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A Reduced Basis Method for Fractional Diffusion Operators

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Abstract

Several authors have proposed and analyzed numerical methods for fractional differential operators, in particular Fourier Galerkin schemes and Caffarelli-Silvestre extensions. In this thesis we consider a different approach. By means of a reduced basis method, the desired operator is projected to a low dimensional space $\mathcal{V}_r$, where the fractional power can be directly evaluated via the eigen-system. The optimal choice of $\mathcal{V}_r$ is provided by the so called *Zolotarëv points*, ensuring exponential convergence. Numerical experiments evaluating the operator and the inverse operator confirm the analysis.

The time-dependent Fractional Cahn-Hilliard Equation (FCHE) is examined for further tests. By a splitting method, the non-linear operator is decoupled from the regular Laplacian, such that the linear parabolic equation is solved exactly on the low dimensional reduced space. Different choices of the fractional power s are discussed and tested.

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Contents

1 Introduction

Numerical simulation of coarsening dynamics is a subject of great interest in computational material science. Phenomena of this kind can be observed in both nature and technology. The behavior of a binary alloy can be modeled by the so-called Allen-Cahn and Cahn–Hilliard equation. In this thesis a generalization of those two models is considered, giving rise to the Fractional Cahn-Hilliard Equation

$$\frac{\partial u}{\partial t}(x,t) + (-\Delta)^s(-\varepsilon^2 \Delta u(x,t) + f(u(x,t))) = 0.$$

Problems evolving from these models are complex and can not be solved analytically in general. Numerical methods have to be installed. To this extent we aim to establish a numerically appealing scheme, such that, in addition to the widely common approaches, efficient implementations for fractional diffusion operators are provided.

Outline of the thesis

In the beginning of this thesis the general framework of intermediate spaces and fractional derivatives is introduced. We consider one special application of interest in terms of the Fractional Cahn-Hilliard Equation, naturally arising from the Allen-Cahn and Cahn-Hilliard model. A coarse overview with respect to its physical derivation in combination with some standard analysis results is provided. We further sketch some present implementation techniques in context of the fractional Laplacian.

The third chapter deals with two different approaches of interpolation theory, Banach and Hilbert space interpolation. We provide both computationally and theoretically convenient settings for the further course of action. Equivalence of those two methods appears to be the main result of this section.

Subsequent, some standard techniques from calculus of variation are applied, giving the K-functional an applicable form in order to make evaluations of interpolation norms possible. Due to extensive computational costs, a reduced basis method is introduced, giving rise to the reduced basis norm. A feasible choice of the reduced space and its efficient implementation is discussed.

In the fifth chapter the connection between interpolation norms and their associated fractional operators is deployed. Methods for inverse operator actions are installed. Moreover, we study a first numerical example in terms of the fractional Poisson equation.

The sixth chapter deals with the involved analysis. An optimal choice of the reduced basis is elaborated, such that exponential convergence rates for the error in the reduced basis norm can be confirmed. Convergence for the reduced basis operator action is naturally obtained. Numerical experiments affirm the analysis.

We finally dedicate our attention to the implementation of the Fractional Cahn-Hilliard Equation itself. A splitting method is installed. The resulting linear parabolic equation is projected to the reduced space where its exact solution can be cheaply computed by means of the matrix exponential function. Coarsening dynamics of FCHE models are studied for several fractional powers.

Implementation

All numerical examples and algorithms where implemented within the Python interface NGS-Py of the open source software packages Netgen and NGSolve[1], see [14] and [15].

Notation

Throughout this thesis we agree on the following notation:

$\langle \cdot, \cdot \rangle_V$	scalar product on the Hilbert space V
$\dim(V)$	dimension of V
$C^\infty_{per}((a,b)^2)$	$\{u \in C^\infty((a,b)^2) \mid u \text{ periodic on } (a,b)^2\}$
$[...]$	matrix in column notation
$[\{...\}]$	linear span of the set $\{...\}$
V_h	H^1-conforming finite element space of uniform mesh-size h
$\mathcal{V}_r$	reduced space of dimension $r+1$
V_r	reduced basis matrix of dimension $(N+1) \times (r+1)$
r	reduced basis dimension downsized by 1
N	finite element space dimension downsized by 1
I_r	$(r+1) \times (r+1)$ unit matrix
I	$(N+1) \times (N+1)$ unit matrix
$\underline{u}$	coefficient vector of $u \in V_h$
$\underline{\underline{u}}$	coefficient vector of $u \in \mathcal{V}_r$
M	mass matrix
A	finite element matrix arising from the H^1-scalar product
$\widehat{A}$	finite element matrix arising from the gradient bilinear form
$\\|\cdot\\|_M$	by M induced norm
ℓ_2	$\left\{x : \mathbb{N} \to \mathbb{R} \,\middle|\, \sum_{k\in\mathbb{N}} \|x(i)\|^2 < \infty \right\}$
v^*	minimizer of the K-functional
v_r^*	minimizer of the reduced basis K-functional
$v^*(t_j)$	snapshot solution of the shifted Laplace problem with respect to t_j
Π_m	space of polynomials on $\mathbb{R}$ up to degree m
$\bar{K}, \bar{K}'$	elliptic integrals
λ_{min}	$\lambda_{min}(M^{-1}A)$
λ_{max}	$\lambda_{max}(M^{-1}A)$
$\mathcal{I}$	refers to the interval $[\sqrt{\lambda_{max}^{-1}}, 1]$
$\hat{\sigma}$	refers to the interval $[1, \sqrt{\lambda_{max}}]$

By $a \preccurlyeq b$ we mean that there exists a constant $c \in \mathbb{R}^+$ independent of a, b and r, such that $a \leq cb$.

[1] https://ngsolve.org/

2 The Fractional Cahn-Hilliard Equation

The goal of this chapter is to elaborate the most common framework of fractional derivatives and interpolation spaces in order to introduce the *Fractional Cahn-Hilliard Equation*. We further establish the Fourier Galerkin method, serving as prototype for the approach performed in subsequent chapters.

2.1 The fractional framework

Successive argumentations follow the outline of [1]. Consider an orthonormal basis $(z_k)_{k\in\mathbb{N}}$ of $L_2(\Omega)$ with $\Omega = (0, 2\pi)^2$, such that

$$-\Delta z_k = \mu_k^2 z_k \tag{2.1}$$

is satisfied in a weak sense with homogeneous Neumann boundary conditions. We apply spectral theory with respect to $(z_k)_{k\in\mathbb{N}}$ in order to establish the fractional framework. Each $u \in L_2(\Omega)$ satisfies the expansion

$$u = \sum_{k\in\mathbb{N}} u_k z_k \qquad u_k := \langle z_k, u\rangle_{L_2},$$

justifying the introduction of fractional spaces

$$H^s(\Omega) := \overline{C^\infty(\Omega)}^{\|\cdot\|_{H^s}} \qquad s \in (0,1), \tag{2.2}$$

whereas the closure is taken with respect to the interpolation norm

$$\|u\|_{H^s}^2 = \sum_{k\in\mathbb{N}} (1+\mu_k^2)^s u_k^2.$$

Motivated by the relation

$$L_2(\Omega) \subseteq H^s(\Omega) \subseteq H^1(\Omega) \qquad s \in (0,1),$$

$H^s(\Omega)$ can be regarded as intermediate space between $H^0(\Omega) = L_2(\Omega)$ and $H^1(\Omega)$.

Remark 2.1. *Along with periodic boundary conditions in* (2.1)*, the choice of* $s \in (1,2)$ *for*

$$H^s_{per}(\Omega) := \overline{C^\infty_{per}(\Omega)}^{\|\cdot\|_{H^s}}$$

indeed gives rise to an intermediate space between the periodic Sobolev spaces $H^1_{per}(\Omega)$ *and* $H^2_{per}(\Omega)$*. We therefore allow* $s \in (1,2)$ *in this case, leading to an extrapolation space*

$$H^2_{per}(\Omega) \subseteq H^{1+\alpha}_{per}(\Omega) \subseteq H^1_{per}(\Omega)$$

for all $\alpha \in (0,1)$.

2.1.1 Fractional Laplacian

Identity (2.1) suggests the following definition.

Definition 2.2. *For all $s \in (0,1)$ and $u \in H^s(\Omega)$ the fractional Laplace operator is defined as*

$$(-\Delta)^s u = \sum_{k\in\mathbb{N}} \mu_k^{2s} u_k z_k.$$

One immediately observes the following property.

Lemma 2.3. *Let $r, s \in (0,1)$ and $u \in H^{r+s}(\Omega)$. Then*

$$(-\Delta)^{r+s} u = (-\Delta)^r (-\Delta)^s u = (-\Delta)^s (-\Delta)^r u.$$

Proof. According to definition 2.2 there holds

$$\begin{aligned}
(-\Delta)^r (-\Delta)^s u &= (-\Delta)^r \left(\sum_{k\in\mathbb{N}} \mu_k^{2s} u_k z_k \right) \\
&= \sum_{k\in\mathbb{N}} \mu_k^{2s} u_k (-\Delta)^r z_k \\
&= \sum_{k\in\mathbb{N}} \mu_k^{2(r+s)} u_k z_k = (-\Delta)^{r+s} u,
\end{aligned}$$

which is why the first identity holds. The second one follows analogously. ■

Another important concept required for posing weak formulations of fractional Cahn-Hilliard models is partial integration for fractional derivatives.

Lemma 2.4 (Fractional integration by parts)**.** *Let $r, s \in (0,1)$ and $u, v \in H^{r+s}(\Omega)$. Then there holds*

$$\langle (-\Delta)^{r+s} u, v \rangle_{L_2} = \langle (-\Delta)^r u, (-\Delta)^s v \rangle_{L_2}.$$

Proof. Since

$$(-\Delta)^{r+s} u = \sum_{k\in\mathbb{N}} \mu_k^{2(r+s)} u_k z_k$$

it follows by spectral decomposition

$$\begin{aligned}
\langle (-\Delta)^{r+s} u, v \rangle_{L_2} &= \langle \sum_{k\in\mathbb{N}} \mu_k^{2(r+s)} u_k z_k, \sum_{k\in\mathbb{N}} v_k z_k \rangle_{L_2} \\
&= \sum_{k\in\mathbb{N}} \mu_k^{2(r+s)} u_k v_k \\
&= \sum_{k\in\mathbb{N}} \left(\mu_k^{2r} u_k\right) \left(\mu_k^{2s} v_k\right) \\
&= \langle (-\Delta)^r u, (-\Delta)^s v \rangle_{L_2}.
\end{aligned}$$

■

Considerations from above justify the further course of action.

2.2 Derivation of the Fractional Cahn-Hilliard Equation

In the following section a physical derivation of the Fractional Cahn-Hilliard Equation is provided. We proceed similarly to [1], [8] and [19].

Multiphase flows in fluid dynamics deal with the simultaneous flow of an alloy which consist either of the same material in different states (gaseous, liquid or solid) or of several materials with different chemical properties but in the same state. We will examine the latter with binary alloys in a bounded domain Ω only, such as phase separations of oil droplets in water.

To this extent let $u(x,t)$ denote the concentration of one of the two components, a so called *order parameter*. The purpose of such parameters is to distinguish between different phases, i.e. spatial areas where the corresponding order parameter (physical or chemical quantity) is constant. u might be expressed in units of $^{\text{mol}}/_{\text{m}^3}$. Under the assumption of mass preservation the opposite concentration is automatically determined as well.

Suppose that there is a pair of values $(\hat{u}_1, \hat{u}_2) \in \mathbb{R}^2$ and a pair of phases referred to as A and B, such that the mixture can only be in equilibrium if and only if A has concentration $\hat{u}_1$ and B concentration $\hat{u}_2$. This issue can be illustrated by a non-linear function F of bistable type, admitting two local minima in $\hat{u}_1$ and $\hat{u}_2$ with

$$F(\hat{u}_1) = F(\hat{u}_2) = F'(\hat{u}_1) = F'(\hat{u}_2) = 0.$$

A common choice of F is given by

$$F(y) = \frac{1}{4}(1-y^2)^2,$$

such that $\hat{u}_1 = -1$ and $\hat{u}_2 = 1$. It is further assumed that the initial state $u(x,0) = u_0(x)$ with $u_0(\Omega) \subseteq (\hat{u}_1, \hat{u}_2)$ provides a uniform, unstable mixture of the components, resulting in the phase separation in which the alloy aims to evolve into phase A with concentration $\hat{u}_1$ and phase B with concentration $\hat{u}_2$. Mathematically spoken, this corresponds to the value of a functional

$$\hat{E}(u(x,t)) = \int_\Omega F(u(x,t))\,dx,$$

decreasing in time, finally reaching a minimum. One widely accepted approach is to deal with the slightly modified functional

$$E(u(x,t)) = \int_\Omega F(u(x,t)) + \frac{\varepsilon^2}{2}|\nabla u(x,t)|^2\,dx$$

with a small parameter $\varepsilon > 0$. From a physical point of view, this corresponds to the common assumption that materials have the tendency to evolve as uniform as possible. The penalty term then restrains large jumps of the gradient.

It is reasonable to further assume that the amount of each component remains constant throughout the evolution, resulting in the constraint

$$\int_\Omega u(x,t)\,dx = const. \tag{2.3}$$

The goal is now to develop a law of evolution for u, such that the energy $E(u)$ decreases in time while (2.3) holds. To this extent we consider the *gradient of* E and hope that mass preservation is obtained.

