Numerical insights on the generalized Steklov problem in planar domains

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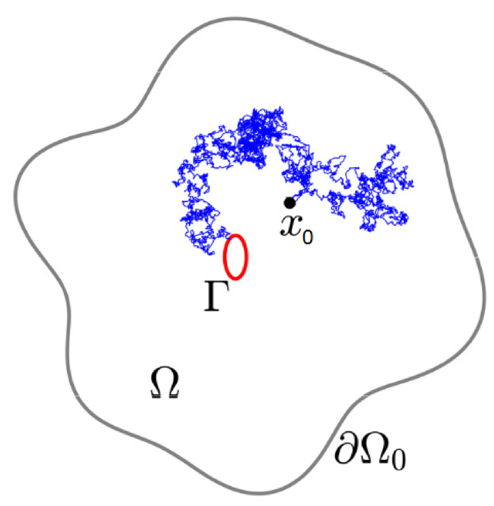
Motivation

Conventional approach to diffusion-controlled reactions



Propagator $G_q(\boldsymbol{x},t|\boldsymbol{x}_0)$ satisfies

$$\begin{cases} \partial_t G_q(\boldsymbol{x},t|\boldsymbol{x}_0) = D\Delta G_q(\boldsymbol{x},t|\boldsymbol{x}_0) \\ -\partial_n G_q(\boldsymbol{x},t|\boldsymbol{x}_0)|_\Gamma = qG_q(\boldsymbol{x},t|\boldsymbol{x}_0)|_\Gamma \\ \partial_n G_q(\boldsymbol{x},t|\boldsymbol{x}_0)|_{\partial\Omega_0} = 0 \\ G_q(\boldsymbol{x},t=0|\boldsymbol{x}_0) = \delta(\boldsymbol{x}-\boldsymbol{x}_0) \end{cases} \quad (1)$$

Spectral decomposition

$$G_q(\boldsymbol{x},t|\boldsymbol{x}_0) = \sum_{k=1}^{\infty} e^{-Dt\lambda_k^{(q)}} u_k^{(q)}(\boldsymbol{x}) \left[u_k^{(q)}(\boldsymbol{x}_0)\right]^*, \quad (2)$$

where $\lambda_k^{(q)}$ and $u_k^{(q)}$ are the eigenvalues and eigenfunctions of the Robin Laplacian.
Main disadvantages:

- dynamics and reactions are coupled via Robin boundary condition
- eigenmodes depend implicitly on the reactivity parameter q

Encounter-based approach [1]

Skorokhod (or Langevin) equation:

$$d\boldsymbol{X}_t = \sqrt{2D}\,\overbrace{d\boldsymbol{W}_t}^{\text{Brownian motion}} + \overbrace{\boldsymbol{n}(\boldsymbol{X}_t)}^{\text{unit normal vector}}\,\overbrace{d\ell_t}^{\text{Boundary local time}} \quad (3)$$

$(\boldsymbol{X}_t,\ell_t) \longleftrightarrow P(\boldsymbol{x},\ell,t|\boldsymbol{x}_0)$ is the encounter propagator

Spectral decomposition

$$\tilde{P}(\boldsymbol{x},\ell,p|\boldsymbol{x}_0) = \tilde{G}_\infty(\boldsymbol{x},p|\boldsymbol{x}_0)\delta(\ell) + \frac{1}{D}\sum_{k=0}^{\infty} V_k^{(p)}(\boldsymbol{x}_0)V_k^{(p)}(\boldsymbol{x})e^{-\mu_k^{(p)}\ell} \quad (4)$$

(where tilde denotes the Laplace transform with respect to time)
The encounter propagator is linked to the conventional propagator

$$G_q(\boldsymbol{x},t\,|\,\boldsymbol{x}_0) = \int_0^\infty e^{-q\ell} P(\boldsymbol{x},\ell,t\,|\,\boldsymbol{x}_0)\,d\ell \quad (5)$$

Advantages:

- explicit dependence on q (decoupling dynamics and reactions)
- possibility of introducing more elaborate surface reactions

The Dirichlet-to-Neumann operator and the Steklov problem [2]

