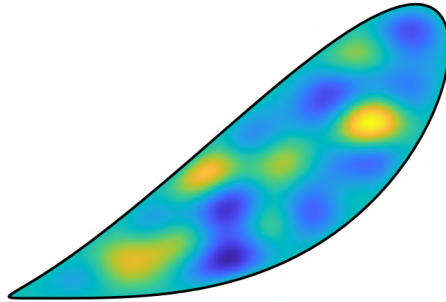


NUMERICAL SOLUTION OF TWO-DIMENSIONAL SPDES

using a Galerkin exponential time differencing scheme

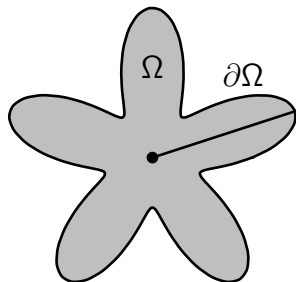
NUMDIFF-16 | September 9, 2021 | Julian Clausnitzer | Jülich Supercomputing Centre, Germany



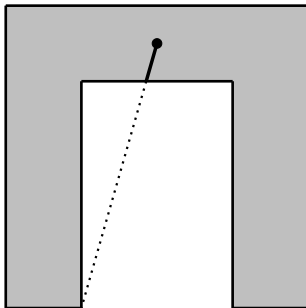
Part I: Introduction & motivation

INTRODUCTION AND OVERVIEW

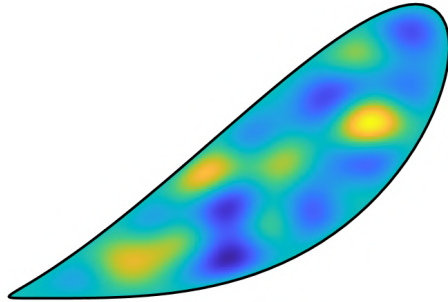
- Aim of the project (joint work with Andreas Kleefeld): Solving parabolic stochastic partial differential equations (SPDEs) on **star-shaped** Lipschitz two-dimensional domains.
- What's new about this: Until now, only relatively simple domains have been considered.



star-shaped



not star-shaped



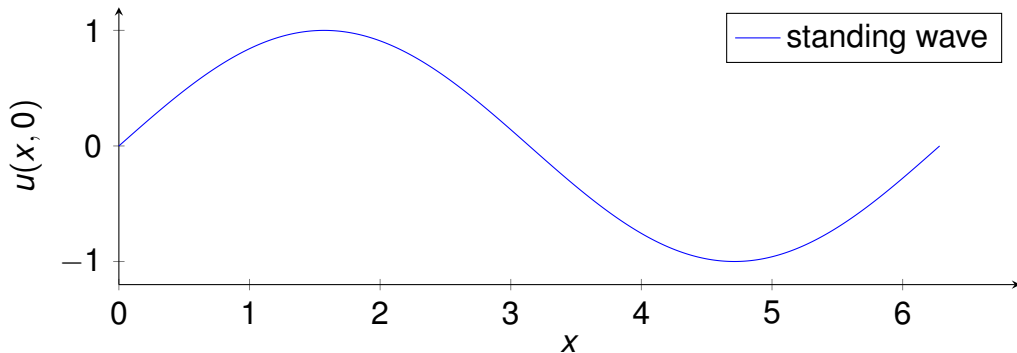
Part II: Theory

THEORY

SPDEs

- Solution of a partial differential equation (PDE): A function. E.g. the vibrating string of a guitar for the wave equation.