Let V be a Hilbert space and $\mathcal{F} : V \longrightarrow \mathbb{R}$, then the gradient $\nabla_V \mathcal{F}$ of $\mathcal{F}$ at point $u \in V$ is defined as the Riesz-representative of its first variation, i.e.

$$\forall v \in V: \quad \langle \nabla_V \mathcal{F}(u), v \rangle_V = \frac{d}{d\varepsilon} \mathcal{F}(u + \varepsilon v) \Big|_{\varepsilon=0}.$$

The proportionality

$$\frac{\partial u}{\partial t} = -\nabla_V E(u) \tag{2.4}$$

ensures decay of energy by means of the chain rule

$$\frac{\partial}{\partial t} E(u(x,t)) = \langle \nabla_V E, \frac{\partial u}{\partial t} \rangle_V = -\|\nabla_V E\|_V^2 \leq 0.$$

We pose the question which choice of V guarantees that (2.3) holds. Direct computations reveal that for $V = L_2(\Omega)$

$$\frac{d}{d\varepsilon} E(u + \varepsilon v) \Big|_{\varepsilon=0} = \langle \varepsilon^2 \nabla u, \nabla v \rangle_{L_2} + \langle F'(u), v \rangle_{L_2} = \langle -\varepsilon^2 \Delta u + F'(u), v \rangle_{L_2}.$$

Together with (2.4) and $f(u) := F'(u) = u^3 - u$ this results in the *Allen-Cahn equation*

$$\frac{\partial u}{\partial t} + (-\varepsilon^2 \Delta u + f(u)) = 0 \text{ in } \Omega.$$

Formal computations confirm that the Allen-Cahn equation fails to preserve mass. This problem can be overwhelmed by the choice $V = H^{-1}(\Omega)$. Again, the associated gradient can be determined

$$\nabla_{H^{-1}} E(u) = (-\Delta)(-\varepsilon^2 \Delta u + f(u)),$$

adding up to the *Cahn-Hilliard equation*

$$\frac{\partial u}{\partial t} + (-\Delta)(-\varepsilon^2 \Delta u + f(u)) = 0 \text{ in } \Omega,$$

which does indeed satisfy (2.3), as shown in Lemma 2.5. To some extent the choice of H^{-1} might occur arbitrary. Therefore we extend the concept from above for $V = H^{-s}(\Omega)$, $s \in [0,1]$, yielding

$$\nabla_{H^{-s}} E = (-\Delta)^s (-\varepsilon^2 \Delta u + f(u)),$$

to finally obtain the *Fractional Cahn-Hilliard Equation* (FCHE)

$$\frac{\partial u}{\partial t} + (-\Delta)^s (-\varepsilon^2 \Delta u + f(u)) = 0 \text{ in } \Omega.$$

This provides the foundation to regard the following problem. For $s \in [0,1]$ and $\Omega = (0, 2\pi)^2$ we aim to find a smooth function $u(x,t)$ on $\Omega \times (0,T]$, such that

$$\forall (x,t) \in \Omega \times (0,T]: \quad \frac{\partial u}{\partial t}(x,t) + (-\Delta)^s (-\varepsilon^2 \Delta u(x,t) + f(u(x,t))) = 0, \tag{2.5a}$$

$$\forall t \in (0,T]: \quad u(\cdot, t) \text{ is } 2\pi\text{-periodic}, \tag{2.5b}$$

$$\forall x \in \Omega: \quad u(x,0) = u_0(x), \tag{2.5c}$$

whereas $f(u) = F'(u) = u^3 - u$. The weak formulation is derived as usual. Multiplying (2.5a) by a test function, integrating over the domain Ω and integration by parts lead to the familiar variational setting: Find $u \in L_2([0,T], H^{1+s}_{per}(\Omega))$, such that for all $t \in (0,T]$

$$\forall v \in H^{1+s}_{per}(\Omega): \quad \langle \frac{\partial u}{\partial t}, v\rangle_{L_2} + \langle \varepsilon^2(-\Delta)^{\frac{1+s}{2}} u, (-\Delta)^{\frac{1+s}{2}} v\rangle_{L_2} + \langle f(u), (-\Delta)^s v\rangle_{L_2} = 0, \tag{2.6}$$

with initial condition (2.5c). The choice of $s = 0$ corresponds to the weak formulation of the classical Allen-Cahn equation whereas $s = 1$ refers to the Cahn-Hilliard equation.

2.3 Properties of the Fractional Cahn-Hilliard Equation

The question arises how the choice of s impacts certain properties of the equation. Especially, we are interested in mass conservation and the non-increasing behavior of the energy $E(u)$. As shown below, both properties hold for all $s \in (0,1]$, such that the FCHE can be regarded as pendent to the Cahn-Hilliard rather than Allen-Cahn equation, no matter how small the choice of s is. We record:

Lemma 2.5. *For all $s \in (0,1]$ the Fractional Cahn-Hilliard Equation is mass preserving.*

Proof. In the following we show that

$$\forall t \geq 0: \quad \int_\Omega u(x,t)\,dx = \int_\Omega u_0(x)\,dx = const. \tag{2.7}$$

holds for the weak solution of FCHE. Since every classical solution trivially satisfies (2.6), this proofs the claim. Taking $v \equiv 1 \in H^{1+s}(\Omega)$ as test function gives

$$\langle \frac{\partial u}{\partial t}, 1\rangle_{L_2} = 0.$$

It follows

$$\frac{\partial}{\partial t}\int_\Omega u(x,t)\,dx = \int_\Omega \frac{\partial u}{\partial t}(x,t)\,dx = \langle \frac{\partial u}{\partial t}, 1\rangle_{L_2} = 0.$$

We conclude that (2.7) is valid. ■

Lemma 2.6. *For all $s \in [0,1]$ the solution u of (2.5a) - (2.5c) satisfies*

$$\forall t \geq 0: \quad E(u(x,t)) \leq E(u_0(x)) \text{ on } \Omega.$$

Proof. Every classical solution also solves the weak formulation. We obtain for all $x \in \Omega$

$$\begin{aligned}
\frac{d}{dt}E(x,t) &= \frac{d}{dt}\int_\Omega F(u(x,t)) + \frac{\varepsilon^2}{2}|\nabla u(x,t)|^2\,dx \\
&= \langle F'(u(x,t)), \frac{\partial u}{\partial t}(x,t)\rangle_{L_2} + \langle \varepsilon^2 \nabla u(x,t), \nabla \frac{\partial u}{\partial t}(x,t)\rangle_{L_2} \\
&= \langle f(u(x,t)), \frac{\partial u}{\partial t}(x,t)\rangle_{L_2} + \langle \varepsilon^2(-\Delta)u(x,t), \frac{\partial u}{\partial t}(x,t)\rangle_{L_2} \\
&= \langle \varepsilon^2(-\Delta)u(x,t) + f(u(x,t)), \frac{\partial u}{\partial t}(x,t)\rangle_{L_2} \\
&= -\langle \varepsilon^2(-\Delta)u(x,t) + f(u(x,t)), (-\Delta)^s(\varepsilon^2(-\Delta)u(x,t) + f(u(x,t)))\rangle_{L_2}.
\end{aligned}$$

Fractional integration by parts yields

$$\frac{d}{dt}E(x,t) = -\|(-\Delta)^{\frac{s}{2}}(\varepsilon^2(-\Delta)u(x,t) + f(u(x,t)))\|^2_{L_2} \leq 0,$$

resulting in the claimed non-increasing property. ■

2.4 Computational state of the art

Several authors have proposed and analyzed numerical methods to implement fractional differential operators in order to solve equations of type (2.6). A widely common approach is given by the *Fourier-spectral Galerkin* scheme which, among many others, has been discussed in [1], [17] and [20]. Its semi-discretization in space for the weak formulation of FCHE can be formulated in the following way: Find $u \in V_N = [\{e^{ikx_1+ilx_2} \,|\, k,l = -N,...,N\}]$, such that

$$\forall t \in (0,T]\, \forall v \in V_N : \quad \langle \frac{\partial u}{\partial t}, v \rangle_{L_2} + \langle \varepsilon^2 (-\Delta)^{\frac{1+s}{2}} u, (-\Delta)^{\frac{1+s}{2}} v \rangle_{L_2} + \langle f(u), (-\Delta)^s v \rangle_{L_2} = 0.$$

Due to the choice of V_N a decoupled system is derived. The fractional Laplace can be applied according to its definition, leaving only derivatives in time but not in space.

A different concept is regarded in [2] and [6], where the fractional Laplace operator is implemented by means of a harmonic extension problem. Consider the smooth and bounded solution u of

$$\begin{aligned} \forall x \in \mathbb{R}^n\colon \quad & u(x,0) = f(x), \\ \forall x \in \mathbb{R}^n,\, y > 0 : \quad & \Delta u(x,y) = 0. \end{aligned}$$

The square root of the Laplacian $(-\Delta)^{\frac{1}{2}}$ can then be identified with the operator

$$T : f \mapsto -\frac{\partial u}{\partial y}(x,0).$$

A generalization for arbitrary (fractional) powers can be performed. The approach illustrated in this thesis is a different one, interpreting fractional operators in context of Banach and Hilbert space interpolation.

3 Interpolation spaces

Interpolation spaces provide several applications in the field of PDEs, especially in context of trace spaces and fractional derivatives. There are numerous ways to define and analyze those kinds of intermediate spaces. In this chapter we examine two approaches in detail. One refers to the classical Hilbert space interpolation based on expansions according to the eigen-system. The other one is also applicable for Banach spaces, known as *real method of interpolation* or *Peetre's method* , see [4], [5] and [12].

3.1 Hilbert space interpolation

In section 2.1 we presumed the existence of an orthonormal basis of eigenfunctions satisfying (2.1) in order to construct intermediate spaces $H^s(\Omega)$ of $L_2(\Omega)$ and $H^1(\Omega)$. For arbitrary Hilbert spaces one works with some well known results from the field of functional analysis.

Theorem 3.1. *Let $(V_0, \langle\cdot,\cdot\rangle_0), (V_1, \langle\cdot,\cdot\rangle_1)$ be Hilbert spaces. The operator $K : V_1 \longrightarrow V_0$ is compact if and only if there exists an orthonormal basis $(z_k)_{k\in\mathbb{N}}$ of V_1 and a sequence $(\mu_k)_{k\in\mathbb{N}}$ of positive real numbers with $\mu_k \xrightarrow{k\to\infty} 0$, such that for all $k, l \in \mathbb{N}$*

$$\langle Kz_k, Kz_l\rangle_0 = \mu_k^2 \delta_{k,l}.$$

Corollary 3.2. *Let $(V_0, \langle\cdot,\cdot\rangle_0), (V_1, \langle\cdot,\cdot\rangle_1)$ be Hilbert spaces, such that V_1 is dense in V_0 and the embedding operator* $\mathrm{id} : V_1 \longrightarrow V_0$ *is compact. Then there exists an orthonormal basis $(z_k)_{k\in\mathbb{N}}$ of V_0 and a family of positive real numbers $(\lambda_k)_{k\in\mathbb{N}}$ with $\lambda_k \xrightarrow{k\to\infty} \infty$, such that for all $k \in \mathbb{N}$*

$$\forall v \in V_1 : \quad \langle z_k, v\rangle_1 = \lambda_k^2 \langle z_k, v\rangle_0. \tag{3.1}$$

Proof. (Sketch) The operator $\mathrm{id} : V_1 \longrightarrow V_0$ is compact, according to Theorem 3.1 there exists a basis $(\tilde{z}_k)_{k\in\mathbb{N}}$ of V_1 and eigenvalues $(\mu_k)_{k\in\mathbb{N}}$, such that for all $k, l \in \mathbb{N}$

$$\langle \tilde{z}_k, \tilde{z}_l\rangle_1 = \delta_{k,l} \quad \text{and} \quad \langle \tilde{z}_k, \tilde{z}_l\rangle_0 = \mu_k^2 \delta_{k,l}.$$

Due to density $(\tilde{z}_k)_{k\in\mathbb{N}}$ is also an orthogonal basis of V_0. We define

$$\lambda_k := \frac{1}{\mu_k} \quad \text{and} \quad z_k := \lambda_k \tilde{z}_k.$$

It easily follows that $(z_k)_{k\in\mathbb{N}}$ is an orthonormal basis of V_0, since

$$\langle z_k, z_l\rangle_0 = \lambda_k \lambda_l \langle \tilde{z}_k, \tilde{z}_l\rangle_0 = \lambda_k^2 \mu_k^2 \delta_{k,l} = \delta_{k,l}.$$

For any $v \in V_1 \subseteq V_0$ we can therefore apply Fourier expansion with respect to $(z_k)_{k\in\mathbb{N}}$ to obtain

$$\langle z_k, v\rangle_1 = \langle z_k, \sum_{l\in\mathbb{N}} v_l z_l\rangle_1 = \sum_{l\in\mathbb{N}} v_l \langle z_k, z_l\rangle_1 = \sum_{l\in\mathbb{N}} \lambda_k \lambda_l v_l \langle \tilde{z}_k, \tilde{z}_l\rangle_1 = \lambda_k^2 v_k = \lambda_k^2 \langle z_k, v\rangle_0.$$

We finally point out that $(\mu_k)_{k\in\mathbb{N}}$ converges to zero, yielding

$$\lambda_k \xrightarrow{k\to\infty} \infty.$$

■

Considerations from above provide all the necessary tools required to introduce the concept of interpolation theory. We define:

Definition 3.3. *A pair of Hilbert spaces* $((V_0, \langle\cdot,\cdot\rangle_0), (V_1, \langle\cdot,\cdot\rangle_1))$ *is called Hilbert interpolation couple if* $V_1 \subseteq V_0$ *is dense and the embedding operator* $\mathrm{id} : V_1 \longrightarrow V_0$ *compact.*

According to corollary 3.2 Hilbert interpolation couples allow the choice of an V_0-orthonormal basis of eigenfunctions $(z_k)_{k\in\mathbb{N}}$, such that

$$\forall v \in V_1 : \quad \langle z_k, v\rangle_1 = \lambda_k^2 \langle z_k, v\rangle_0. \tag{3.2}$$

$(z_k)_{k\in\mathbb{N}}$ is a complete system, ensuring that every $u \in V_0$ admits the expansion

$$u = \sum_{k=1}^{\infty} u_k z_k.$$

For all $u \in V_0$ and $v \in V_1 \subseteq V_0$ there holds

$$\|u\|_0^2 = \langle\sum_{k=1}^{\infty} u_k z_k, \sum_{l=1}^{\infty} u_l z_l\rangle_0 = \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} u_k u_l \langle z_k, z_l\rangle_0 = \sum_{k=1}^{\infty} u_k^2,$$
$$\|v\|_1^2 = \langle\sum_{k=1}^{\infty} v_k z_k, \sum_{l=1}^{\infty} v_l z_l\rangle_1 = \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} v_k v_l \langle z_k, z_l\rangle_1 = \sum_{k=1}^{\infty} \lambda_k^2 v_k^2.$$

The identity

$$V_1 = \{u \in V_0 \mid \sum_{k=1}^{\infty} \lambda_k^2 u_k^2 < \infty\}$$

suggests the introduction of the following definition.

