highly skewed degree distributions displaying fat tails. We will characterise degree distribution in an undirected graph via the probability density function $p(k)$ that describes the number vertices in the graph with degree $k$. 
Random properties of complex networks

For many real-world complex graphs, $p(k)$ follows a power law:

\[ p(k) \propto k^{-\gamma}, \quad \gamma \geq 1. \]

By elementary calculus, we have that $\mathcal{E}(k)$, the expected value (or mean) of the degree, behaves as

\[ \mathcal{E}(k) \approx \frac{C}{\gamma - 2} \left( 1 - N^{2-\gamma} \right). \]

Therefore, in order to have sparse graphs (sparse adjacency matrices and sparse matrices in general), we need to take $\gamma > 2$ so that $\mathcal{E}(k)$ remains bounded by a constant as $N \to \infty$. (The value $\gamma = 2$ is a critical value, for which the mean degree grows logarithmically with $N$; for $1 \leq \gamma < 2$, the mean degree grows like a fractional power of $N$ and the graph becomes dense in the limit of large $N$.)
Random properties of complex networks

Many complex graphs follow a power law degree distribution with $2 < \gamma \leq 3$. and we will work under this assumption. Note that, for values of $\gamma$ between 2 and 3, the corresponding value of the variance $\mathcal{V}(k)$ will approximated by

$$\mathcal{V}(k) \approx \frac{C_1}{\gamma - 3} \left(1 - N^{3-\gamma}\right)$$

which for $N \uparrow \infty$ diverges.
Random properties of complex networks

We observe that the fairly regular graphs obtained by meshing 2D or 3D domains in the approximation of PDEs do not follow a power law, owing to the requirement that the triangles or the tetrahedra must preserve the minimum angle condition which imposes a bound the maximum number of edges incident in a vertex, independent of $N$. 
E. Estrada, The Structure of Complex Network, Oxford University Press, 2011,

http://www.maths.strath.ac.uk/research/groups/numerical_analysis/contest
Degree, Diameter, Centrality

A from pref.m (CONTEST); Scale free random graph.
Degree, Diameter, Centrality

$A$ from pref.m (CONTEST); Scale free random graph. DIAMETER OF $A = 5$. 
Degree, Diameter, Centrality

\[ A \text{ from pref.m (CONTEST); Scale free random graph.} \]

\[ \text{DIAMETER OF } A = 5. \]

Centrality: \( \text{diag}(\exp(A)) \)
Degree, Diameter, Centrality

A from pref.m (CONTEST); Scale free random graph.
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Why this may be not enough?

The 1318 transnational corporations that form the core of the economy in 2007. Superconnected companies are red, very connected companies are yellow. The size of the dot represents revenue (Image: PLoS One) (New Scientist)
Why this may be not enough?

The network of global corporate control S. Vitali, J. B. Glattfelder, and S. Battiston ETH Zurich, Kreuzplatz 5, 8032 Zurich, Switzerland.

"In effect, less than 1 per cent of the companies were able to control 40 per cent of the entire network," says Glattfelder.
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One of the 147 (in position 34) was Lehman Brothers Holdings Inc.
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Combinatorial and metric Graphs

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- A graph $\Gamma$ 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 $s_e$. 
Remarks

- We can remove vertices of degree 2 after we fuse the 2 edges into one
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- We can remove vertices of degree 2 after we fuse the 2 edges into one.
- The graph $\Gamma$ is a topological manifold (or a 1D simplicial complex) having singularities at the vertices, i.e. it is NOT a differentiable manifold. Let $E^+ = \frac{1}{2}(|E| + E)$ and $E^- = \frac{1}{2}(|E| - E)$. Let $Z \in \mathbb{R}^{N \times n}$ with $N$ number of vertices and $n$ number of co-ordinates for each vertex the representation of of the vertices in $\Gamma$. Then

$$Z(s) = (E^+)^T Z - s E^T Z$$

$s \in [0, 1]$ is the 1-D simplicial complex and $Z(1) = (E^-)^T Z$. 


Remarks

» We can remove vertices of degree 2 after we fuse the 2 edges into one

» The graph $\Gamma$ is a topological manifold (or a 1D simplicial complex) having singularities at the vertices, i.e. it is NOT a differentiable manifold.