$$\partial_{tt}u(x, t) = c^2 \partial_{xx}u(x, t)$$

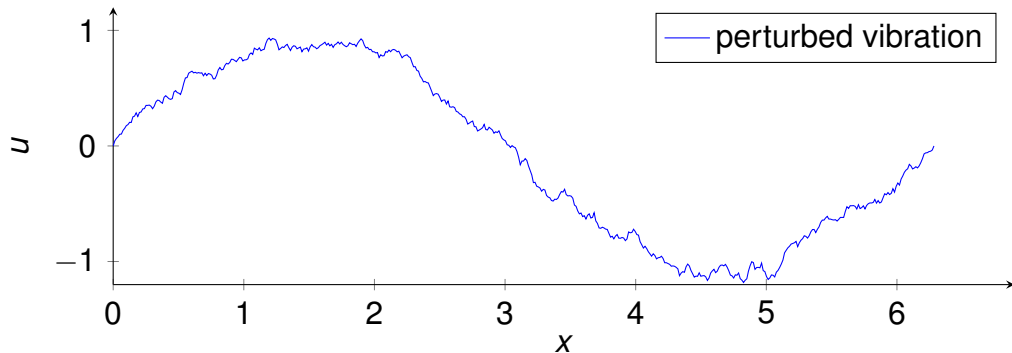


THEORY

SPDEs

- Solution of an SPDE: A stochastic process. E.g. a vibrating string fluctuating randomly.

$$\partial_{tt}u(x, t) = c^2 \partial_{xx}u(x, t) + \xi_t$$



THEORY

Setting

- 1 **Stochastic analysis** and Wiener processes in Hilbert spaces
- 2 **Approximation** of SPDEs: Projection and temporal discretization
- 3 **Boundary integral formulation** and **Beyn integral algorithm** for more general 2D domains

THEORY

1. Stochastic analysis

In SPDEs, the process X_t does not take values in \mathbb{R} , but in a general Hilbert space H (here, e.g. $H = H^2(\Omega) \cap H_0^1(\Omega) \subset L^2(\Omega)$). We consider

$$dX(t) = AX(t)dt + dW(t), \quad X(0) = x_0$$

or, equivalently:

$$X(t) = x_0 + \int_0^t AX(s)ds + \int_0^t dW^Q(s),$$

where

- 1 $(X(t))_{t \in [0, T]}$, $T > 0$, is a stochastic process taking values in H ,
- 2 $A : H \rightarrow H$ is a linear operator (typically, $A = \Delta$), and generates an analytical semigroup $(S(t))_{t \in [0, T]}$.
- 3 $(W^Q(t))_{t \in [0, T]}$ a **Wiener process** (Brownian motion) taking values in H .

The $dW^Q(s)$ integral is called **stochastic integral**.

Under the

THEORY

1. Stochastic analysis: Wiener processes

The H -valued Q -cylindrical Wiener process $(W(t))_{t \in [0, T]}$ has a series representation

$$W^Q(t) = \sum_{i=1}^{\infty} \sqrt{q_i} \beta_i(t) \phi_i, \quad (1)$$

with $q_i \geq 0$ are the eigenvalues of Q , $\{\phi_i\}_{i \in \mathbb{N}}$ an ONB of H (usually assumed to be the eigenfunctions of A) and β_k one-dimensional Brownian motions.

To satisfy the condition (Jentzen, Kloeden 2008)

$$\sum_{i=1}^{\infty} (\lambda_i)^{2\gamma-1} q_i < \infty, \quad (2)$$

in the 2D case (where $\lambda_N \sim N$ are Dirichlet eigenvalues and $\gamma \in (0, 1)$) it must be assumed that $q_i \sim i^{-\eta}$ for $\eta > 0$ or that $q_i = 0$ for some $i > K \in \mathbb{N}$ (smooth noise).

The **mild solution** of the SPDE is given by the implicit equation

$$X(t) = S(t)x_0 + \int_0^t S(t-s)dW^Q(s) \quad (3)$$

with $S(t) = e^{At}$ the analytic semigroup.

Under these assumptions (and possibly, suitable assumptions on a nonlinearity F), there exists a unique mild solution (Jentzen, Kloeden 2008).

THEORY

2. Approximation

The approximation of the solution is done in two steps:

- 1 Projection onto a finite-dimensional subspace of H .
- 2 Discretization in time.

THEORY

2. Approximation: Projection

For our equations, we assume **Dirichlet boundary conditions**, i.e.,

$$X|_{\partial\Omega} = 0.$$

Galerkin approach: The solution $(X(t))_{t \in [0, T]}$ is extended in a Fourier-like series, the base functions being the **Dirichlet eigenfunctions** u of Δ in Ω satisfying

$$\Delta u = \lambda u \tag{4}$$

for a real number $\lambda \in \mathbb{R}_{>0}$. They form an orthonormal basis (ONB) of $L^2(\Omega)$.