Definition 3.4. *Let* (V_0, V_1) *be a Hilbert interpolation couple. For each* $s \in (0,1)$ *the Hilbert interpolation norm of* (V_0, V_1) *is defined as*

$$\|u\|_{H^s(V_0,V_1)} := \left(\sum_{k=1}^{\infty} \lambda_k^{2s} u_k^2\right)^{\frac{1}{2}}.$$

Its associated Hilbert interpolation space is

$$[V_0, V_1]_{H^s} := \{u \in V_0 \mid \|u\|_{H^s(V_0,V_1)} < \infty\}.$$

Remark 3.5. *The interpolation space* $([V_0, V_1]_{H^s}, \|\cdot\|_{H^s(V_0,V_1)})$ *is a Hilbert space itself.*

As long as it is clear from the context we will neglect the dependency in V_0 and V_1. $[V_0, V_1]_{H^s}$ is indeed an intermediate space, since for all $s \in (0,1)$ there holds

$$V_1 \subseteq [V_0, V_1]_{H^s} \subseteq V_0.$$

The most important case for further applications is given by the Hilbert interpolation couple $(L_2(\Omega), H^1(\Omega))$. Notice that the constriction of $[L_2(\Omega), H^1(\Omega)]_{H^s}$ coincides with the approach performed in section 2.

Example: Let $V_1 = H_0^1([0,1])$ and $V_0 = L_2([0,1])$. Then the eigen-pairs in (3.2) have the form

$$\lambda_k = k \qquad \text{and} \qquad z_k(x) = \sqrt{2}\sin(k\pi x) \qquad k \in \mathbb{N}.$$

Example: Let $V_1 = H^1(\Omega)$ and $V_0 = L_2(\Omega)$ with $\Omega = [0,1]^2$. Then there holds

$$\lambda_{k,l} = \pi^2(k^2 + l^2) \qquad \text{and} \qquad z_{k,l}(x,y) = 2\cos(k\pi x)\cos(l\pi y) \qquad k,l \in \mathbb{N}.$$

The associated Hilbert interpolation norm on $[L_2(\Omega), H^1(\Omega)]_{H^s}$ is plotted in figure 1.

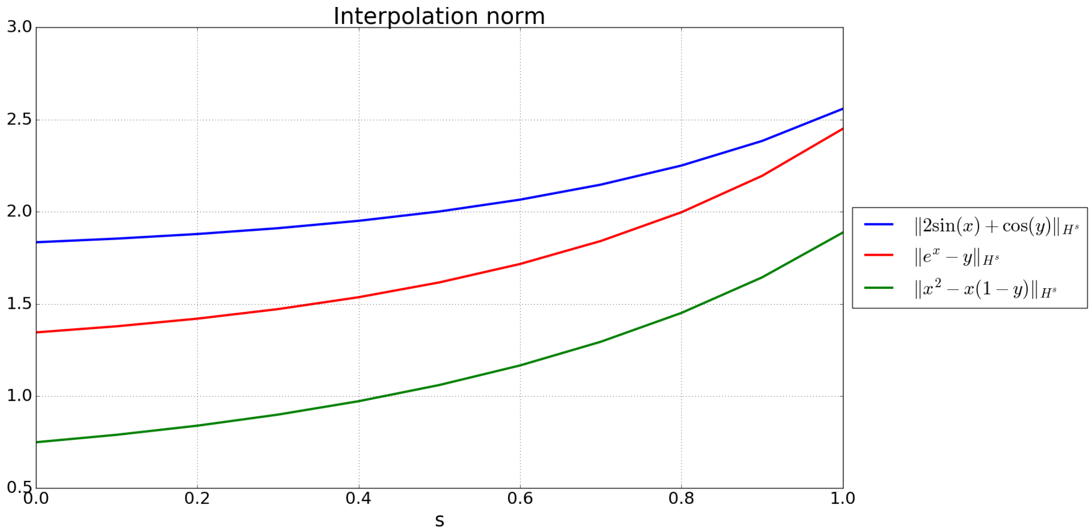


Figure 1: Hilbert interpolation norm of $[L_2(\Omega), H^1(\Omega)]_{H^s}$ with $\Omega = [0,1]^2$ for different function $u \in L_2(\Omega)$.

3.2 Banach space interpolation

Argumentations from above are only applicable for Hilbert spaces. An alternative introduction is provided which also works for feasible Banach spaces. Analogously to before we define under which conditions a pair of Banach spaces is admissible for space interpolation.

Definition 3.6. *A pair of Banach spaces $((B_0, \|\cdot\|_0), (B_1, \|\cdot\|_1))$ is called Banach interpolation couple if $B_1 \subseteq B_0$ is dense and the embedding operator continuous.*

Interpolation between Banach spaces is based on the following definition.

Definition 3.7. *Let (B_0, B_1) be a Banach interpolation couple. Then the K-functional of (B_0, B_1) is defined as*

$$\begin{aligned} K(B_0, B_1) : \mathbb{R}^+ \times B_0 &\longrightarrow \mathbb{R} \\ (t, u) &\mapsto \inf_{v \in B_1} \sqrt{\|u - v\|_0^2 + t^2 \|v\|_1^2}. \end{aligned}$$

Whenever possible we will suppress the dependency in B_0 and B_1 and write $K(t,u)$ instead of $K(B_0, B_1)(t,u)$. Trivially there holds

$$\forall u \in B_1: \quad K(t,u) \leq \|u\|_0 \quad \text{and} \quad K(t,u) \leq t\|u\|_1, \tag{3.3}$$

ensuring that the integral (3.4) is well-defined.

Definition 3.8. *Let (B_0, B_1) be a Banach interpolation couple. For each $s \in (0,1)$ the Banach interpolation norm of (B_0, B_1) is defined as*

$$\|u\|_{B^s(B_0,B_1)} := \left(\int_0^\infty t^{-2s-1} K^2(t,u)\, dt \right)^{\frac{1}{2}}. \tag{3.4}$$

Its associated Banach interpolation space is

$$[B_0, B_1]_{B^s} := \{u \in B_0 \,|\, \|u\|_{B^s(B_0,B_1)} < \infty\}.$$

Remark 3.9. *The interpolation space* $([B_0, B_1]_{B^s}, \|\cdot\|_{B^s(B_0,B_1)})$ *is a Banach space itself.*

As long as it is clear from the context we will neglect the dependency in B_0 and B_1. Similarly to before it holds for all $s \in (0,1)$

$$B_1 \subseteq [B_0, B_1]_{B^s} \subseteq B_0.$$

For each fixed $u \in B_0$ the K-functional is a non-decreasing, continuous and concave function in t, converging to $\|u\|_0$ as $t \to \infty$.

Example: In figure 2 we consider the to $(L_2(\Omega), H^1(\Omega))$ associated K-functional on $\Omega = [0,1]^2$ for different functions $u \in L_2(\Omega)$.

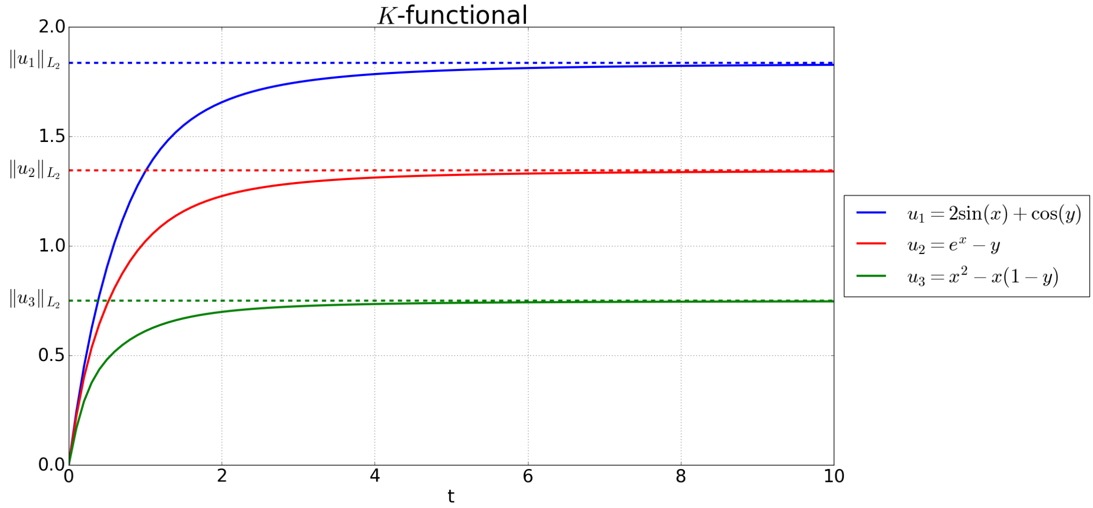


Figure 2: $K(L_2(\Omega), H^1(\Omega))(t, u_i)$ for different u_i, $i = 1, 2, 3$, with $t \in [0, 10]$ on the unit square.

Even though definition 3.8 makes interpolation theory applicable for feasible Banach spaces, we will rather consider its application in context of Hilbert interpolation couples, providing an alternative approach to definition 3.4.

An important result for further applications is stated in the following Theorem. It guarantees that in the Hilbert space case both interpolation methods coincide.

Theorem 3.10. *Let* (V_0, V_1) *be a Hilbert interpolation couple. Then*

$$\|\cdot\|_{B^s(V_0,V_1)} = C_s \|\cdot\|_{H^s(V_0,V_1)} \quad \textit{with} \quad C_s = \sqrt{\frac{\pi}{2\sin(\pi s)}}.$$

Proof. We proceed similarly to [7] and [13]. For each $u \in [V_0, V_1]_{H^s}$ with

$$u = \sum_{k \in \mathbb{N}} u_k z_k$$

one observes

$$\begin{aligned} K^2(t,u) &= \inf_{v \in V_1} \|u - v\|_0^2 + t^2 \|v\|_1^2 \\ &= \inf_{\substack{(v_k) \in \ell_2 \\ (\lambda_k v_k) \in \ell_2}} \sum_{k \in \mathbb{N}} (u_k - v_k)^2 + t^2 \lambda_k^2 v_k^2 \\ &= \sum_{k \in \mathbb{N}} \inf_{v_k \in \mathbb{R}} (u_k - v_k)^2 + t^2 \lambda_k^2 v_k^2. \end{aligned}$$

The minimum for each summand is taken for those v_k which satisfy

$$-2(u_k - v_k) + 2t^2\lambda_k^2 v_k = 0 \quad \Longleftrightarrow \quad v_k = \frac{1}{1 + t^2\lambda_k^2} u_k.$$

Hence

$$\begin{aligned}
K^2(t,u) &= \sum_{k\in\mathbb{N}} u_k^2 - 2\frac{u_k^2}{1+t^2\lambda_k^2} + \frac{(1+t^2\lambda_k^2)u_k^2}{(1+t^2\lambda_k^2)^2} \\
&= \sum_{k\in\mathbb{N}} u_k^2 \frac{(1+t^2\lambda_k^2)}{(1+t^2\lambda_k^2)} - 2u_k^2 \frac{(1+t^2\lambda_k^2)}{(1+t^2\lambda_k^2)^2} + u_k^2 \frac{(1+t^2\lambda_k^2)}{(1+t^2\lambda_k^2)^2} \\
&= \sum_{k\in\mathbb{N}} u_k^2 \frac{(1+t^2\lambda_k^2)}{(1+t^2\lambda_k^2)} - u_k^2 \frac{1}{(1+t^2\lambda_k^2)} \\
&= \sum_{k\in\mathbb{N}} u_k^2 \frac{t^2\lambda_k^2}{(1+t^2\lambda_k^2)}.
\end{aligned}$$