» $\Gamma$ 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 $\Gamma$ are the vertices and all the points on the edges. The Lebesgue’s measure is well defined on all of $\Gamma$ for finite graphs.
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Berkolaiko and Kuchment, Introduction to Quantum Graphs, AMS186, 2012
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 $u$ at a distance less than $r$ from $v$. 
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Hilbert spaces

Definition-$L^2(\Gamma)$: \( (L^2_e = \{ f \mid \int_e f^2 ds < \infty \}) \)

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

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

Definition-$H^1(\Gamma)$ (Sobolev space): \( (H^1_e = \{ f \mid \int_e \left( \frac{df}{ds} \right)^2 ds < \infty \}) \)

\[H^1(\Gamma) = \left( \bigoplus_{e \in \mathcal{E}} H^1(e) \right) \cap C^0(\Gamma)\]

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

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


Berkolaiko and Kuchment, Introduction to Quantum Graphs, AMS186, 2012
Hamiltonian

Operators ($s$ denotes the coordinate on an edge)

Second derivative $f \rightarrow -\frac{d^2 f}{ds^2}$

A natural condition is to assume that $f(e) \in H^2(e)$, $\forall e \in \mathcal{E}$.
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**Second derivative**  $f \rightarrow -\frac{d^2 f}{ds^2}$

**Schrödinger**  $f \rightarrow -\frac{d^2 f}{ds^2} + V(s)f$

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Magnetic Schrödinger \( f \rightarrow \left( \frac{1}{i} \frac{d}{ds} - A(s) \right)^2 f + V(s)f \)

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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
Hamiltonian

Operators ($s$ denotes the coordinate on an edge)

**Second derivative** We will focus on $f \mapsto -\frac{d^2 f}{ds^2}$

A natural condition is to assume that $f(e) \in H^2(e), \ \forall e \in \mathcal{E}$. 
We are interested in local conditions at the vertices. Let $d_v$ 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 $A \in \mathbb{R}^{d_v \times d_v}$ and $B \in \mathbb{R}^{d_v \times d_v}$, $F = (f_1(v), \ldots, f_{d_v}(v))$ and $F' = (f'_1(v), \ldots, f'_{d_v}(v))$. 
Boundary conditions

We are interested in local conditions at the vertices. Let $d_v$ 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 $v$:

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

\textit{Theorem}

Let $\Gamma$ be a metric graph with finitely many edges. Consider the operator $\mathbf{h}$ acting as $-\frac{d^2}{ds^2}$ 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 $\{ A_v \in \mathbb{R}^{d_v \times d_v}, B_v \in \mathbb{R}^{d_v \times d_v} | v \in \mathcal{V} \}$ a collection of matrices such that $\text{Rank}(A_v, B_v) = d_v$ for all $v$.

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

(Kostrykin Schrader, 1999) (Berkolaiko and Kuchment, Introduction to Quantum Graphs, AMS186, 2012)
A linear algebra bit (1)

We drop the subscript \( v \) for a moment

\[
B = 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} \quad \text{(SVD)}
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A = WRV^T \quad R = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix}
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\[ W^T(A, B) \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & \Sigma_1 & 0 \\ 0 & R_{22} & 0 & 0 \end{pmatrix} \]
A linear algebra bit (2)

\[
W^T(A, B) \begin{pmatrix} V^T F \\ V^T F' \end{pmatrix} = 0 \iff \begin{pmatrix} R_{11} & R_{12} & \Sigma_1 & 0 \\ 0 & R_{22} & 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T F \\ V_2^T F \\ V_1^T F' \\ V_2^T F' \end{pmatrix} = 0
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\[ \text{Rank}((A, B)) = d \implies R_{22} \text{ invertible } \implies V_2^T F = 0 \implies F \in \text{span}(V_1) \]
A linear algebra bit (2)

\[ W^T(A, B) \left( \begin{array}{c} V^T F \\ V^T F' \end{array} \right) = 0 \iff \left( \begin{array}{ccc} R_{11} & R_{12} & \Sigma_1 \\ 0 & R_{22} & 0 \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{c} V_1^T F \\ V_2^T F \\ V_1^T F' \\ V_2^T F' \end{array} \right) = 0 \]

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\[ \implies R_{11} V_1^T F + \Sigma_1 V_1^T F' = 0 \implies V_1^T F' = -\Sigma_1^{-1} R_{11} V_1^T F \]

\[ \implies F' = -V_1 \Sigma_1^{-1} R_{11} V_1^T \iff F' = LF \quad (\text{min norm solution}) \]

\[ (AB^T = BA^T) \implies L = L^T \]
A linear algebra bit (3)