THEORY

2. Approximation: Spatial Projection

There is an orthonormal basis $\{\phi_i\}_{i \in \mathbb{N}}$ of $L^2(\Omega)$ satisfying

$$\Delta \phi_i = \lambda_i \phi_i, \quad i \in \mathbb{N}$$

for real eigenvalues $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots$. We use a projection

$$P_N : H \rightarrow H_N = \text{span}\{\phi_1, \dots, \phi_N\}$$

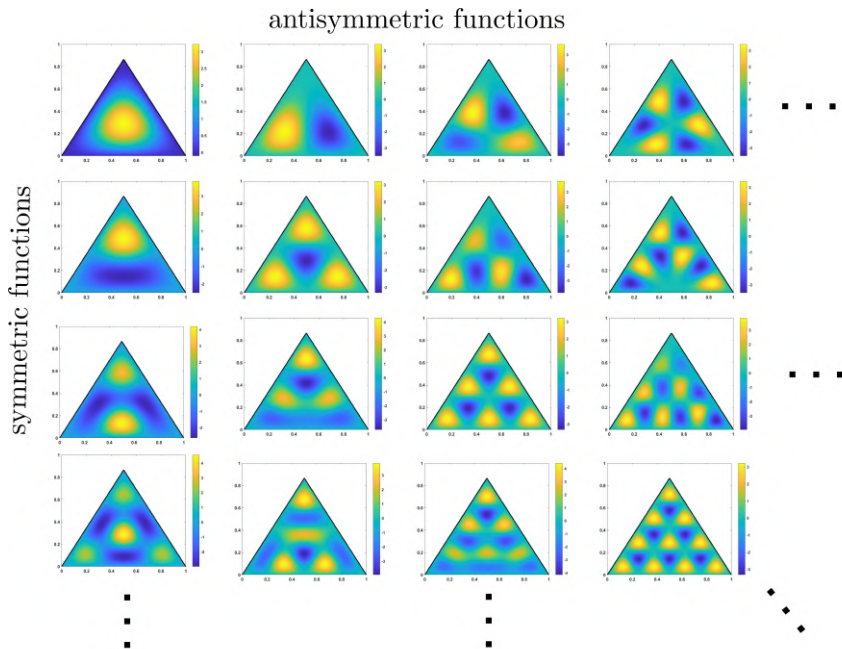
$$u(x) = \sum_{i=1}^{\infty} \langle \phi_i, u \rangle \phi_i(x) \mapsto \sum_{i=1}^N \langle \phi_i, u \rangle \phi_i(x)$$

and consider the projected equation

$$dX_N(t) = A_N X_N(t) dt + dW_N(t), \quad X_N(0) = x_0,$$

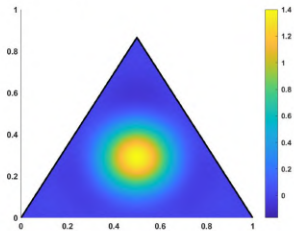
$$X_N = P_N \circ X, \quad A_N = P_N \circ A, \quad W_N = P_N \circ W.$$

Orthonormal basis for $L^2(\Omega)$, where Ω is an equilateral triangle:

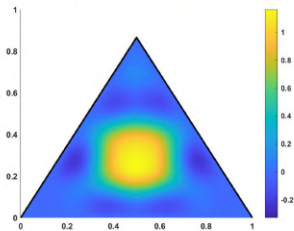


Fourier approximations for a centered square in Ω , $f(x) = \mathbb{1}_{[0.35,0.65] \times [0.139,0.439]}(x)$

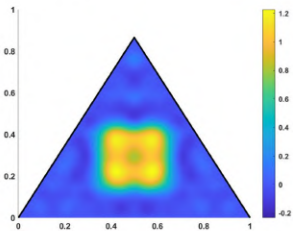
$$\sum_{i=1}^{10} \langle f, \phi_i \rangle_{L^2(\Omega)} \phi_i(x)$$