Plugging in reveals

$$\begin{aligned}
\|u\|_{B^s}^2 &= \int_0^\infty t^{-2s-1} K^2(t,u)\, dt \\
&= \int_0^\infty t^{-2s-1} \sum_{k\in\mathbb{N}} u_k^2 \frac{t^2\lambda_k^2}{(1+t^2\lambda_k^2)}\, dt \\
&= \sum_{k\in\mathbb{N}} \int_0^\infty t^{-2s-1} u_k^2 \frac{t^2\lambda_k^2}{(1+t^2\lambda_k^2)}\, dt.
\end{aligned}$$

Substitution $\tau = \lambda_k t$ yields

$$\begin{aligned}
\|u\|_{B^s}^2 &= \sum_{k\in\mathbb{N}} \int_0^\infty \left(\frac{\tau}{\lambda_k}\right)^{-2s-1} u_k^2 \frac{\tau^2}{1+\tau^2} \frac{d\tau}{\lambda_k} \\
&= \sum_{k\in\mathbb{N}} \lambda_k^{2s} u_k^2 \int_0^\infty \frac{\tau^{1-2s}}{1+\tau^2}\, d\tau \\
&= \left(\int_0^\infty \frac{\tau^{1-2s}}{1+\tau^2}\, d\tau\right) \|u\|_{H^s}^2.
\end{aligned}$$

Verifying the identity

$$\int_0^\infty \frac{\tau^{1-2s}}{1+\tau^2}\, d\tau = \frac{\pi}{2\sin(\pi s)}$$

concludes the proof. ■

Theorem 3.10 justifies the definition of

$$[V_0, V_1]_s := [V_0, V_1]_{H^s} = [V_0, V_1]_{B^s}$$

for Hilbert interpolation couples (V_0, V_1). Both $([V_0, V_1]_s, \|\cdot\|_{H^s})$ and $([V_0, V_1]_s, \|\cdot\|_{B^s})$ are Hilbert spaces itself, such that the norms are equivalent involving only the constant C_s. For the further course of action we will agree on the slightly modified notation

$$[V_0, V_1]_{H^s} := ([V_0, V_1]_s, \|\cdot\|_{H^s}) \qquad [V_0, V_1]_{B^s} := ([V_0, V_1]_s, \|\cdot\|_{B^s})$$

in order to indicate which norm is involved.

Examples show that the construction of intermediate spaces accords to the natural understanding of interpolation. Under the assumption of Ω being a Lipschitz domain, one can proof that

$$[L_2(\Omega), H^2(\Omega)]_{H^{\frac{1}{2}}} = H^1(\Omega).$$

In a sense, boundary values are accounted as well, since

$$[L_2(\Omega), H_0^2(\Omega)]_{H^{\frac{1}{2}}} = H_0^1(\Omega) \qquad [L_2(\Omega), H_{per}^2(\Omega)]_{H^{\frac{1}{2}}} = H_{per}^1(\Omega).$$

Remark 3.11. *Analogously to remark 2.1 extrapolation can only be applied to* $(L_2(\Omega), H^1_{per}(\Omega))$*, such that the identity* $H^2_{per}(\Omega) \subseteq [L_2(\Omega), H^1_{per}(\Omega)]_{H^{1+\alpha}} \subseteq H^1_{per}(\Omega)$ *holds for all* $\alpha \in (0, 1)$.

4 Implementation of interpolation norms

Section 3 holds for general Banach and Hilbert interpolation couples. Throughout this thesis though, we will be satisfied to deal with the case $V_0 = L_2(\Omega)$ and $V_1 = H^1(\Omega)$ primary. Argumentation from before suggests two different approaches in order to compute their associated interpolation norm. Either of those comes with its own difficulties attached. While the Banach space method requires both the evaluation of an infimum and the computation of an improper integral, the Hilbert approach involves extensive eigenvalue problems. It turns out that the latter one is preferable for computational aspects, whereas the analysis better applies to the Banach space framework.

4.1 Evaluation of the K-functional

Throughout what follows let $\Omega \subseteq \mathbb{R}^d$, $d = 1, 2, 3$, denote a bounded Lipschitz domain. Consider the Banach interpolation couple $(L_2(\Omega), H^1(\Omega))$ together with its associated K-functional

$$K^2(t, u) = \inf_{v \in H^1} \|u - v\|_{L_2}^2 + t^2 \|v\|_{H^1}^2.$$

Evaluations of K involve the computations of a minimizer $v^*(u, t)$, such that

$$K^2(t, u) = \|u - v^*(u, t)\|_{L_2} + t^2 \|v^*(u, t)\|_{H^1}.$$

It will be shown that $v^*(u, t)$ is the weak solution of a partial differential equation, giving $K^2(t, u)$ a computationally applicable form.

4.1.1 The variational framework

One immediately observes the following property.

Lemma 4.1. *Let $t \in \mathbb{R}^+$ and $u \in L_2(\Omega)$. $v^* \in H^1(\Omega)$ minimizes $K(t, u)$ if and only if v^* minimizes*

$$\mathcal{F}_{(u,t)}(v) := \int_\Omega -2uv + v^2 + t^2(v^2 + (\nabla v)^2)\, dx \qquad v \in H^1(\Omega). \tag{4.1}$$

Proof. Direct computations reveal

$$\begin{aligned}
K^2(t, u) &= \inf_{v \in H^1} \|u - v\|_{L_2}^2 + t^2 \|v\|_{H^1}^2 \\
&= \inf_{v \in H^1} \langle u - v, u - v \rangle_{L_2} + t^2 \|v\|_{H^1}^2 \\
&= \inf_{v \in H^1} \|u\|_{L_2}^2 - 2\langle u, v \rangle_{L_2} + \|v\|_{L_2}^2 + t^2 \|v\|_{H^1}^2 \\
&= \inf_{v \in H^1} \int_\Omega u^2 - 2uv + v^2 + t^2 \left(v^2 + (\nabla v)^2\right) dx.
\end{aligned}$$

Since $\|u\|_{L_2}^2$ affects the functional's value only, but not the choice of the infimum itself, we can neglect the first summand in the integral to conclude the claim. ■

The problem is set in the framework of calculus of variation. For fixed $u \in H^1(\Omega)$ and $t > 0$ find $v^* \in H^1(\Omega)$, such that

$$\mathcal{F}_{(u,t)}(v^*) = \inf_{v \in H^1} \mathcal{F}_{(u,t)}(v), \tag{4.2}$$

with

$$\begin{aligned}\mathcal{F}_{(u,t)} : H^1(\Omega) &\longrightarrow \mathbb{R} \\ v &\mapsto \int_\Omega F_{(u,t)}(v(x), \nabla v(x))\, dx\end{aligned}$$

and

$$\begin{aligned}F_{(u,t)} : \mathbb{R} \times \mathbb{R}^d &\longrightarrow \mathbb{R} \\ (z,p) &\mapsto -2u(x)z + z^2 + t^2\left(z^2 + p^2\right).\end{aligned}$$

Due to readability reasons we will neglect the subscript (u, t) in further notations, keeping in mind that the problem holds a dependency in both u and t. Existence and uniqueness properties of (4.2) follow by some standard results from calculus of variation.

Theorem 4.2 (Existence)**.** *Let $X \neq \emptyset$ be a linear space, $F \in C^\infty(\mathbb{R} \times \mathbb{R}^d)$ convex in p and its variational integral*

$$\begin{aligned}\mathcal{F} : X &\longrightarrow \mathbb{R} \\ v &\mapsto \int_\Omega F(v(x), \nabla v(x))\, dx\end{aligned}$$

coercive, i.e.

$$\exists \alpha, \beta \in \mathbb{R}^+ \forall u \in X : \quad \mathcal{F}(v) \geq \alpha \|\nabla v\|_{L_2}^2 - \beta. \tag{4.3}$$

Then there exists a minimizer $v^* \in X$, such that

$$\mathcal{F}(v^*) = \inf_{v \in X} \mathcal{F}(v).$$

Proof. See [3, Theorem 5.9]. ■

Theorem 4.3 (Uniqueness)**.** *Let X be a linear space, $F \in C(\mathbb{R} \times \mathbb{R}^d)$ convex in each of its arguments and $\mathcal{F} : X \longrightarrow \mathbb{R}$ the associated variational integral. Then*

$$v^* \in X \text{ minimizes } \mathcal{F} \quad \Longrightarrow \quad v^* \text{ is unique.}$$

Proof. See [3, Theorem 5.10]. ■

Both Theorems can be applied to the minimization problem of interest.

Corollary 4.4. *For each $t \in \mathbb{R}^+$ and $u \in H^1(\Omega)$ there exists a unique $v^* \in H^1(\Omega)$, such that*

$$\mathcal{F}(v^*) = \inf_{v \in H^1} \mathcal{F}(v)$$

with

$$\mathcal{F}(v) := \int_\Omega -2uv + v^2 + t^2\left(v^2 + (\nabla v)^2\right)\, dx.$$

Proof. We check the assumptions of Theorem 4.2. $X = H^1(\Omega) \neq \emptyset$ is a linear space and

$$F(z,p) := -2u(x)z + z^2 + t^2\left(z^2 + |p|^2\right)$$

satisfies $F \in C^\infty(\mathbb{R}, \mathbb{R}^d)$ and is convex in p. The non-trivial part is the coercivity. Cauchy-Schwarz inequality reveals

$$\begin{aligned}\mathcal{F}(v) &= -2\int_\Omega uv\,dx + (1+t^2)\int_\Omega v^2\,dx + t^2\int_\Omega (\nabla v)^2\,dx \\ &\geq -\underbrace{2\|u\|_{L_2}}_{=:C_1}\|v\|_{L_2} + \underbrace{(1+t^2)}_{=:C_2}\|v\|_{L_2}^2 + t^2\|\nabla v\|_{L_2}^2.\end{aligned}$$

We distinguish between two possible cases.

1. $\|v\|_{L_2} > \max\left\{\frac{C_1}{C_2}, 1\right\} \quad \Longrightarrow \quad -C_1\|v\|_{L_2} + C_2\|v\|_{L_2}^2 > 0$
2. $\|v\|_{L_2} \leq \max\left\{\frac{C_1}{C_2}, 1\right\} \quad \Longrightarrow \quad -C_1\|v\|_{L_2} \geq -C_1\max\{\frac{C_1}{C_2}, 1\} =: -\beta$
   It follows

$$-C_1\|v\|_{L_2} + C_2\|v\|_{L_2} \geq -\beta + C_2\|v\|_{L_2} \geq -\beta.$$

Setting $\alpha := t^2$ yields

$$\mathcal{F}(v) \geq \alpha\|\nabla v\|_{L_2} - \beta,$$

for all $v \in H^1(\Omega)$, granting the existence of a minimizer $v^* \in H^1(\Omega)$. Since $F(z,p)$ is convex in z as well, Theorem 4.3 provides uniqueness. ■

The question arises whether the unique minimizer v^* can be computed explicitly. To this extent we specify the following definition (not in its most general form but in the one that fits our setting adequately).

Definition 4.5. *Let X be a linear function space over $\mathbb{R}$ with $v, \xi \in X$ and $\mathcal{F} : X \longrightarrow \mathbb{R}$ a functional on X. Further let*

$$\phi(\varepsilon) := \mathcal{F}(v + \varepsilon\xi)$$

for all $\varepsilon \in \mathbb{R}$. If $\phi'(0)$ does exist, we define the first variation of $\mathcal{F}$ at v in direction ξ as

$$\delta\mathcal{F}(v,\xi) := \phi'(0).$$

The first variation can be considered as a weaker form of the concept of derivatives, where no topology on X is required. Similarly to the smooth case one can derive a necessary condition to detect local minimizer. Along with some technical assumptions it can be shown that each minimizer v^* satisfies

$$\forall \xi \in C^\infty(\Omega) : \quad \delta\mathcal{F}(v^*, \xi) = 0. \tag{4.4}$$

This condition can be formulated as partial differential equation, referred to as *weak Euler-Lagrange equation.* It holds for all candidates satisfying (4.4)

$$\begin{aligned}
0 &= \delta\mathcal{F}(v^*, \xi) \\
&= \frac{d}{d\varepsilon}\mathcal{F}(v^* + \varepsilon\xi)\big|_{\varepsilon=0} \\
&= \frac{d}{d\varepsilon}\int_\Omega F(v^*(x) + \varepsilon\xi(x), \nabla v^*(x) + \varepsilon\nabla\xi(x))\, dx \Big|_{\varepsilon=0} \\
&= \int_\Omega \frac{\partial F}{\partial z}(v^*(x), \nabla v^*(x))\xi(x) + \sum_{i=1}^{d}\frac{\partial F}{\partial p_i}(v^*(x), \nabla v^*(x))\frac{\partial \xi}{\partial x_i}(x)\, dx. \qquad (4.5)
\end{aligned}$$

For sufficiently smooth functions this is also true in the strong sense, resulting in the *classical Euler-Lagrange equation*

$$\frac{\partial F}{\partial z}(x, v^*(x), \nabla v^*(x)) + \sum_{i=0}^{d}\frac{\partial}{\partial x_i}\left[\frac{\partial F}{\partial p_i}(x, v^*(x), \nabla v^*(x))\right] = 0.$$

Elaborations from above enable us to set the minimizer of the K-functional in correspondence with the solution of a shifted Laplace problem, providing the essential information of this section.