Let $P_v = I - Q_v$ and $Q_v = B_v^+ B_v$ ($B_v^+$ is the Moore-Penrose pseudo inverse) be the (symmetric) orthogonal projectors relative to node $v$ then

$$A_v F + B_v F' = 0 \iff \begin{cases} P_v F = 0 \\ Q_v F' + L_v F = 0 \end{cases} \tag{*}$$

where

$$L_v = B_v^+ A_v Q_v$$

and

$$L_v = L_v^T.$$  

All self-adjoint realizations of $\mathfrak{h}$ (the negative second derivative) on $\Gamma$, 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 $f \in \mathcal{D}(\mathfrak{h}) \subset \bigoplus H^2(e)$ are described by (*)
The Quadratic form $h$ of $\mathfrak{h}$ is

$$ h[f, f] = \sum_{e \in \mathcal{E}} \int_{e} \left| \frac{df}{ds} \right|^2 ds - \sum_{v \in \mathcal{V}} \sum_{e \in \mathcal{E}} (L_v)_{jk} f_j(v) \overline{f_k(v)} $$

$$ = \sum_{e \in \mathcal{E}} \int_{e} \left| \frac{df}{ds} \right|^2 ds - \sum_{v \in \mathcal{V}} \langle L_v F, F \rangle, $$

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 $P_v F = 0$. 
Symmetric vertex conditions: a classification

We want to classify the cases for which the conditions

\[
\begin{align*}
PF &= 0 \\
QF' + LF &= 0
\end{align*}
\]

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

\[
\vec{\psi} = \frac{1}{\sqrt{d}} (1, \ldots, 1)^T \in \mathbb{C}^d.
\]

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. $P = 0, \quad Q = I, \quad L = \alpha \vec{\psi} \vec{\psi}^T + \beta I$
   - $\beta = 0$ $\delta'$-conditions
   - $\alpha = \beta = 0$ Neumann-conditions
Symmetric vertex conditions: a classification

2. $P = I, \quad Q = 0 \ (L \text{ irrelevant})$ Dirichlet-conditions
Symmetric vertex conditions: a classification

3. \( P = I - \bar{\psi}\bar{\psi}^T, \quad Q = \bar{\psi}\bar{\psi}^T, \quad L = \alpha Q \quad \delta\)-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?
Are these all the possible cases?

NO!!
Examples of b.c.

\( \delta \text{-type conditions} \)

\[
\begin{aligned}
\left\{ \begin{array}{l}
    f(s) \text{ is continuous on } \Gamma \\
    \forall v \in \Gamma \quad \sum_{e \in \mathcal{E}_v} \frac{df}{ds_e}(v) = \alpha_v f(v)
\end{array} \right.
\end{aligned}
\]

\( \mathcal{E}_v \) is the subset of the edges having \( v \) as a boundary point.

\( \alpha_v \) are real fixed numbers

We describe the case for a node \( v \) of degree 3 (generalization is easy)
Examples of b.c.

\[ A_v = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -\alpha_v & 0 & 0 \end{pmatrix} \quad B_v = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix} \]
Examples of b.c.

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\[ A_v B_v^T = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\alpha_v \end{pmatrix} \]

The self-adjoint condition is satisfied iff \( \alpha \in \mathbb{R} \)
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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 $h$

$$h[f, f] = \sum_{e \in E} \left( \int_{e} \left| \frac{df}{ds} \right|^2 ds - \sum_{v \in V} \langle L_v F, F \rangle \right)$$

$$= \sum_{e \in E} \left( \int_{e} \left| \frac{df}{ds} \right|^2 ds + \sum_{v \in V} \alpha_v |f(v)|^2 \right).$$
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$$\begin{cases} f(s) \text{ is continuous on } \Gamma \\ \forall v \in \Gamma \quad \sum_{e \in \mathcal{E}_v} \frac{df}{ds_e}(v) = 0 \end{cases}$$

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

\( \delta' \)-type conditions

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

\( \mathcal{E}_v \) is the subset of the edges having \( v \) as a boundary point.

\( \alpha_v \) are real fixed numbers

We describe the case for a node \( v \) of degree 3 (generalization is easy)
Examples of b.c.

\[
B_v = \begin{pmatrix}
1 & -1 & 0 \\
0 & 1 & -1 \\
-\alpha_v & 0 & 0
\end{pmatrix} \quad A_v = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
1 & 1 & 1
\end{pmatrix}
\]
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The self-adjoint condition is satisfied iff \( \alpha \in \mathbb{R} \)

If \( \alpha_v = 0 \) for some \( v \) then \( L_v = 0 \).

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

\[ B_v = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -\alpha_v & 0 & 0 \end{pmatrix} \quad A_v = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix} \]

\[ A_v B_v^T = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\alpha_v \end{pmatrix} \]

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 \( Q_v = I \).