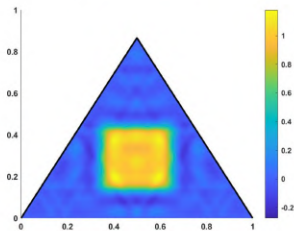
$$\sum_{i=1}^{20} \langle f, \phi_i \rangle_{L^2(\Omega)} \phi_i(x)$$



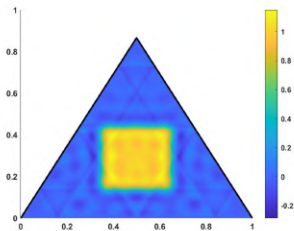
$$\sum_{i=1}^{50} \langle f, \phi_i \rangle_{L^2(\Omega)} \phi_i(x)$$



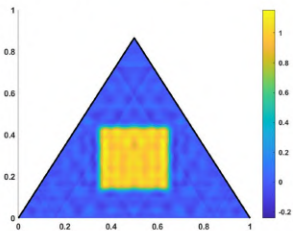
$$\sum_{i=1}^{100} \langle f, \phi_i \rangle_{L^2(\Omega)} \phi_i(x)$$



$$\sum_{i=1}^{200} \langle f, \phi_i \rangle_{L^2(\Omega)} \phi_i(x)$$



$$\sum_{i=1}^{500} \langle f, \phi_i \rangle_{L^2(\Omega)} \phi_i(x)$$



THEORY

2. Approximation: Temporal discretization

$$dX_N(t) = A_N X_N(t) dt + dW_N(t), \quad X_N(0) = x_0 \quad (5)$$

We consider a running Fourier expansion

$$X_N(t) = \sum_{i=1}^N v_i^N(t) \cdot \phi_i.$$

We divide (5) into M time steps, step size $h = T/M$, $t_j = j \cdot h$, $j = 1, \dots, M$.

We consider a running Fourier expansion

$$X_N(t) = \sum_{i=1}^N v_i^N(t) \cdot \phi_i.$$

The full scheme for the coefficients $v_{i,j}^{N,M} = v_i^N(t_j)$, $t_j = j \cdot \frac{T}{M}$, is (Jentzen, Kloeden 2008)

$$v_{i,j+1}^{N,M} = \exp(-\lambda_i h) v_{i,j}^{N,M} + \left(\frac{1}{2\lambda_i} (1 - \exp(-2\lambda_i h)) \right)^{1/2} R_{i,j},$$

where $R_{i,j} \sim N(0, 1)$ i.i.d., $i = 1, \dots, N$, $j = 0, \dots, M - 1$.

THEORY

3. Boundary integral formulation and Beyn integral algorithm

For the presented scheme, the eigenvalues λ_i and eigenfunctions ϕ_i , $i = 1, \dots, N$, are needed.

- For simple shapes (disk, square, triangle), λ_i and ϕ_i are known exactly
- For more general domains: The eigenvalue problem

$$\begin{aligned}\Delta u + \kappa^2 u &= 0 \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega, \\ u &\neq 0.\end{aligned}$$

is solved with a double-layer ansatz

$$u(\mathbf{x}) = \text{DL}_\kappa[\psi](\mathbf{x}) = \int_{\partial\Omega} \psi(\mathbf{y}) \cdot \partial_{\nu(\mathbf{y})} \Phi_\kappa(\mathbf{x}, \mathbf{y}) \, d\mathbf{s}(\mathbf{y}).$$

THEORY

3. Boundary integral formulation and Beyn integral algorithm

We use a double layer ansatz

$$u(x) = \text{DL}_\kappa[\psi](x) = \int_{\partial\Omega} \psi(y) \cdot \partial_{\nu(y)} \Phi_\kappa(x, y) \, d\mathbf{s}(y), \quad x \in \Omega$$

with a density function $\psi \in C(\partial\Omega)$ and the fundamental solution

$$\Phi_\kappa(x, y) = \frac{i}{4} H_0^{(1)}(\kappa \|x - y\|). \quad (6)$$

Using the jump relation of the double layer potential, we have the equation

$$-\frac{1}{2}\psi(x) + \int_{\partial\Omega} \psi(y) \cdot \partial_{\nu(y)} \Phi_\kappa(x, y) \, d\mathbf{s}(y) = 0, \quad x \in \partial\Omega \quad (7)$$

which is discretized using a boundary element collocation method. This gives rise to a nonlinear eigenvalue problem

$$M(\kappa)\vec{\psi} = 0, \quad (8)$$

where $\vec{\psi}$ contains the values of ψ at the collocation nodes.