Theorem 4.6. *For each $u \in H^1(\Omega)$ and $t \in \mathbb{R}^+$ the minimizer v^* of* (4.2) *(or equivalently of the K-functional) is the unique solution of the variational problem: Find $v \in H^1(\Omega)$, such that*

$$\forall w \in H^1(\Omega): \quad \langle v, w\rangle_{L_2} + t^2\langle v, w\rangle_{H^1} = \langle u, w\rangle_{L_2}. \qquad (4.6)$$

Proof. The weak Euler-Lagrange equation provides a necessary condition for minimizer of (4.2).

$$\begin{aligned}
\frac{\partial F}{\partial z} &= -2u + 2z + 2t^2 z, \\
\frac{\partial F}{\partial p_i} &= 2t^2 p_i.
\end{aligned}$$

Plugging into (4.5) and division by 2 leads to the claimed variational problem, which is uniquely solvable. Corollary 4.4 concludes the proof. ■

4.2 The finite element setting

Results from above can be applied to the discrete framework. Throughout what follows let $V_h \subseteq H^1(\Omega)$ be a finite element space of dimension $N + 1$. For each $u \in V_h$ denote $\underline{u} \in \mathbb{R}^{N+1}$ the uniquely assigned Galerkin vector, such that $G(\underline{u}) = u$, whereas G denotes the Galerkin isomorphism

$$\begin{aligned}
G : \mathbb{R}^{N+1} &\longrightarrow V_h \\
\underline{u} &\longmapsto u = \sum_{i=0}^{N}\underline{u}_i\varphi_i
\end{aligned}$$

with a basis $(\varphi_i)_{i=0}^N$ of V_h. We consider the interpolation space $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{B^s}$ together with its associated K-functional

$$K^2(t, u) = \inf_{v\in V_h}\|u - v\|_{L_2}^2 + t^2\|v\|_{L_2}^2 \qquad t > 0, u \in V_h. \qquad (4.7)$$

Analogously to section 2.1 one shows that the minimizer $v^*(u,t)$ of (4.7) is the unique solution of the shifted Laplace problem: Find $v \in V_h$, such that

$$\forall w \in V_h : \quad \langle v, w\rangle_{L_2} + t^2 \langle v, w\rangle_{H^1} = \langle u, w\rangle_{L_2},$$

giving rise to the linear system of equations

$$(M + t^2 A)\underline{v}^* = M\underline{u} \tag{4.8}$$

with mass matrix M and H^1-matrix A, arising from the H^1-bilinear form. The K-functional's value is

$$\begin{aligned} K^2(t,u) &= \|u - v^*\|_{L_2}^2 + t^2\|v^*\|_{H^1}^2 \\ &= \|\underline{u} - \underline{v}^*\|_M^2 + t^2\|\underline{v}^*\|_A^2. \end{aligned}$$

Together with (4.8) this yields

$$K^2(t,u) = \|\underline{u} - (M + t^2 A)^{-1} M\underline{u}\|_M^2 + t^2 \|(M + t^2 A)^{-1} M\underline{u}\|_A^2. \tag{4.9}$$

Due to this feasible handling of $K(t,u)$ we are now able to dedicate our attention to the evaluation of the associated interpolation norms.

4.3 Implementation of interpolation norms

The goal of this section is to provide an efficient implementation of the Banach interpolation norm

$$\|u\|_{B^s}^2 = \int_0^\infty t^{-2s-1} K^2(t,u)\, dt \tag{4.10}$$

on the Banach interpolation space $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{B^s}$. Due to (4.9) the integrand in (4.10) can be evaluated for each $t > 0$. Ad hoc, one could aim to compute the interpolation norm by means of numerical integration rules for improper integrals. However, this involves plenty of evaluations in t, requiring each the solution of the associated shifted Laplace problem. Ideas for improvement are discussed in the next section.

4.3.1 The reduced basis approach

We are now confronted with two major problems.

1. Improper integrals are difficult to solve accurately and might lead to substantial approximation errors.

2. Computational costs might exceed reasonable capacity since many evaluations for different parameters t are required.

Both issues can be overwhelmed by a reduced basis approach. The concept is the following. We introduce a subspace $\mathcal{V}_r \subseteq V_h$ of dimension $r+1$, referred to as *reduced space*, and define its associated *reduced basis K-functional* on V_h as

$$K_r^2(t,u) := \inf_{v_r \in \mathcal{V}_r} \|u - v_r\|_{L_2}^2 + t^2\|v_r\|_{H^1}^2 \qquad t > 0, u \in V_h \tag{4.11}$$

together with its induced *reduced basis Banach interpolation norm*

$$\|u\|_{B_r^s}^2 := \int_0^\infty t^{-2s-1} K_r^2(t,u)\, dt. \tag{4.12}$$

Remark 4.7. *For all $u \in \mathcal{V}_r$ the introduced norm $\|u\|_{B_r^s}$ coincides with the Banach interpolation norm on the intermediate space*

$$[(\mathcal{V}_r, \|\cdot\|_{L_2}), (\mathcal{V}_r, \|\cdot\|_{H^1})]_s.$$

Analogously to both the continuous and the finite element setting, evaluations of $K_r(t, u)$ can be related to the variational problem: Find $v_r \in \mathcal{V}_r$, such that

$$\forall w_r \in \mathcal{V}_r: \quad \langle v_r, w_r\rangle_{L_2} + t^2\langle v_r, w_r\rangle_{H^1} = \langle u, w_r\rangle_{L_2}.$$

By means of the reduced basis Galerkin isomorphism

$$\begin{aligned} G_r : \mathbb{R}^{r+1} &\longrightarrow \mathcal{V}_r \\ \underline{\underline{u}} &\longmapsto u = \sum_{i=0}^{r} \underline{\underline{u}}_i \varphi_i^{\mathcal{V}_r} \end{aligned}$$

according to a basis $(\varphi_i^{\mathcal{V}_r})_{i=0}^r$ of $\mathcal{V}_r$, the arising linear system of equations reads as

$$(M_r + t^2 A_r)\underline{\underline{v}}_r^* = M_r \underline{\underline{u}}, \tag{4.13}$$

with $M_r, A_r \in \mathbb{R}^{(r+1)\times(r+1)}$. The linear system (4.13) naturally arises (under the right choice of the basis $(\varphi_i^{\mathcal{V}_r})_{i=0}^r$) from (4.8). In order to establish this connection we state the following definition.

Definition 4.8. *Let $\{v_0, ..., v_r\}$ be an L_2-orthonormal basis of $\mathcal{V}_r$. Then the associated reduced basis matrix V_r is defined as*

$$V_r := [\underline{v}_0, ..., \underline{v}_r] \in \mathbb{R}^{(N+1)\times(r+1)}.$$

Remark 4.9. *Due to*

$$\delta_{k,l} = \langle v_k, v_l\rangle_{L_2} = \int_\Omega v_k v_l \, dx = \underline{v_k}^T M \underline{v_l}$$

there holds

$$V_r^T M V_r = I_r \in \mathbb{R}^{(r+1)\times(r+1)}.$$

V_r can be regarded as prolongation, its transposed as restriction matrix between V_h and $\mathcal{V}_r$, operating on the related coefficient vectors.

The identity $\underline{v}_r^* = V_r \underline{\underline{v}}_r^*$ plugged into (4.8) together with multiplication of V_r^T from the left yields

$$(V_r^T M V_r + t^2 V_r^T A V_r)\underline{\underline{v}}_r^* = V_r^T M \underline{u},$$

such that (under the assumption that the matrices M_r and A_r have been assembled with respect to the to V_r associated basis, which we from now agree on) $M_r = V_r^T M V_r = I_r$ and $A_r = V_r^T A V_r$ holds.

Remark 4.10. *Even though $M_r = I_r$, at some points we will insist on writing M_r instead of I_r in order to emphasize relevant aspects.*

The value of $K_r^2(t,u)$ can be expressed as

$$\begin{aligned} K_r^2(t,u) &= \|u - v_r^*\|_{L_2}^2 + t^2\|v_r^*\|_{H^1}^2 \\ &= \|\underline{u} - \underline{v}_r^*\|_M^2 + t^2\|\underline{v}_r^*\|_{A_r}^2 \\ &= \|\underline{u} - V_r(I_r + t^2A_r)^{-1}V_r^TM\underline{u}\|_M^2 + t^2\|V_r(I_r + t^2A_r)^{-1}V_r^TM\underline{u}\|_A^2. \end{aligned}$$

Along with a feasible choice of $\mathcal{V}_r$ we hope that

$$\begin{aligned} v_r^*(t,u) \approx v^*(t,u) &\implies K_r(t,u) \approx K(t,u), \\ &\implies \|u\|_{B_r^s} \approx \|u\|_{B^s}. \end{aligned}$$

The subsequent section gives rise to the question how a proper space $\mathcal{V}_r$ is constructed, such that the required approximation properties hold in the best possible way.

4.3.2 Choice of the reduced space

Since both v^* and v_r^* involve a dependency in u and t, it is rather unlikely that any choice of $\mathcal{V}_r \subseteq V_h$ with $r \ll \dim(V_h)$ provides reasonable approximation properties for all $u \in V_h$ and $t > 0$. The clue is to choose $\mathcal{V}_r = \mathcal{V}_r(u)$ in dependency of u, such that at least

$$v_r^*(t) \approx v^*(t)$$

for all $t \in \mathbb{R}^+$ is satisfied appropriately. To this extent let $u \in V_h$ be fixed throughout the entire section. For given snapshots $t_0 = 0$ and $t_1, ..., t_r \in \mathcal{I} := [t_{min}, t_{max}] \subseteq \mathbb{R}^+$, t_{min}, t_{max} to be determined later, we consider the related snapshot solutions $v^*(t_j)$ of the shifted Laplace problem: Find $v \in V_h$, such that

$$\forall w \in V_h : \quad \langle v, w\rangle_{L_2} + t_j^2\langle v, w\rangle_{H^1} = \langle u, w\rangle_{L_2} \qquad j = 0, ..., r. \tag{4.14}$$

We set

$$\mathcal{V}_r := [\{v^*(t_0), ..., v^*(t_r)\}] \subseteq V_h,$$

such that

$$v^*(t) \approx \sum_{j=0}^{r} \alpha_j v^*(t_j) \qquad \alpha_j = \alpha_j(t)$$

and further

$$\|u\|_{B_r^s} \approx \|u\|_{B^s}.$$

Remark 4.11. *Due to $\mathcal{V}_r = \mathcal{V}_r(u)$ we will occasionally write $\|u\|_{H^s_{r(u)}}$ instead of $\|u\|_{H_r^s}$ in order to emphasize the dependency in u.*

Setting $t_0 = 0$ guarantees that $u = v^*(t_0)$ is contained in the reduced space itself. This choice can be justified in the following way. If $u \in \mathcal{V}_r$, then

$$K_r^2(t,u) = \inf_{v_r \in \mathcal{V}_r} \|u - v_r\|_{L_2}^2 + t^2\|v_r\|_{H^1}^2 \le t^2\|u\|_{H^1}^2,$$

yielding

$$\forall s \in (0,1)\, \exists \varepsilon > 0\, \forall t \in (0,1): \quad t^{-2s-1} K_r^2(t,u) \leq t^{-2+\varepsilon-1} K_r^2(t,u) \leq \|u\|_{H^1}^2 \frac{1}{t^{1-\varepsilon}},$$

such that the limit

$$\lim_{c \to 0} \int_c^1 t^{-2s-1} K_r(t,u)^2 \, dt$$

exists. Due to $K_r^2(t,u) \leq \|u\|_{L_2}^2$ one further obtains

$$\forall s \in (0,1)\, \exists \varepsilon > 0\, \forall t \in (1,\infty): \quad t^{-2s-1} K_r^2(t,u) \leq t^{-\varepsilon-1} K_r^2(t,u) \leq \|u\|_{L_2}^2 \frac{1}{t^{1+\varepsilon}},$$

such that again

$$\lim_{c \to \infty} \int_1^c t^{-2s-1} K_r^2(t,u) \, dt < \infty$$

holds. Summing up, the choice of $t_0 = 0$ ensures the convergence of the induced reduced basis integral

$$\int_0^\infty t^{-2s-1} K_r^2(t,u) \, dt, \tag{4.15}$$

which does not necessarily hold if $u \notin \mathcal{V}_r$.

The latter sampling points $t_1, ..., t_r$ are taken with respect to the interval $\mathcal{I} = [t_{min}, t_{max}]$ with

$$t_{min} := \frac{1}{\sqrt{\lambda_{max}(M^{-1}A)}} \quad \text{and} \quad t_{max} := 1 \approx \frac{1}{\sqrt{\lambda_{min}(M^{-1}A)}}. \tag{4.16}$$

A deeper understanding of this choice will be given in section 6. The question arises how to distribute $t_1, ..., t_r$ across the interval, such that

$$\|u\|_{B_r^s} \approx \|u\|_{B^s}$$

holds in the best possible way. For the moment we assume the snapshots to be geometrically scattered across $\mathcal{I}$ and again refer to section 6 for further elaborations.

Before computational aspects are discussed we show that the term *basis* is indeed justified for $\{v^*(t_0), ..., v^*(t_r)\}$.