\( (L_v)_{i,j} = -\frac{1}{\alpha d_v} \quad \forall i, j \)
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 \( \sigma(\mathcal{H}) \)

\[
\sigma(\mathcal{H}) = \left\{ \frac{n^2 \pi^2}{l^2} \mid e \in (E), \ n \in \mathbb{Z} - 0 \right\}
\]
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

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

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

$\Omega_d$ fat graph ($l_e$ length of edge $e$)
Modelling (Neumann Schrödinger example)

On $\Omega_d$ we define the Schrödinger operator

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

with Neumann conditions on $\partial \Omega_d$ ($q$ scalar electric and $A$ vector magnetic potentials)
Modelling (Neumann Schrödinger example)

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

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

where $A^t_e$ 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

$$\sum_{\{k | v \in e_k\}} p_k \left( \frac{df_k}{ds_k} - i A_k^t f_k \right) (v) = 0$$

$p_k$ 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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Modelling (Neumann Schrödinger example)

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

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

where $\lambda_n$ is the $n$-th eigenvalue counted in increasing order (accounting multiplicity)
Finally, among our goals is the analysis of parabolic problems on metric graphs. In this case, we assume that the functions we use also depend on a second variable $t$ representing time, i.e. (see Raviart-Thomas 1983),

$$f(t, x) : [0, T] \times \Gamma \to \mathbb{R}.$$
Let \( V \) denote either \( L^2(\Gamma) \) or \( H^1(\Gamma) \). Let \( C^0([0, T]; V) \) be the space of functions \( f(t, x) \) that are continuous in \( t \) with values in \( V \), i.e., for each fixed value \( t^* \) of \( t \) we have that \( f(t^*, \cdot) \in V \). This space is equipped with the norm

\[
\| f \|_{C^0([0, T]; V)} = \sup_{0 \leq t \leq T} \| f(t, \cdot) \|_V.
\]
Parabolic problems

Let $L^2([0, T]; V)$ be the space of functions $f(t, x)$ that are square-integrable in $t$ for the $dt$ measure with values in $V$, i.e. for each fixed value $t^*$ of $t$ we have that $f(t, \cdot) \in V$. This space is equipped with the norm

$$
\| f \|_{L^2([0, T]; V)} = \left( \int_0^T \| f(t, \cdot) \|_V^2 \, dt \right)^{\frac{1}{2}}
$$

and scalar product

$$
(f, g)_{L^2([0, T]; V)} = \int_0^T \left( f(t, \cdot), g(t, \cdot) \right)_V \, dt.
$$
Parabolic problems

We note that all these definitions can be easily modified to deal with self-adjoint operators acting on spaces of complex-valued functions, as required by quantum mechanics.
Parabolic equation

Given $u_0 \in H^1(\Gamma)$ and a $f \in L^2([0, T], L^2(\Gamma))$ find

$$ u \in L^2([0, T], H^1(\Gamma)) \cup C^0([0, T]; H^1(\Gamma))$$

and

$$ \begin{cases} 
\forall v \in H^1(\Gamma) \\
\frac{d}{dt} (u(t), v)_{L^2([0, T], L^2(\Gamma))} + h[u(t), v] = (f(t), v)_{L^2([0, T], L^2(\Gamma))} & \text{on } ]0, T[ \\
u(0) = u_0 
\end{cases} $$

$$ h[u, v] = \sum_{e \in \mathcal{E}} \int_e \frac{\partial u(t, s)}{\partial s} \frac{\partial v}{\partial s} ds + \sum_{e \in \mathcal{E}} \int_e m(s)u(t)v(s) ds. $$

Neumann-Kirchhoff conditions
Parabolic equation

\[
\begin{aligned}
\frac{\partial u(t, s)}{\partial t} - \frac{\partial^2 u(t, s)}{\partial s^2} + mu(t, s) &= f & \text{on } \Gamma \\

u(0, s) &= u_0.
\end{aligned}
\]
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:
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:

**Theorem**

Let $\Gamma$ 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 $\sigma(\hbar)$ is discrete.
An interesting connection

\[ hf = \lambda f \quad f \in L^2(\Gamma) \]

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

\[ f_e = \frac{1}{\sin \sqrt{\lambda l_e}} (f_e(v) \sin \sqrt{\lambda}(l_e - s) + f_e(w) \sin \sqrt{\lambda}s) \]
An interesting connection