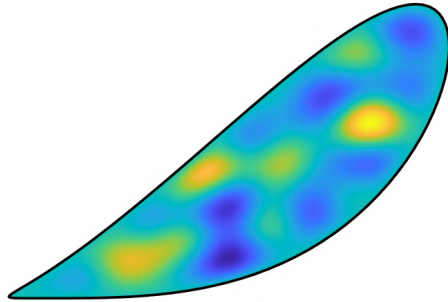
The nonlinear eigenvalue problem

$$M(\kappa)\vec{\psi} = 0 \quad (9)$$

is solved using the **Beyn algorithm** (Beyn, 2012), which makes use of Keldysh's theorem from complex analysis to retrieve the eigenvalues from contour integrals of the form

$$\frac{1}{2\pi i} \int_{\gamma} f(z)M(z)^{-1} dz, \quad (10)$$

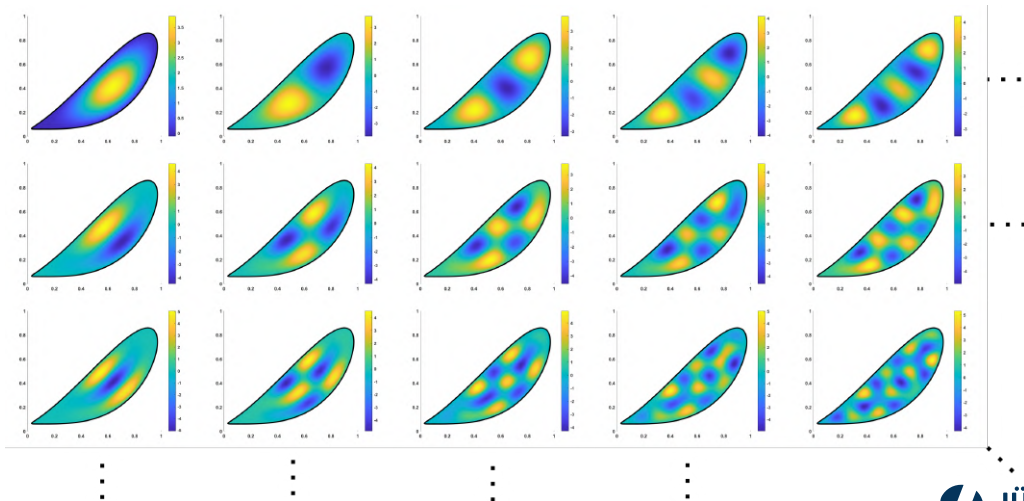
where f is a holomorphic function and γ is a contour containing an eigenvalue.



Part III: Numerical results

We show the first elements of the ONB for $L^2(\Omega)$ for the wing-shaped domain whose boundary inside $[0, 1] \times [0, 1]$ is given by