Theorem 4.12. *Assume that $0 = t_0 < t_1 < ... < t_r$ and let $v^*(t_j)$ denote the solution of* (4.14) *and $(\lambda_k, z_k)_{k=0}^N$ the L_2-orthonormal eigen-pairs of V_h, such that*

$$\forall w \in V_h: \quad \langle z_k, w \rangle_{H^1} = \lambda_k^2 \langle z_k, w \rangle_{L_2}.$$

Further let $u \in V_h$, $m \leq N$ with $u \in [\{z_0, ..., z_m\}]$ and $\langle z_k, u \rangle_{L_2} \neq 0$ for all $k = 0, ..., m$. Then

$$r \leq m \quad \Longrightarrow \quad \{v^*(t_0), ..., v^*(t_r)\} \text{ is linearly independent.}$$

Proof. Fourier expansion yields (see Lemma 6.3)

$$v^*(t_j) = \sum_{k=0}^{N} \frac{u_k}{1 + t_j^2 \lambda_k^2} z_k.$$

Assume that

$$\sum_{j=0}^{r} \alpha_j v^*(t_j) = \sum_{j=0}^{r} \alpha_j \sum_{k=0}^{N} \frac{u_k}{1 + t_j^2 \lambda_k^2} z_k = 0$$

for some coefficients $\alpha_0, ..., \alpha_r \in \mathbb{R}$. Permutation of the summation yields

$$\sum_{k=0}^{N} \sum_{j=0}^{r} \alpha_j \frac{u_k}{1 + t_j^2 \lambda_k^2} z_k = 0.$$

Since $u \in [\{z_0, ..., z_m\}]$ there holds $u_k = \langle z_k, u \rangle_{L_2} = 0$ for $k > m$. It follows

$$\sum_{k=0}^{m} \sum_{j=0}^{r} \alpha_j \frac{u_k}{1 + t_j^2 \lambda_k^2} z_k = 0.$$

Due to orthonormality of $(z_k)_{k=0}^m$ and division by $u_k \neq 0$ one observes

$$\forall k \in \{0, ..., m\} : \quad \sum_{j=0}^{r} \alpha_j \frac{1}{1 + t_j^2 \lambda_k^2} = 0. \tag{4.17}$$

Reformulation of (4.17) gives rise to the linear system of equations

$$\begin{pmatrix} \frac{1}{1+t_0^2\lambda_0^2} & \cdots & \frac{1}{1+t_r^2\lambda_0^2} \\ \vdots & & \vdots \\ \frac{1}{1+t_0^2\lambda_m^2} & \cdots & \frac{1}{1+t_r^2\lambda_m^2} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_r \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}.$$

For the case $m = r$ one can easily proof (for example by induction with the Laplacian determinant expansion by minors) that the matrix is regular. In this case the equation can only hold for

$$\alpha_0 = ... = \alpha_r = 0. \tag{4.18}$$

We conclude that $\{v^*(t_0), ..., v^*(t_r)\}$ is linearly independent for $r = m$. Every subset of a linearly independent set is linearly independent itself which is why (4.18) also holds for all $r < m$, proofing the claim. ■

So far we have achieved to establish a procedure approximating the K-functional by means of a reduced basis approach. Nevertheless, the reduced basis interpolation norm itself has a rather inconvenient form from a computational point of view. This problem can be avoided by reinterpreting (4.12) in context of Hilbert space interpolation.

4.3.3 Computational aspects

The definition of $\mathcal{V}_r$ suggests a canonical choice of the associated reduced basis matrix V_r. We agree on the following convention. Whenever V_r is noted in the subsequent, we refer to the matrix arising from Gramm-Schmidt M-orthonormalization applied to $[\underline{v}^*(t_0), ..., \underline{v}^*(t_r)]$.

The main result of this section is given in Theorem 4.14. The necessary preparation is provided in the following.

Lemma 4.13. *Let $t \in \mathbb{R}^+$, $u \in V_h$, $\beta = \|u\|_{L_2}$ and $e_1 \in \mathbb{R}^{r+1}$ the first unit vector. Then*

$$K_r^2(t,u) = \inf_{y \in \mathbb{R}^{r+1}} \|\beta e_1 - y\|_{M_r}^2 + t^2 \|y\|_{A_r}^2.$$

Proof. Since $u = v^*(t_0) \in \mathcal{V}_r = [\{v^*(t_0), ..., v^*(t_r)\}]$ there holds

$$\begin{aligned} K_r^2(t,u) &= \inf_{v_r \in \mathcal{V}_r} \|u - v_r\|_{L_2}^2 + t^2 \|v_r\|_{H^1}^2 \\ &= \inf_{y \in \mathbb{R}^{r+1}} \|V_r(\beta e_1 - y)\|_M^2 + t^2 \|V_r y\|_A^2 \\ &= \inf_{y \in \mathbb{R}^{r+1}} (V_r(\beta e_1 - y))^T M V_r(\beta e_1 - y) + t^2 (V_r y)^T A V_r y \\ &= \inf_{y \in \mathbb{R}^{r+1}} (\beta e_1 - y)^T V_r^T M V_r (\beta e_1 - y) + t^2 y^T V_r^T A V_r y \\ &= \inf_{y \in \mathbb{R}^{r+1}} \|\beta e_1 - y\|_{M_r}^2 + t^2 \|y\|_{A_r}^2. \end{aligned}$$

■

Theorem 4.14. *Let $u \in V_h$, $s \in (0,1)$ and $\beta = \|u\|_{L_2}$. Then*

$$\|u\|_{B_r^s} = C_s \|\beta e_1\|_{A_r^s},$$

with C_s as defined in Theorem 3.10.

Proof. Lemma 4.13 yields

$$\|u\|_{B_r^s}^2 = \int_0^\infty t^{-2s-1} \inf_{y \in \mathbb{R}^{r+1}} \left(\|\beta e_1 - y\|_{M_r}^2 + t^2 \|y\|_{A_r}^2 \right) dt = \|\beta e_1\|_{B^s}^2,$$

whereas the latter norm is taken with respect to the interpolation space

$$[(\mathbb{R}^{r+1}, \|\cdot\|_{M_r}), (\mathbb{R}^{r+1}, \|\cdot\|_{A_r})]_{B^s}.$$

Equivalence of the norms (Theorem 3.10) reveals

$$\|u\|_{B_r^s} = \|\beta e_1\|_{B^s} = C_s \|\beta e_1\|_{H^s} = C_s \|\beta e_1\|_{A_r^s},$$

whereas $\|\cdot\|_{H^s}$ denotes the norm of $[(\mathbb{R}^{r+1}, \|\cdot\|_{M_r}), (\mathbb{R}^{r+1}, \|\cdot\|_{A_r})]_{H^s}$. For the last equality we refer to Theorem 5.2 and the identity $M_r = I_r$. ■

Analogously to before we relate the Banach setting with the Hilbert case in a reduced basis sense. To this extent we define:

Definition 4.15. *The reduced basis Hilbert interpolation norm of $u \in V_h$ is defined as*

$$\|u\|_{H_{r(u)}^s} := \|u\|_{H^s((\mathcal{V}_r(u), \|\cdot\|_{L_2}), (\mathcal{V}_r(u), \|\cdot\|_{H^1}))}.$$

Again, we will occasionally neglect the dependency in u in following discussions. The proof of Theorem 4.14 immediately reveals:

Corollary 4.16. *Let $u \in V_h$, $s \in (0,1)$ and $\beta = \|u\|_{L_2}$. Then there holds*

$$\|u\|_{H_r^s} = \|\beta e_1\|_{A_r^s}.$$

Due to norm equivalence there is no reason to favor one of the interpolation norms over the other. We therefore stick to the Hilbert space setting when it comes to computations in order to avoid the inconvenient form of (4.12).

We summarize all the steps required to approximate the Hilbert interpolation norm of a finite element function $u \in V_h$ in a reduced basis sense:

1. For $t_0 = 0$ and $t_1, ..., t_r \in \mathcal{I}$ compute the snapshot solutions $v^*(t_j)$ of the associated shifted Laplace problems, i.e.

$$\underline{v}^*(t_j) = (M + t_j^2 A)^{-1} M \underline{u},$$

and set $\hat{V}_r = [\underline{v}^*(t_0), ..., \underline{v}^*(t_r)]$.

2. Apply Gramm-Schmidt orthonormalization to $\hat{V}_r$ with respect to the M-scalar product in order to obtain the reduced basis matrix V_r.

3. Compute the projected H^1-matrix

$$A_r = V_r^T A V_r.$$

4. Compute $A_r^s = Z_r \Lambda_r^s Z_r^T$ by means of its small eigen-system.

5. Compute $\|u\|_{H_r^s} = \sqrt{\beta^2 e_1^T A_r^s e_1}$.

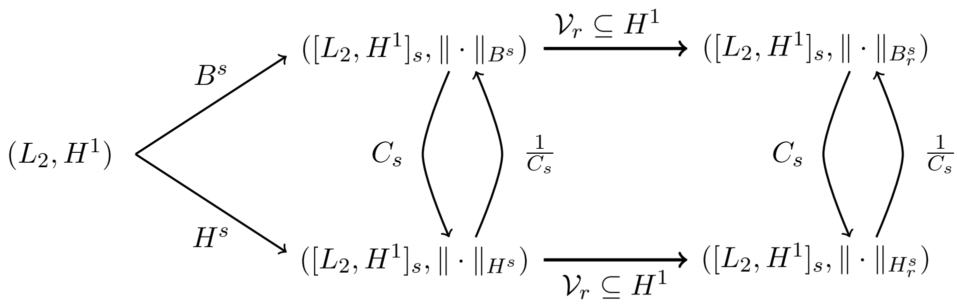


Figure 3: Schematic structure of interpolation spaces and norms.

A computationally beneficial observation is that the convergence behavior of our method is relatively robust in the choice of $\mathcal{I}$. Numerical tests affirmed that in most cases it is sufficient to take $\tilde{\lambda} \approx \lambda_{max}(M^{-1}A)$ and set $\mathcal{I} = [\sqrt{\tilde{\lambda}^{-1}}, 1]$ without loosing substantial approximation properties. In this way expensive computations of $\lambda_{max}(M^{-1}A)$ can be spared.

Under certain conditions the reduced basis norm is already exact for $r < N$.

Theorem 4.17. *Let* $(\lambda_k, z_k)_{k=0}^N$ *be* L_2*-orthonormal eigen-pairs of* V_h*, such that*

$$\forall w \in V_h: \quad \langle z_k, w\rangle_{H^1} = \lambda_k^2 \langle z_k, w\rangle_{L_2}.$$

Assume that $m \leq N$ *and* $u \in V_h$ *with* $u \in [\{z_0, ..., z_m\}]$*. Then*

$$r \geq m \quad \implies \quad \|u\|_{H_r^s} = \|u\|_{H^s}.$$

Proof. We show that

$$\mathcal{V}_r = [\{v^*(t_0), ..., v^*(t_r)\}] = [\{z_0, ..., z_m\}]$$

for $r \geq m$. The snapshot solutions $v^*(t_j) \in V_h$ satisfy

$$\forall w \in V_h: \quad \langle v^*(t_j), w\rangle_{L_2} + t_j^2 \langle v^*(t_j), w\rangle_{H^1} = \langle u, w\rangle_{L_2}. \tag{4.19}$$

Again, we refer to Lemma 6.3 to provide the expansion

$$v^*(t_j) = \sum_{k=0}^{N} \frac{u_k}{1 + t_j^2 \lambda_k^2} z_k.$$

Since $u \in [\{z_0, ..., z_m\}]$ it follows $v^*(t_j) \in [\{z_0, ..., z_m\}]$ for all $j = 0, ..., r$. We obtain

$$[\{v^*(t_0), ..., v^*(t_r)\}] \subseteq [\{z_0, ..., z_m\}].$$

Due to Theorem 4.12 the set $\{v^*(t_0), ..., v^*(t_r)\}$ is linearly independent for $r \leq m$, yielding

$$[\{v^*(t_0), ..., v^*(t_r)\}] \supseteq [\{z_0, ..., z_m\}]$$

for $r \geq m$, proofing the claim. ■

Remark 4.18. *Theorem 4.17 shows that increasing the reduced space dimension is reasonable as long as* $r < m$*. There holds*

$$r \geq m \quad \implies \quad \forall l \geq 0: \quad \mathcal{V}_r = \mathcal{V}_{r+l}. \tag{4.20}$$

5 Implementation of fractional diffusion operators

So far we have achieved to provide approximations for the interpolation norms on the intermediate space $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_s$ by means of a reduced basis method. This approach naturally involves the definition of a fractional operator. It will be clarified that this operator satisfies the desired requirements to realize a feasible approximation of $(-\Delta)^s$.

5.1 Fractional operators

Throughout what follows let again $V_h \subseteq H^1(\Omega)$ denote a conforming finite element space. The normed space

$$[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{B^s}$$

is not only a Banach but also a Hilbert space. Hence, $\|\cdot\|_{B^s}$ induces a scalar product which is inquired in the following Lemma.