The Dirichlet-to-Neumann operator $\mathcal{M}_p$ associates to a function f on the boundary Γ another function on that boundary:

$$\begin{aligned} \mathcal{M}_p : \mathcal{H}^{1/2}(\Gamma) &\to \mathcal{H}^{-1/2}(\Gamma) \\ f &\mapsto (\partial_n u)|_\Gamma , \end{aligned} \quad (6)$$

where $u(\boldsymbol{x})$ is the solution of the boundary value problem (with $p \geq 0$),

$$(p-\Delta)u(\boldsymbol{x}) = 0 \text{ in } \Omega, \quad u(\boldsymbol{x}) = f(\boldsymbol{x}) \text{ on } \Gamma, \quad \partial_n u(\boldsymbol{x}) = 0 \text{ on } \partial\Omega_0 \quad (7)$$

The spectrum of $\mathcal{M}_p$ is closely related to the spectrum of the (generalized) Steklov problem:

$$(p-\Delta)V_k^{(p)} = 0 \text{ in } \Omega, \quad \partial_n V_k = \mu_k V_k^{(p)} \text{ on } \Gamma, \quad \partial_n V_k^{(p)} = 0 \text{ on } \partial\Omega_0 \quad (8)$$

Decay of Steklov eigenfunctions $V_k^{(p)}$ [4, 5, 6]

Steklov eigenfunctions (with sufficiently high k) have an upper bound that decays exponentially, i.e., there exist constants $B > 0$, $\eta > 0$, $\epsilon > 0$ and k_0 such that $\forall k > k_0,\ \forall \boldsymbol{x} \in \Omega$

$$|\sqrt{\partial\Omega}||V_k^{(p)}(\boldsymbol{x})| \leq B\left(\mu_k^{(p)}\right)^{\frac{d}{2}-\frac{1}{4}} \exp\left(-\eta\,\mu_k^{(p)} \min\{\epsilon, |\boldsymbol{x}-\partial\Omega|\}\right), \quad (10)$$

In practice what are the values of B and ϵ? Is η close to 1?

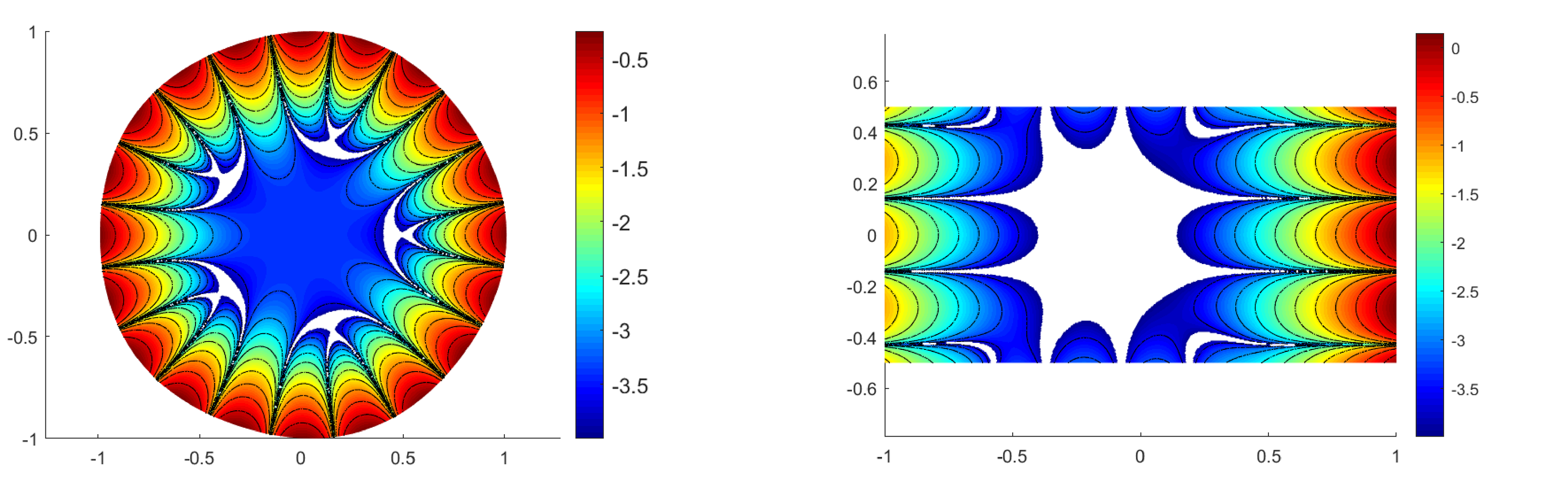


Figure 1 – *Decay of $\lg|V_{20}^{(0)}|$ away from the boundary for a slighlty deformed disk and a rectangle.*