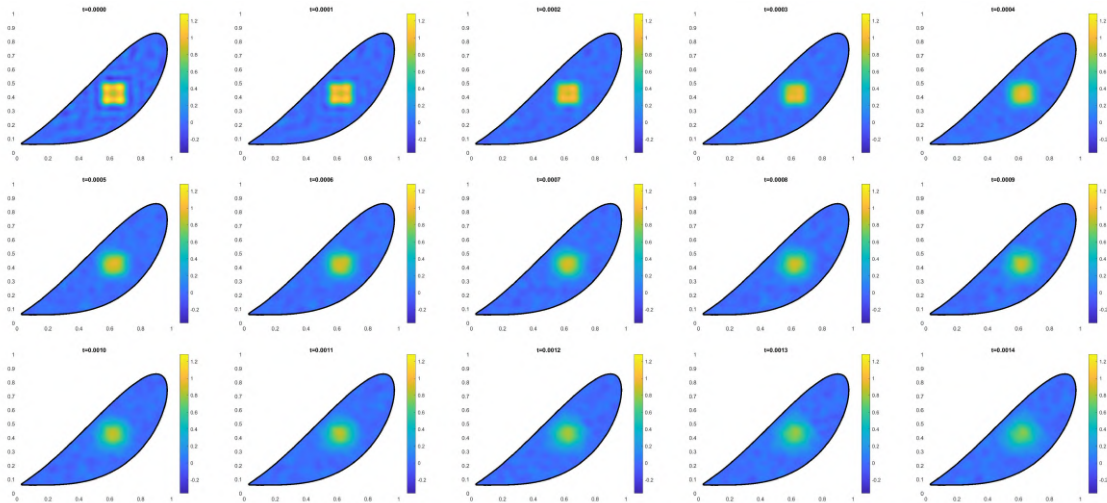
$$\gamma(t) = \begin{pmatrix} 0.25 \sin(t) - 0.4 \cos(t) + 0.5 \\ 0.2(\cos(t) - 1)^2 + 0.3 \end{pmatrix}, \quad t \in [0, 2\pi). \quad (11)$$



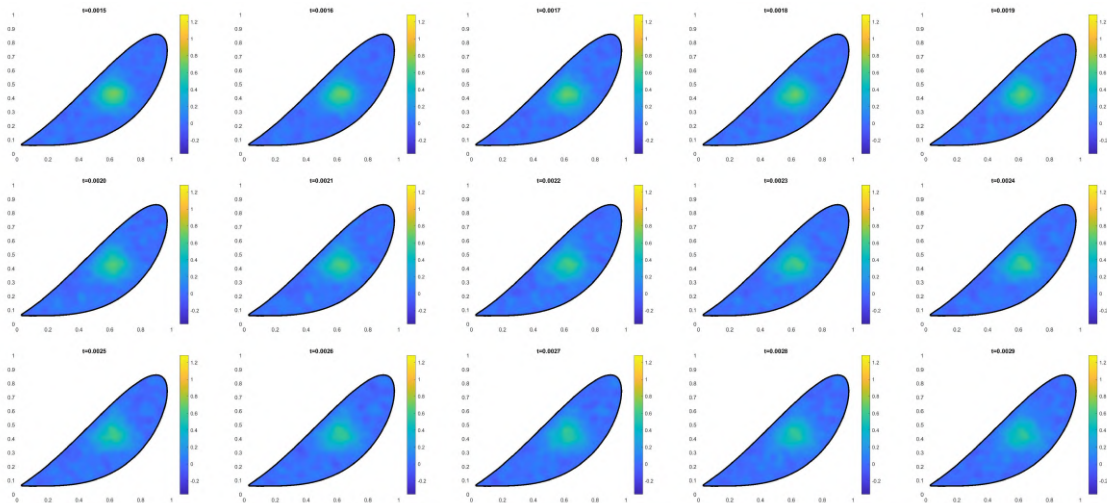
A plot for the heat equation

$$dX(t) = \Delta X(t)dt + 0.1dW(t), \quad X(0) = \mathbb{1}_{[0.55,0.7] \times [0.35,0.5]}, \quad t \in [0, 0.01] \quad (12)$$

with $N = 200$ eigenfunctions and $M = 100$ time steps:



For $t \in [0.0015, 0.0029]$



NUMERICAL RESULTS

Error analysis

We perform the Galerkin-ETD scheme with perturbed eigenvalues and eigenfunctions. Hence, there are three error sources:

- 1 The error of the Galerkin-ETD scheme,
- 2 The approximation of the eigenvalues in the Galerkin scheme,
- 3 The approximation of the eigenfunctions in the Galerkin scheme.

NUMERICAL RESULTS

Error analysis

The following can be said about the errors:

- 1 The error of the Galerkin-ETD scheme: This error has been shown to be (Jentzen, Kloeden 2008)

$$\sup_{j=0,\dots,M} \left(\mathbb{E} \|X(t_j) - \tilde{X}_{M,N}(t_j)\|_{L^2(\Omega)}^2 \right)^{1/2} \leq C_T \left(\lambda_N^{\epsilon-1} + \frac{\log(M)}{M} \right) \quad (13)$$

for any $\epsilon > 0$ (spatial error, temporal error). This means that the scheme should have a strong convergence order of $1 - \epsilon$ for any $\epsilon > 0$ w.r.t. λ_N and M . (In two dimensions, $\lambda_N \sim N$ asymptotically.)