Lemma 5.1. *The Banach interpolation norm $\|\cdot\|_{B^s}$ on the Banach interpolation space $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{B^s}$ satisfies*

$$\forall u \in V_h : \quad \langle u, u\rangle_{B^s} = \|u\|_{B^s}^2,$$

with

$$\langle v, u\rangle_{B^s} = \underline{v}^T M \int_0^\infty t^{-2s-1} \left(M^{-1} - (M + t^2 A)^{-1}\right) dt\, M\underline{u}.$$

Proof. The minimizer of the K-functional $v^* \in V_h$ corresponds to the solution of the linear system

$$(M + t^2 A)\underline{v}^* = M\underline{u}.$$

Direct computations reveal

$$\begin{aligned}
\|u - v^*\|_{L_2}^2 &= \|\underline{u} - (M + t^2A)^{-1}M\underline{u}\|_M^2 \\
&= \left(\underline{u} - (M + t^2A)^{-1}M\underline{u}\right)^T M\left(\underline{u} - (M + t^2A)^{-1}M\underline{u}\right) \\
&= \underline{u}^T M\underline{u} - 2\underline{u}^T M(M + t^2A)^{-1}M\underline{u} + \underline{u}^T M(M + t^2A)^{-1}M(M + t^2A)^{-1}M\underline{u},
\end{aligned}$$

$$\begin{aligned}
t^2\|v^*\|_{H^1}^2 &= t^2\|(M + t^2A)^{-1}M\underline{u}\|_A^2 \\
&= \left((M + t^2A)^{-1}M\underline{u}\right)^T \underbrace{t^2A}_{=(M+t^2A)-M} \left((M + t^2A)^{-1}M\underline{u}\right) \\
&= \underline{u}^T M(M + t^2A)^{-1}M\underline{u} - \underline{u}^T M(M + t^2A)^{-1}M(M + t^2A)^{-1}M\underline{u}.
\end{aligned}$$

This yields

$$\begin{aligned}
K^2(t, u) &= \|u - v^*\|_{L_2}^2 + t^2\|v^*\|_{H^1}^2 \\
&= \underline{u}^T M\underline{u} - \underline{u}^T M(M + t^2A)^{-1}M\underline{u} = \underline{u}^T M(M^{-1} - (M + t^2A)^{-1})M\underline{u}.
\end{aligned}$$

Hence

$$\begin{aligned}
\|u\|_{B^s}^2 &= \int_0^\infty t^{-2s-1} K^2(t,u)\,dt \\
&= \int_0^\infty t^{-2s-1} \underline{u}^T M \left(M^{-1} - (M + t^2 A)^{-1}\right) M \underline{u}\,dt \\
&= \underline{u}^T M \int_0^\infty t^{-2s-1} \left(M^{-1} - (M + t^2 A)^{-1}\right) dt\, M \underline{u}.
\end{aligned}$$

■

Although Lemma 5.1 provides a suitable representation for theoretical considerations, it is again favorable to work in the Hilbert space framework when it comes to numerical computations. To this purpose we state the following Theorem.

Theorem 5.2. *The Hilbert interpolation norm $\|\cdot\|_{H^s}$ on the Hilbert interpolation space $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{H^s}$ satisfies*

$$\forall u \in V_h\colon \quad \langle u, u\rangle_{H^s} = \|u\|_{H^s}^2,$$

with

$$\langle v, u\rangle_{H^s} = \underline{v}^T M (M^{-1}A)^s \underline{u}. \tag{5.1}$$

Proof. Let $(\lambda_k, z_k)_{k=0}^N$ denote the L_2-orthonormal eigensystem with the property

$$\forall w \in V_h : \quad \langle z_k, w\rangle_{H^1} = \lambda_k^2 \langle z_k, w\rangle_{L_2}.$$

Further let

$$Z = (\underline{z}_0, ..., \underline{z}_N) \qquad \text{and} \qquad \Lambda = \mathrm{Diag}(\lambda_0^2, ..., \lambda_N^2).$$

We show that

$$M^{-1}A = Z\Lambda Z^{-1} \tag{5.2}$$

holds. Since

$$Z^T M Z = I \qquad \text{and} \qquad Z^T A Z = \Lambda$$

it follows

$$M = Z^{-T} Z^{-1} \qquad \text{and} \qquad A = Z^{-T} \Lambda Z^{-1}.$$

All together

$$M^{-1}A = (Z^{-T}Z^{-1})^{-1} Z^{-T}\Lambda Z^{-1} = Z Z^T Z^{-T} \Lambda Z^{-1} = Z\Lambda Z^{-1},$$

which proofs (5.2). Computations of the right hand side of (5.1) reveal

$$\underline{u}^T M (M^{-1}A)^s \underline{u} = \underline{u}^T Z^{-T} Z^{-1} Z \Lambda^s Z^{-1} \underline{u} = \underline{u}^T Z^{-T} \Lambda^s Z^{-1} \underline{u}.$$

Basis transformation yields

$$\underline{u} = \sum_{k=0}^{N} \langle u, z_k \rangle_{L_2} \underline{z}_k = Z\underline{\hat{u}}$$

with

$$\underline{\hat{u}} := (\langle z_0, u \rangle_{L_2}^2, ..., \langle z_N, u \rangle_{L_2}^2)^T \in \mathbb{R}^{N+1}.$$

Applying Z^{-1} from the left gives

$$Z^{-1}\underline{u} = \underline{\hat{u}}$$

to finally obtain

$$\underline{u}^T M(M^{-1}A)^s \underline{u} = \underline{\hat{u}}^T \Lambda^s \underline{\hat{u}} = \sum_{k=0}^{N} \lambda_k^{2s} \langle u, z_k \rangle_{L_2}^2 = \|u\|_{H^s}^2.$$

■

Trivially there holds

$$M(M^{-1}A)^s = \begin{cases} M(M^{-1}A)^0 = M, & s = 0 \\ M(M^{-1}A)^1 = A, & s = 1 \end{cases}.$$

M and A are the finite element matrices arising from the bilinear forms

$$\langle \cdot, \cdot \rangle_{H^0} = \langle \cdot, \cdot \rangle_{L_2} \qquad \text{and} \qquad \langle \cdot, \cdot \rangle_{H^1} = \langle \cdot, \cdot \rangle_{L_2} + \langle \nabla \cdot, \nabla \cdot \rangle_{L_2}.$$

Therefore, $M(M^{-1}A)^s$ can be regarded as interpolation operator between M and A. In a strong sense, this refers to

$$M(M^{-1}A)^s \approx (I + (-\Delta))^s = I + (-\Delta)^s. \tag{5.3}$$

Direct computations of $(M^{-1}A)^s \in \mathbb{R}^{(N+1)\times(N+1)}$ according to the eigen-system are not applicable for large N. Again, the reduced basis setting can be installed to overwhelm this inconvenience.

5.2 Reduced basis methods for fractional operators

In order to make computations of (5.3) affordable, we consider the following approach. Analogously to Theorem 5.1, one can show that $\|\cdot\|_{B^s_{r(\cdot)}}$ induces an operator on the finite element intermediate space. The reduced basis norm gives a good approximation to the original interpolation norm, granting good chances that the same holds for the induced fractional operators. In chapter 6 we will proof that this is indeed the case.

Lemma 5.3. *The reduced basis Banach interpolation norm* $\|\cdot\|_{B^s_{r(\cdot)}}$ *on the Banach interpolation space* $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{B^s}$ *satisfies*

$$\forall u \in V_h\colon \quad \langle u, u \rangle_{B^s_{r(u)}} = \|u\|_{B^s_{r(u)}}^2$$

with

$$\langle v, u \rangle_{B^s_{r(u)}} = \underline{v}^T M V_r \int_0^\infty t^{-2s-1} \left(I_r - (I_r + t^2 A_r)^{-1} \right) dt \, V_r^T M \underline{u}. \tag{5.4}$$

Proof. The relations $\underline{u} = V_r\underline{\underline{u}}$ and $M_r = V_r^T M V_r = I_r$ reveal

$$\begin{aligned}\|u - v_r^*\|_{L_2}^2 &= \|\underline{u} - V_r(I_r + t^2 A_r)^{-1} V_r^T M \underline{u}\|_M^2\\ &= \|\underline{u} - V_r(I_r + t^2 A_r)^{-1} \underline{\underline{u}}\|_M^2\\ &= \big(\underline{u} - V_r(I_r + t^2 A_r)^{-1} \underline{\underline{u}}\big)^T M \big(\underline{u} - V_r(I_r + t^2 A_r)^{-1} \underline{\underline{u}}\big)\\ &= \underline{u}^T M \underline{u} - 2\underline{\underline{u}}^T (I_r + t^2 A_r)^{-1} \underline{\underline{u}} + \underline{\underline{u}}^T (I_r + t^2 A_r)^{-1} M_r (I_r + t^2 A_r)^{-1} \underline{\underline{u}},\end{aligned}$$

$$\begin{aligned}t^2\|v_r^*\|_{H^1}^2 &= t^2\|V_r(I_r + t^2 A_r)^{-1} V_r^T M \underline{u}\|_A^2\\ &= \big(V_r(I_r + t^2 A_r)^{-1} \underline{\underline{u}}\big)^T t^2 A \big(V_r(I_r + t^2 A_r)^{-1} \underline{\underline{u}}\big)\\ &= \big(\underline{\underline{u}}^T (I_r + t^2 A_r)^{-1} V_r^T\big)\big((M + t^2 A) - M\big)\big(V_r(I_r + t^2 A_r)^{-1} \underline{\underline{u}}\big).\end{aligned}$$

Due to $V_r^T(M + t^2 A)V_r = (I_r + t^2 A_r)$ it follows

$$t^2\|v_r^*\|_{H^1} = \underline{\underline{u}}^T (I_r + t^2 A_r)^{-1} \underline{\underline{u}} - \underline{\underline{u}}^T (I_r + t^2 A_r)^{-1} I_r (I_r + t^2 A_r)^{-1} \underline{\underline{u}}^T.$$

Hence

$$K_r^2(t, u) = \underline{u}^T M \underline{u} - \underline{\underline{u}}^T (I_r + t^2 A_r)^{-1} \underline{\underline{u}}^T. \tag{5.5}$$

Since $u \in \mathcal{V}_r$ it follows

$$\underline{u}^T M \underline{u} = \underline{\underline{u}}^T V_r^T M V_r \underline{\underline{u}} = \underline{\underline{u}}^T M_r \underline{\underline{u}} = \underline{\underline{u}}^T I_r \underline{\underline{u}}.$$

Identity (5.5) reveals

$$K_r^2(t, u) = \underline{\underline{u}}^T (I_r - (I_r + t^2 A_r)^{-1}) \underline{\underline{u}}.$$

Resubstituting $\underline{\underline{u}} = V_r M \underline{u}$ concludes the proof. ∎

The reduced basis pendant to Theorem 5.2 reads as follows.

Theorem 5.4. *The reduced basis Hilbert interpolation norm $\|\cdot\|_{H^s_{r(\cdot)}}$ on the Hilbert interpolation space $[(V_h, \|\cdot\|_{L_2}), (V_h, \|\cdot\|_{H^1})]_{H^s}$ satisfies*

$$\forall u \in V_h\colon \quad \langle u, u\rangle_{H^s_{r(u)}} = \|u\|^2_{H^s_{r(u)}},$$

with

$$\langle v, u\rangle_{H^s_{r(u)}} = \underline{v}^T M V_r A_r^s V_r^T M \underline{u}.$$

Proof. Let $(\lambda_k, z_k)_{k=0}^r$ be L_2-orthonormal eigenpairs of $\mathcal{V}_r$, such that

$$\forall w_r \in \mathcal{V}_r : \quad \langle z_k, w_r\rangle_{H^1} = \lambda_k^2 \langle z_k, w_r\rangle_{L_2} \qquad k = 0, ..., r.$$

Define the matrices

$$Z_r := (\underline{\underline{z}}_0, ..., \underline{\underline{z}}_r) \in \mathbb{R}^{(r+1)\times(r+1)} \qquad \Lambda_r := \mathrm{Diag}(\lambda_0^2, ..., \lambda_r^2) \in \mathbb{R}^{(r+1)\times(r+1)},$$

such that

$$Z_r^T M_r Z_r = Z_r^T Z_r = I_r \qquad \text{and} \qquad Z_r^T (M_r^{-1} A_r) Z_r = \Lambda_r,$$

to obtain

$$\begin{aligned}
\|u\|_{H_r^s}^2 &= \sum_{k=0}^{r} \lambda_k^{2s} \langle u, z_k \rangle_{L_2}^2 \\
&= \underline{u}^T M (V_r Z_r) \Lambda_r^s (V_r Z_r)^T M \underline{u} \\
&= \underline{u}^T M V_r (M_r^{-1} A_r)^s V_r^T M \underline{u} \\
&= \underline{u}^T M V_r A_r^s V_r^T M \underline{u}.
\end{aligned}$$

■

Considerations from above provide all the necessary tools to introduce fractional operators in a reduced basis sense. The action

$$\underline{u} \mapsto M V_r (M_r^{-1} A_r)^s V_r^T M \underline{u} = M V_r A_r^s V_r^T M \underline{u}$$

can be regarded as an approximation of the fractional operator action

$$\underline{u} \mapsto M (M^{-1} A)^s \underline{u}, \tag{5.6}$$

requiring only the computation of the small eigen-system

$$A_r^s = Z_r \Lambda_r^s Z_r^T$$

on the reduced space $\mathcal{V}_r$. We state the following definition.