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Substituting

\[ f'_e(v) = \frac{l_e \sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( f_e(w) - f_e(v) \cos l_e \sqrt{\lambda} \right) \]

in (*) and eliminating the derivatives we compute a system of algebraic relations
An interesting connection

\[ \mathcal{H}f = \lambda f \quad f \in L^2(\Gamma) \]

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

\[ f_e = \frac{1}{\sin \sqrt{\lambda}l_e} (f_e(v) \sin \sqrt{\lambda}(l_e - s) + f_e(w) \sin \sqrt{\lambda}s) \]

Substituting

\[ f_e'(v) = \frac{l_e\sqrt{\lambda}}{\sin \sqrt{\lambda}} (f_e(w) - f_e(v) \cos l_e \sqrt{\lambda}) \]

in (*) and eliminating the derivatives we compute a system of algebraic relations

\[ T(\lambda)F = 0 \]
An interesting connection

\textbf{Theorem}
\[ \lambda \neq n^2 \pi^2 l_e^{-2} \quad \text{with} \quad n \in \mathbb{Z} - \{0\} \quad \text{belongs to the spectrum of } \mathcal{H} \iff \text{zero belongs to the spectrum of } T(\lambda) \]
An interesting connection

**Theorem**

\[ \lambda \neq n^2 \pi^2 l_e^{-2} \text{ with } n \in \mathbb{Z} - \{0\} \text{ belongs to the spectrum of } \h \text{ iff } \]

zero belongs to the spectrum of \( T(\lambda) \)

This results connects quantum graph theory to combinatorial graph theory
An interesting connection

Theorem
\[ \lambda \neq n^2 \pi^2 l_e^{-2} \text{ with } n \in \mathbb{Z} - \{0\} \text{ belongs to the spectrum of } \hat{\mathcal{H}} \text{ iff} \]
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What about \( \lambda = n^2 \pi^2 l_e^{-2} \)?
An interesting connection

**Theorem**

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zero belongs to the spectrum of \( T(\lambda) \)

What about \( \lambda = n^2 \pi^2 l_e^{-2} \)?

If we have only Dirichlet conditions they are the only eigenvalues, otherwise ??????
Summary

- We have defined the analytical structure of a Quantum Graph
  - the metric properties
  - the operators
  - the boundary conditions
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We assume that at the vertices of degree $d = 1$ we have Dirichlet conditions.
Summary

- We have defined the analytical structure of a Quantum Graph
  - the metric properties
  - the operators
  - the boundary conditions
- We will focus in the last part on finite graphs and we will give some hints on:
  - Solution of differential equations
  - Eigenvalues problems

We assume that at the vertices of degree $d = 1$ we have Dirichlet conditions. Only Neumann-Kirchhoff conditions for sake of simplicity.
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 $u(s) \in H^1(\Gamma)$. 

Differential equations
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- On each edge $e \in \mathcal{E}$ we solve the local problem and we denote by $u_e(s_e)$ the solution.
Differential equations

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\[
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- On each edge \( e \in \mathcal{E} \) we solve the local problem and we denote by \( u_e(s_e) \) the solution.
- Using the Neumann-Kirchhoff conditions and the values of the derivative at the vertices, we form and solve an algebraic system on the vertices.
Differential equations

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

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- On each edge $e \in E$ we solve the local problem and we denote by $u_e(s_e)$ the solution.
- Using the Neumann-Kirchhoff conditions and the values of the derivative at the vertices, we form and solve an algebraic system on the vertices.

We have described an abstract Domain Decomposition approach.
Finite-element basis

On each edge of the quantum graph it is possible to use the classical 1D finite-element method. Let $e$ be a generic edge identified by two vertices, which we denote by $v_a$ and $v_b$. The parameter $x$ will map the edge such that for $x = 0$ we have the vertex $v_a$ and for $x = \ell_e$ we have the vertex $v_b$. The first step is to subdivide the edge in $n^e$ intervals of length $h^e$. The points

$$\left\{ \mathcal{E}_e = \{x^e_j\}_{j=1}^{n-1} \right\} \cup \{v_a^e\} \cup \{v_b^e\}$$

form a chain linking the $v_a^e$ to $v_b^e$ lying on the edge $e$. Denoting by $\left\{ \psi^e_j \right\}_{j=0}^{n+1}$ the standard hat basis functions we have
Finite-element basis

\[
\psi_0^e(x) = \begin{cases} 
1 - \frac{x}{h} & \text{if } 0 \leq x \leq h^e \\
0 & \text{otherwise}
\end{cases}
\]