NUMERICAL RESULTS

Error analysis

- 2 Approximate eigenvalue error: For an error tolerance

$$\tilde{\epsilon} = \max_{i=1,\dots,N} \{|\lambda_i - \tilde{\lambda}_i|\} \quad (14)$$

between the approximate eigenvalues $\tilde{\lambda}_i$ and the exact eigenvalues λ_i , it can be shown that the resulting error behaves as $\mathcal{O}(\tilde{\epsilon} \cdot M \cdot N)$.

- 3 Approximate eigenfunction error: Likewise, for an error tolerance

$$\tilde{\epsilon} = \max_{i=1,\dots,N} \{\|e_i - \tilde{e}_i\|_{L^2(\Omega)}\} \quad (15)$$

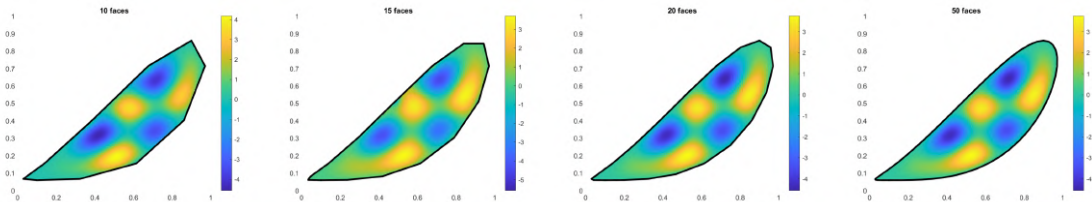
between the approximate eigenfunctions \tilde{e}_i and the exact eigenfunctions e_i , it can be shown that the resulting error also behaves as $\mathcal{O}(\tilde{\epsilon} \cdot M \cdot N)$.

NUMERICAL RESULTS

Error analysis

Note that the first error term 'competes' against the other two in the sense that it decreases as M, N grow, while the other two grow as M, N grow.

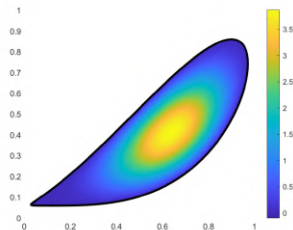
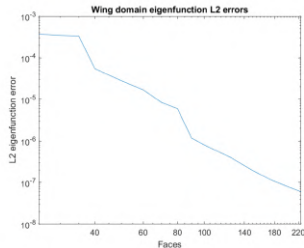
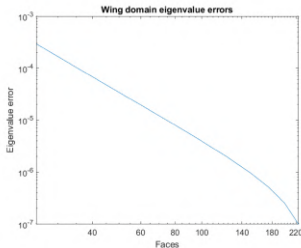
This necessitates a high accuracy for the eigenvalues and eigenfunctions. The accuracy depends on the number of boundary elements.



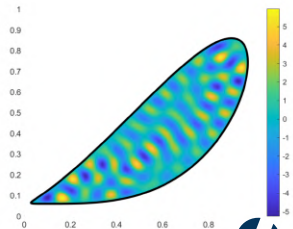
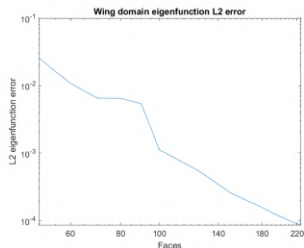
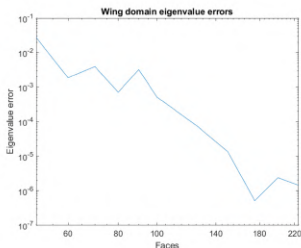
From high-frequency scattering theory (e.g. Bruno, Reitich 2008) it is known that to maintain a given accuracy, the number n_f of boundary elements must rise linearly with $\kappa_N = \sqrt{\lambda_N}$.