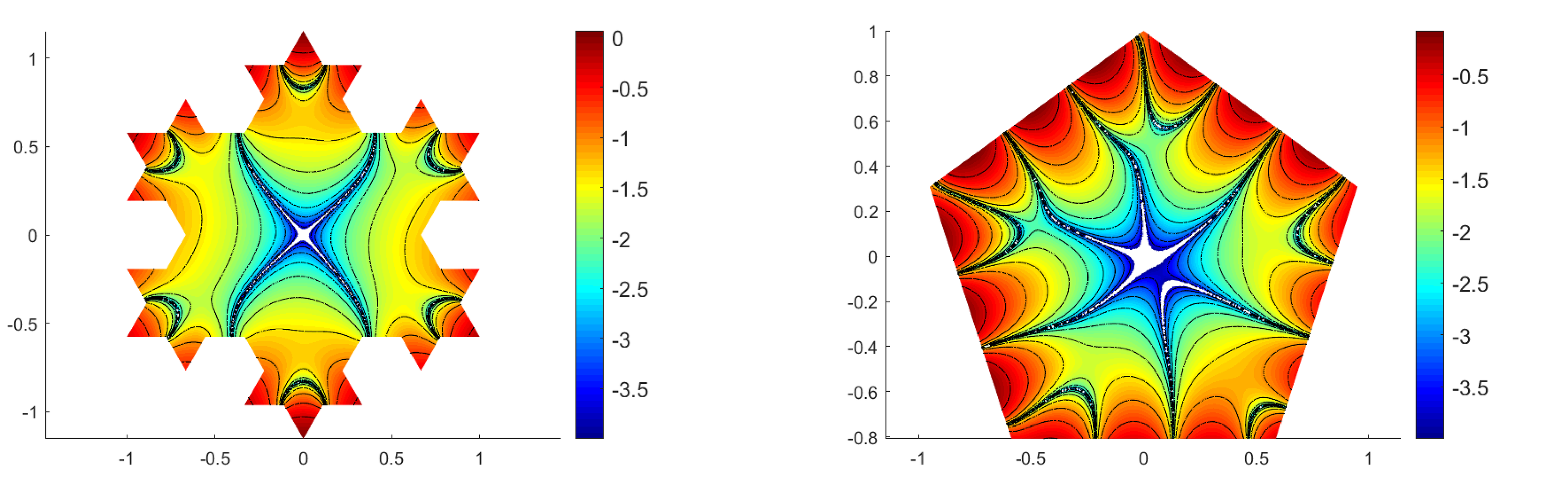


Figure 2 – *Decay of $\lg|V_{15}^{(0)}|$ away from the boundary for two polygonal shapes.*

Asymptotic behavior of eigenvalues for polygonal domains

We relate the asymptotic behavior of eigenvalues to the angles of a polygonal domain via coefficients c_k as

$$\mu_k^{(p)} \simeq c_k\sqrt{p} \quad (p \gg 1). \quad (9)$$

The coefficients c_k are obtained thanks to an iterative procedure [3]:

- Let $a_0 = \{\alpha_0^{(0)}, \ldots, \alpha_{N-1}^{(0)}\}$ be a sequence of all angles of a polygonal domain with N vertices.
- The coefficient c_0 is set to be $c_0 = \sin(\min\{\pi, a_0\}/2)$, it is determined by the smallest angle of the domain, say $\alpha_i^{(0)}$
- Update: the i-th element of the sequence a_0 is increased by $2\alpha_i^{(0)}$
- The next coefficient is determined by $c_1 = \sin(\min\{\pi, a_1\}/2)$, the smallest angle in the already constructed sequence a_1, say $\alpha_j^{(1)}$
- Update: the j-th element of this sequence is increased by $2\alpha_j^{(0)}$ to produce a new sequence a_{k+1}, and so on ...

Open problems in the non self-adjoint setting with complex parameter p

In diffusion-oriented applications, the complex parameter p naturally emerges in the computation of inverse Laplace transforms. In this case, the Dirichlet-to-Neumann operator is no longer self-adjoint, and previous results may not be valid.

- *What is the behavior of eigenvalues $\mu_k^{(p)}$ and eigenfunctions $V_k^{(p)}$?*
- *Do exist branching points in the spectrum?*
- *Does it make sense to perform the inverse Laplace transform of $V_k^{(p)}$ with respect to p?*

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