\[
\psi_j^e(x) = \begin{cases} 
1 - \frac{|x_j - x|}{h} & \text{if } x_{j-1} \leq x \leq x_{j+1} \\
0 & \text{otherwise}
\end{cases}
\] \quad (1)

\[
\psi_{n^e+1}(x) = \begin{cases} 
1 - \frac{l^e - x}{h} & \text{if } l^e - h^e \leq x \leq l^e \\
0 & \text{otherwise}
\end{cases}
\]
Finite-element basis

\[
\psi_0^e(x) = \begin{cases} 
1 - \frac{x}{h} & \text{if } 0 \leq x \leq h^e \\
0 & \text{otherwise}
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\[
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0 & \text{otherwise}
\end{cases}
\]

\[
\psi_{n^e+1}^e(x) = \begin{cases} 
1 - \frac{\ell^e - x}{h} & \text{if } \ell^e - h^e \leq x \leq \ell^e \\
0 & \text{otherwise}
\end{cases}
\]

The functions \( \psi_j^e \) are a basis for the finite-dimensional space

\[
V_h^e = \left\{ w \in H^1(e); \ w_{|[x_j^e,x_{j+1}^e]} \in P_1, \ j = 0, \ldots, n + 1 \right\},
\]

where \( P_1 \) is the space of linear functions.
Finite-element framework

In practice, we subdivide each edge forming a chain made of node of degree 2 and we build the usual hat functions extending them to the vertices.
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Finite-element framework

Globally, we can construct the space

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

that is a finite dimensional space of functions that belong to $H^1(\Gamma)$. 
Finite-element framework

Globally, we can construct the space

\[ V_h(\Gamma) = \bigoplus_{e \in \mathcal{E}} V^e_h \]

that is a finite dimensional space of functions that belong to \( H^1(\Gamma) \). The continuity on \( \Gamma \) of the functions in \( V_h \) follows from construction: at each vertex \( v \) we have \( d_v \) (degree of the vertex \( v \)) linear functions that have values 1 on \( v \) each one belonging to an independent \( V^e_h \) with \( e \in \mathcal{E}_v \).
Finite-element framework

Globally, we can construct the space

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

that is a finite dimensional space of functions that belong to $H^1(\Gamma)$. Any function $f_h(x) \in V_h(\Gamma)$ is then a linear combination of the $\psi_j^e$:

$$f_h(x) = \sum_{e \in \mathcal{E}} \sum_{j=0}^{n+1} \alpha_j^e \psi_j^e(x_e).$$

The quadratic form $\mathcal{h}$ of the Hamiltonian operator can be tested on all the $\psi$ and we have the following finite dimensional (discrete) bilinear form

$$\mathcal{h}_h(f_h, \psi_k^e) = \sum_{e \in \mathcal{E}} \sum_{j=0}^{n+1} \alpha_j^e \left\{ \int_e \frac{d\psi_j^e}{dx} \frac{d\psi_k^e}{dx} dx + \int_e V(x) \psi_j^e \psi_k^e dx \right\}. $$

In $\mathcal{h}$ and $\mathcal{h}_h$ the Kirchhoff’s conditions at each vertices are the natural conditions and they are satisfied.
Extended Graph

The nodes on the edges will describe a chain path between two vertices. We can then think of introducing a new (combinatorial) graph in which the nodal discretization points become additional vertices and the edges are obtained by subdividing the edges of the original (metric) graph. We call this the extended graph associated with \( \Gamma \) and denote it by \( \mathcal{G} \).

Assuming for simplicity that all edges \( e \in \mathcal{E} \) have equal length and that the same number \( n - 1 \) of internal nodes are used for each edge, the new graph \( \mathcal{G} \) will have \( (n - 1) \times M + N \) vertices and \( n \times M \) edges, where \( N \) is the number of vertices and \( M \) the number of edges in \( \Gamma \).

The extended graph can be huge, but it has a lot of structure.
Extended Graph: The matrix

Reordering the nodes such that the internal nodes in a edge are consecutive and the vertices are at the end we have that the resulting Gramian matrix $H = (h[h[\psi^e_k, \psi^e_k]])$ is of the form

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^T & H_{22} \end{bmatrix}$$

where $H_{11}$ is block diagonal symmetric and positive definite where each diagonal block is of size $n - 1$ and tridiagonal, and $H_{22}$ is a diagonal matrix with positive diagonal entries. The sparsity pattern of $H_{12}^T$ is that of the incidence matrix of the extended graph $G$.