Absolute eigenvalue errors and L^2 eigenfunction errors to a reference for $n_f = 250$ faces for the wing domain:

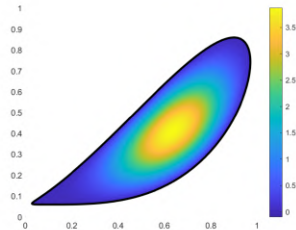
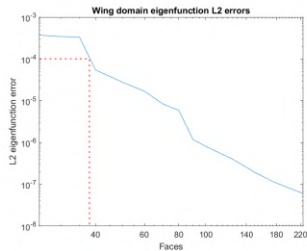
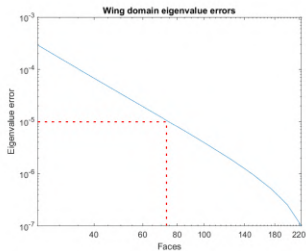
Wave number $\kappa_1 = \sqrt{\lambda_1} \approx 9.7614$:



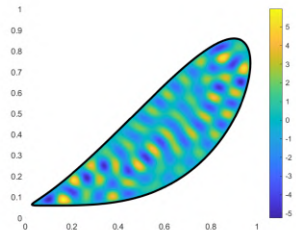
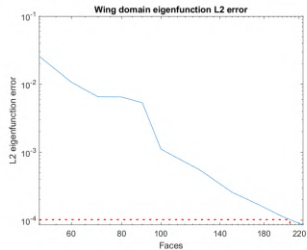
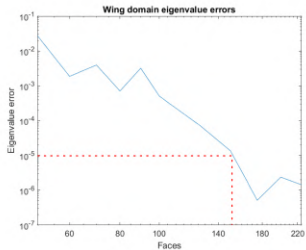
Wave number $\kappa_{112} = \sqrt{\lambda_{112}} \approx 70.9452$:



Suppose that we set as tolerances $\epsilon_1 = 10^{-5}$ for the eigenvalues and $\epsilon_2 = 10^{-4}$ for the eigenfunctions. Wave number $\kappa_1 = \sqrt{\lambda_1} \approx 9.7614$:



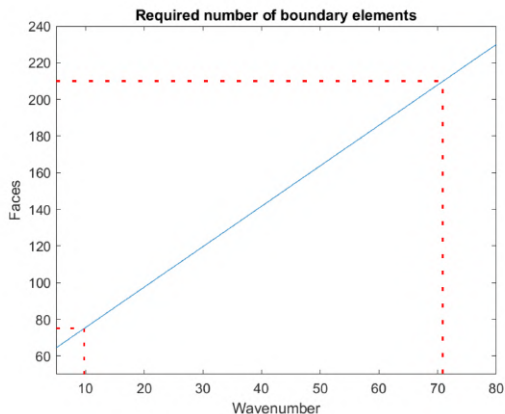
Wave number $\kappa_{112} = \sqrt{\lambda_{112}} \approx 70.9452$:



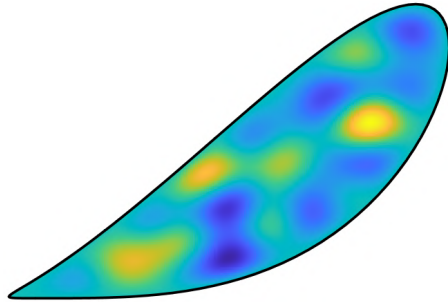
We create a linear fit between the found required face numbers

$$\kappa_1 \approx 9.7614, \quad n_f(\kappa_1) = 75, \quad (16)$$

$$\kappa_2 \approx 70.9452, \quad n_f(\kappa_{112}) = 210. \quad (17)$$



In this way, we can compute eigenvalues and an ONB to a prescribed accuracy for any domain.



Part IV: Outlook, references

OUTLOOK, REFERENCES

Other aspects:

- Effect of nonlinear functions in the SPDE (e.g. reaction-diffusion equations) (work in progress)
- Parallelization of the implementation (work in progress)
- Possible applications: Investigation of pattern formation under perturbations
- Adaptive time-stepping schemes

References, further reading:

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- O. P. Bruno and F. Reitich. High-order methods for high-frequency scattering applications. *Modeling and Computations in Electromagnetics*. Springer, 2008. 129–163.

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