Important: We are assuming that the potential $V(s)$ is positive.
Extended Graph: A simple example

Figure: Example of a simple metric planar graph and of its incidence matrix.
Extended Graph: A simple example

Figure: Example of the extension of the graph when 4 nodes chain is added internally to each edge (left) and of its incidence matrix (right).
Extended Graph: A simple example

Figure: The matrix $H$ pattern where the red bullets correspond to the original vertices and the blue one to the internal nodes on each edge.
Extended Graph

In the special case $V = 0$ (that is, $\hbar = -\frac{d^2}{ds^2}$), we obtain the discrete (negative) Laplacian (stiffness matrix) $L$ on $G$. When the same number of (equidistant) discretization points is used on each edge of $\Gamma$, $L$ coincides (up to the factor $h^{-1}$) with the combinatorial graph Laplacian $L_G$. Both the stiffness matrix $L$ and the mass matrix $M = (h_{jk}, e_k i)$ have a block structure matching that of $H$. For example, if $V(s) = k$ (constant) then $H = L + kM$. Minimization of the discrete quadratic form

$$J_h(u_h) := h[u_h, u_h] - \langle g_h, u_h \rangle, \quad u_h \in V_h(\Gamma)$$

is equivalent to solving the extended linear system $Hu_h = g_h$, of order $(n - 1)M + N$. 
Solution of the extended linear system

The extended linear system can be solved efficiently by block LU factorization, by first eliminating the interior edge nodes (this requires solving, in parallel if one wishes, a set of \( M \) independent tridiagonal systems of order \( n - 1 \)), and then solving the \( N \times N \) Schur complement system

\[
\mathbf{S} \mathbf{u}_h^v = \mathbf{g}_h^v - \mathbf{H}_{12}^\top \mathbf{H}_{11}^1 \mathbf{g}_h^e \equiv \mathbf{c}_h
\]

for the unknowns associated with the vertices of \( \Gamma \) and

\[
\mathbf{S} = \mathbf{H}_{22} - \mathbf{H}_{12}^\top \mathbf{H}_{11}^1 \mathbf{H}_{12}.
\]
Solution of the extended linear system

The block LU factorization of $H$ is given by

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^T & H_{22} \end{bmatrix} = \begin{bmatrix} H_{11} & 0 \\ H_{12}^T & S \end{bmatrix} \begin{bmatrix} I & H_{11}^{-1}H_{12} \\ 0 & I \end{bmatrix}$$

and crucial $S$ is SPARSE.
Solution of the extended linear system

Figure: The pattern of the Schur complement $S$. 
Solution of the extended linear system

**Theorem:** The nonzero pattern of the Schur complement

\[ S = H_{22} - H_{12}^T H_{11}^{-1} H_{12} \]

coincides with that of \( L_\Gamma \), the (combinatorial) graph Laplacian of the (combinatorial) graph \( \Gamma \). In the special case \( V = 0 \), we actually have \( S = L_\Gamma \).
Solution of the extended linear system

Note that $S$ is SPD, unless $V = 0$ (in which case $S$ is only positive semidefinite). For $\Gamma$ not too large, we can solve the Schur complement system by sparse Cholesky factorization with an appropriate reordering. However, for large and complex graphs (for example, scale-free graphs), Cholesky tends to generate enormous amounts of fill-in, regardless of the ordering used. Hence, we need to solve the Schur complement system by iterative methods, like the preconditioned conjugate gradient (PCG) algorithm.
Preconditioning of matrices arising from complex graphs is an active area of research. Some of the techniques that work well for other types of problems (like Incomple Cholesky Factorization) are useless here. Here we consider two simple preconditioners:

- **diagonal scaling** with $D = \text{diag}(S)$
- a first degree polynomial preconditioner:

$$P^{-1} = D^{-1} + D^{-1}(D - S)D^{-1}.$$ 

**Note:** For the very sparse matrices considered here, each iteration of PCG with polynomial preconditioning costs about the same as 1.5 iterations with diagonal preconditioning.
Numerical experiments

We present first results for a simple steady-state (equilibrium) problem

$$-\frac{d^2 u}{ds^2} + Vu = g$$

on $\Gamma$

with Neumann-Kirchhoff conditions at the vertices, for three different choices of $\Gamma$:

- yeast, the PPI (Protein-Protein Interaction) network of beer yeast ($N = 2224$, $M = 6609$)
- drugs, a social network of drug addicts ($N = 616$, $M = 2012$)
- pref2000, a synthetic scale-free graph constructed using the preferential attachment scheme ($N = 2000$, $M = 3974$)

In each case we assume that all edges have unit length and we use 20 interior discretization points per edge ($h = \frac{1}{21}$).

For the potential we use $V(s) = K$ (const.) and $V(s) = K(s - \frac{1}{2})^2$ for $K = 0.1, 1, 10$. 
PPI network of Saccharomyces cerevisiae (beer yeast)
Social network of injecting drug users in Colorado Springs

Figure courtesy of Ernesto Estrada.
Scale-free BarabásiAlbert graph (pref)
Numerical experiments

The sizes of the extended system $Hu_h = g_h$ and of the reduced system $Su_h = c_h$ are, respectively:

- $n = 134,404, N = 2224$ for yeast;
- $n = 40,856, N = 616$ for drugs;
- $n = 81,480, N = 2000$ for pref2000.

The Schur complement can be formed efficiently since it is very sparse and we know the location of the nonzero entries in advance. Since the original graphs are very small, the Schur complement system is best solved by sparse Cholesky factorization, but we also experiment with PCG. Without preconditioning, convergence can be slow.

For each problem we also need to solve $M$ uncoupled tridiagonal systems of order 20.
Numerical Experiments

Matrix $S^{-1}$ for pref graph, $K = 0.1.$
Numerical Experiments

Matrix $S^{-1}$ for pref graph, $K = 1$. 
Numerical Experiments

Matrix $S^{-1}$ for pref graph, $K = 10$. 
## Numerical experiments

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**Table:** Results of running pcg ($TOL = \sqrt{eps}$) on Schur complement system, diagonal preconditioner. The “exact” solution is the one returned by backslash.
Numerical experiments

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Table: Results of running \texttt{pcg} (\( TOL = \sqrt{\text{eps}} \)) on Schur complement system, polynomial preconditioner.
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Table: Results of running pcg ($TOL = \epsilon^{1/2}$) on Schur complement system, diagonal preconditioner.
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Table: Results of running gmres ($TOL = eps^{1/2}$) on Schur complement system, polynomial preconditioner.
Numerical experiments

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<tr>
<td>10000</td>
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**Table:** PCG iteration counts for pref graph, increasing $N$ ($TOL = \text{eps}^{1/2}$).

**Note:** Here $h$ is constant, the size $N$ of the graph $\mathcal{G}$ is increasing. The size of the extended graph $\mathcal{G}$ is $n = 81, 480, n = 204, 360$, and $n = 409, 300$. 
### Numerical experiments

<table>
<thead>
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<th>$h^{-1}$</th>
<th>No prec.</th>
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</tr>
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</tr>
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**Table:** PCG iteration counts for prefixed graph, increasing $V(s) = K = 0.1$, $N = 2000$.

**Note:** Here $h$ is decreasing, the size $N$ of the graph $G$ is fixed. The size of the extended graph $G$ increases from 81, 480 to 399, 400. With diagonal or polynomial preconditioning the solution algorithm is scalable with respect to both $N$ and $h$ for these graphs.
The parabolic case with FE

Space discretization using finite elements leads to the semi-discrete system

$$M\dot{u}_h = Hu_h + f_h, \quad u_h(0) = u_{h,0},$$

where $u_h = u_h(t)$ is a vector function on the extended graph $G$, and the mass matrix $M$ and Hamiltonian $H$ are as before. A variety of methods are available for solving this linear system of ODEs: backward Euler, Crank-Nicolson, exponential integrators based on Krylov subspace methods, etc.

Note that for large graphs and/or small $h$, this can be a huge system.

We have obtained some preliminary results using Stefan Güttels code `funm_kryl` for evaluating the action of the matrix exponential on a vector.
... And we can compute the solutions!!!
... And we can compute the solutions!!!
Conclusion

- Quantum graphs are independent from the embedding space and his make them a good candidate to model complex phenomena depending on many variables.
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- Non linear operators: p-Laplacian,..
- Integro-differential operators (fractional derivatives and visco-elasticity, ....)
- Interesting numerical linear algebra and potential high parallelism
- Strong interaction between different expertises ...
I hope the journey was pleasant, interesting, and without too many bumps.

Piacciavi, ... aggradir questo che vuole
e darvi sol può l’umil servo vostro.
(from Ariosto (1474-1533), Orlando Furioso, Canto I)
A Final Remark from an Old Book and a Very Wise Man

Si, avons nous beau monter sur des échasses, car sur des échasses encore faut-il marcher de nos jambes. Et au plus élevé trône du monde, si ne sommes assis que sur notre cul.

(Michel Eyquem de Montaigne (1533-1592), Les Essais, Ch 13)