Definition 5.5. *The associated reduced basis operator of* (5.6) *with respect to* $u \in V_h$ *is defined as*

$$M(M^{-1}A)_{r(u)}^s := M V_r A_r^s V_r^T M.$$

As long as it is clear from the context we will again neglect the dependency in u. One observes that

$$(M^{-1}A)^s \underline{u} \approx (M^{-1}A)_r^s \underline{u} = V_r A_r^s V_r^T M \underline{u}.$$

Remark 5.6. *This construction provides a nonlinear dependency in the input vector* $\underline{u}$*, resulting in a nonlinear operator* $(M^{-1}A)_{r(\cdot)}^s$*, such that*

$$(M^{-1}A)_{r(u+v)}^s (\underline{u} + \underline{v}) \neq (M^{-1}A)_{r(u)}^s \underline{u} + (M^{-1}A)_{r(v)}^s \underline{v} \qquad \text{for } v \neq u.$$

Whenever the application $\underline{u} \mapsto (M^{-1}A)_r^s \underline{u}$ *is performed, the corresponding reduced basis matrices* V_r *have to be deployed for each* $u \in V_h$ *separately.*

5.2.1 The inverse Operator

Implementation of the inverse reduced basis operator is apparently simple. Consider the vector $\underline{\mathrm{f}} \in \mathbb{R}^{N+1}$ arising from finite element discretization applied to the right-hand side functional $\langle f, \cdot \rangle_{L_2} \in V_h^*$. The goal is to provide an efficient procedure for the inverse action

$$\underline{\mathrm{f}} \mapsto [M(M^{-1}A)^s]^{-1} \underline{\mathrm{f}}.$$

This can be achieved by slightly adapted reduced basis techniques. As done before, we apply M-orthonormalization to the matrix

$$\hat{V}_r := [\underline{v}^*(t_0), ..., \underline{v}^*(t_r)],$$

but this time with

$$\underline{v}^*(t_j) = (M + t^2 A)^{-1}\underline{\mathrm{f}} \qquad j = 0, ..., r$$

in order to obtain V_r. This setting enables us to sate the following Theorem.

Theorem 5.7. *Assume that $f \in L_2(\Omega)$ with its associated reduced basis matrix V_r. Further let $u \in V_h$ be the L_2-projection of f on V_h, i.e*

$$\forall w \in V_h : \quad \langle u, w \rangle_{L_2} = \langle f, w \rangle_{L_2},$$

such that $M^{-1}\underline{\mathrm{f}} = \underline{u}$ holds. Then

$$[M(M^{-1}A)^s_{r(u)}]^{-1}\underline{\mathrm{f}} = V_r A_r^{-s} V_r^T \underline{\mathrm{f}}. \tag{5.7}$$

Proof. Identification of V_h with $\mathbb{R}^{N+1}$ gives

$$M(M^{-1}A)^s_r : V_h \longrightarrow V_h^* \quad \Longrightarrow \quad [M(M^{-1}A)^s_r]^{-1} : V_h^* \longrightarrow V_h.$$

The identity $(M^{-1}A)^s_r = V_r A_r^s V_r^T M$ reveals

$$V_r A_r^s V_r^T : V_h^* \longrightarrow V_h.$$

What remains to be proofed is that (5.7) holds.

$$\begin{aligned}
\left(M(M^{-1}A)^s_r\right)\left(V_r A_r^{-s} V_r^T\right)\underline{\mathrm{f}} &= \left(M V_r A_r^s V_r^T M\right)\left(V_r A_r^{-s} V_r^T\right)\underline{\mathrm{f}} \\
&= M V_r A_r^s M_r A_r^{-s} V_r^T \underline{\mathrm{f}} \\
&= M V_r A_r^s A_r^{-s} V_r^T \underline{\mathrm{f}} \\
&= M V_r V_r^T \underline{\mathrm{f}} \\
&= M V_r V_r^T M M^{-1} \underline{\mathrm{f}} \\
&= M V_r V_r^T M \underline{u} = M V_r \underline{\underline{u}} = M \underline{u} = \underline{\mathrm{f}}
\end{aligned}$$

■

Theorem 5.7 justifies the following definition.

Definition 5.8. *Let $f \in L_2(\Omega)$ with its associated reduced basis matrix V_r. Then the inverse reduced basis operator of* (5.6) *with respect to f is defined as*

$$(M^{-1}A)^{-s}_{r(f)} := V_r A_r^{-s} V_r^T.$$

Definition 5.5 and 5.8 provide computationally appealing approximations for the fractional operator actions

$$\underline{u} \mapsto M(M^{-1}A)^s \underline{u} \qquad \text{and} \qquad \underline{u} \mapsto [M(M^{-1}A)^s]^{-1}\underline{u}.$$

So far we have only regarded fractional operators with respect to the full H^1-matrix, resulting in a finite element approximation to the fractional differential operator $I + (-\Delta)^s$. We now aim to replace A by the matrix $\widehat{A}$ arising from the gradient bilinear form in order to obtain

$$(-\Delta)^s u \approx M(M^{-1}\widehat{A})\underline{u}.$$

5.3 Fractional Laplace operator

This section is dedicated to the efficient implementation of fractional powers of the Laplacian itself. Ad hoc one could assume that the fractional norm of the interpolation space between $(V_h, \|\cdot\|_{L_2})$ and $(V_h, |\cdot|_{H^1})$ induces the desired fractional operator action

$$\underline{u} \mapsto M(M^{-1}\widehat{A})\underline{u} \approx M(M^{-1}\widehat{A})^s_{r(u)}\underline{u} = MV_r\widehat{A}_r^s V_r^T M\underline{u},$$

whereas $\widehat{A}$ denotes the matrix arising from the gradient bilinear form $\langle \nabla\cdot, \nabla\cdot\rangle_{L_2}$. Unfortunately, the H^1-semi-norm neither is a norm on general finite element spaces V_h nor does it satisfy the continuous embedding "$(V_h, |\cdot|_{H^1}) \subseteq (V_h, \|\cdot\|_{L_2})$".

This inconvenience might be avoided by either postulating homogeneous Dirichlet data on the boundary $\partial\Omega$ with $V_h \subseteq H^1_0(\Omega)$ or rather consider the averaged subspace

$$\bar{H}^1(\Omega) := \left\{ u \in H^1(\Omega) \,\middle|\, \int_\Omega u\, dx = 0 \right\} \subseteq H^1(\Omega)$$

and choose $V_h \subseteq \bar{H}^1(\Omega)$. In both cases Poincaré, respectively Friedrichs inequality provide equivalence of the semi-norm and the H^1-norm. Compact embedding $(V_h, |\cdot|_{H^1}) \subseteq (V_h, \|\cdot\|_{L_2})$ is guaranteed.

The question arises whether discussed techniques from section 5.2 can be interpreted reasonably if the embedding is not continuous, sparing manipulations of the finite element space V_h in terms of boundary conditions or averaging techniques. To this extent we consider once more the finite element eigenvalue problem: Find an orthonormal basis $(z_k)_{k=0}^N$ of $(V_h, \|\cdot\|_{L_2})$ and eigenvalues $(\widehat{\lambda}_k)_{k=0}^N$, such that

$$\forall w \in V_h: \quad \langle \nabla z_k, \nabla w\rangle_{L_2} = \widehat{\lambda}_k^2 \langle z_k, w\rangle_{L_2} \qquad k = 0, ..., N.$$

Obviously, $z_0 \equiv 1$ is an eigenfunction to the eigenvalue $\widehat{\lambda}_0^2 = 0$. One immediately observes

$$\|z_0\|_{H^0} = \|z_0\|_{L_2} = |\Omega| \neq 0,$$

while for all $s > 0$ there holds

$$|z_0|^2_{H^s} := \sum_{k=0}^N \widehat{\lambda}_k^{2s} \langle z_k, z_0\rangle^2_{L_2} = \widehat{\lambda}_0^{2s}\|z_0\|^2_{L_2} = 0.$$

This involves a discontinuity in $s = 0$ with respect the mapping

$$s \mapsto \|u\|_{H^s}$$

for any $u \in \mathcal{K}_0 := \{u \in V_h \,|\, \langle \nabla u, \nabla u\rangle_{L_2} = 0\} = \{u \in V_h \,|\, u = \textit{const.}\}$, causing division by zero as the inverse operator is applied. Analogously to the regular case with $s = 1$, the fractional Laplacian is not invertible among general boundary conditions. Nevertheless, operator application can still be given sense. Orthogonal decomposition of $u \in V_h \subseteq H^1(\Omega)$, $u = u_0 + u_1$ with $u_0 \in \mathcal{K}_0$ and $u_1 \in \mathcal{K}_0^{\perp_{L_2}}$, holds for all $s \in (0, 1)$

$$(-\Delta)^s u = (-\Delta)^s(u_0 + u_1) = (-\Delta)^s u_1,$$

justifying the definition

$$[(V_h, \|\cdot\|_{L_2}), (V_h, |\cdot|_{H^1})]_{B^s} := [(\mathcal{K}_0^{\perp_{L_2}}, \|\cdot\|_{L_2}), (\mathcal{K}_0^{\perp_{L_2}}, |\cdot|_{H^1})]_{B^s}. \tag{5.8}$$

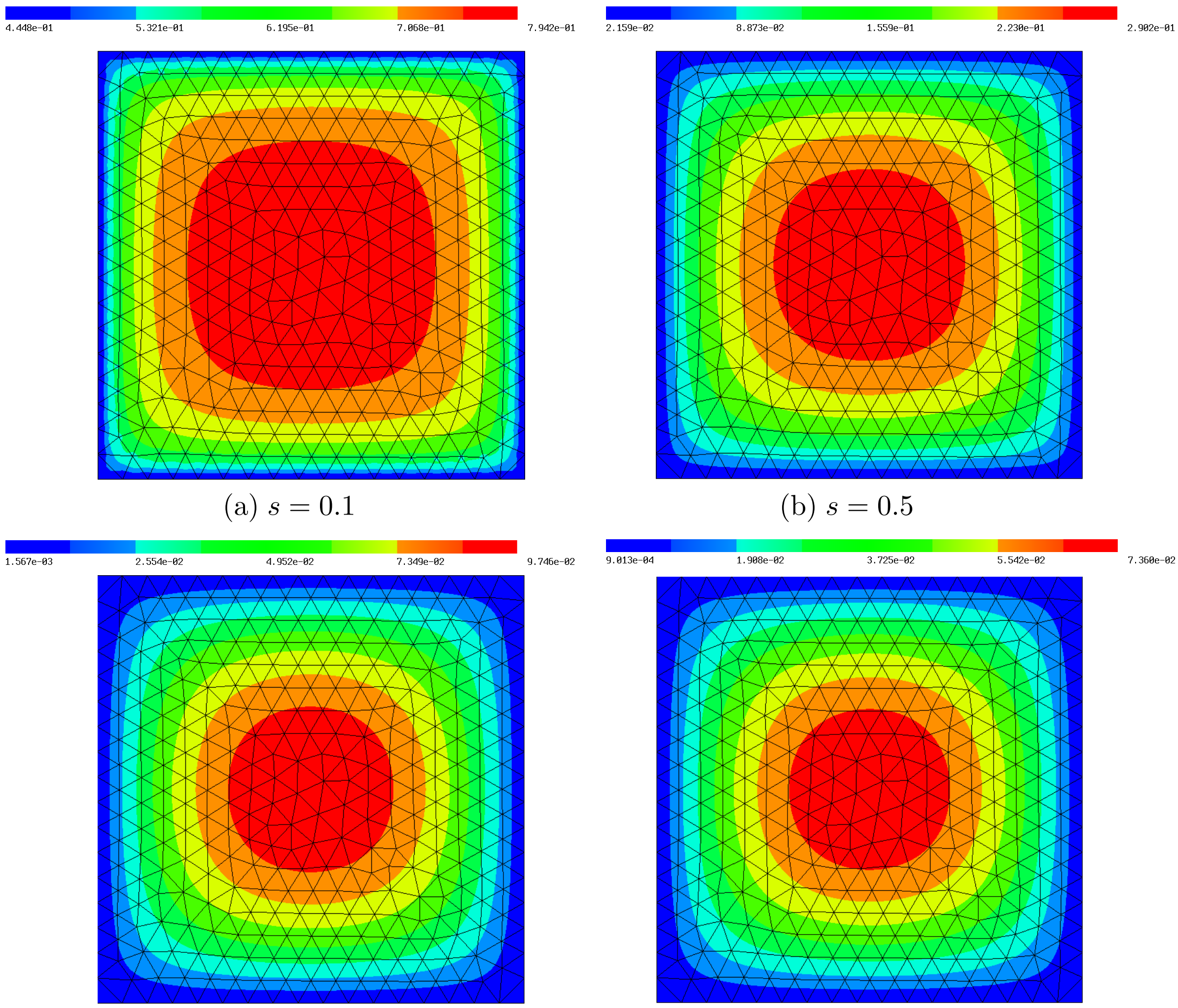
Since $\mathcal{K}_0^{\perp_{L_2}}$ is a closed subspace of $H^1(\Omega)$ and thus a Hilbert space itself, (5.8) is well defined. Hilbert space interpolation in this context is installed analogously. The induced reduced basis operator gives rise to an approximation of the fractional Laplacian according to

$$\underline{u} \mapsto M V_r \widehat{A}_r^s V_r^T M \underline{u} \approx M(M^{-1}\widehat{A})^s \underline{u}.$$

Example. Consider the fractional Poisson equation

$$(-\Delta)^s u = f \text{ on } \Omega, \quad (5.9a)$$
$$u = 0 \text{ on } \partial\Omega. \quad (5.9b)$$

The behavior of u for various exponents s is surveyed in figure 4 for $\Omega = [0,1]^2$ and $f \equiv 1$.



(a) $s = 0.1$ (b) $s = 0.5$

(c) $s = 0.9$ (d) $s = 1$

Figure 4: Solution of the fractional Poisson problem for different powers s.

A continuous transition for changing exponents s is observed. One notices that for small fractional powers the solutions of (5.9a) - (5.9b) tends to approach a constant state in the interior of Ω, rapidly decreasing closer to the boundary due to the postulated boundary conditions. This is based on the fact that $M(M^{-1}\widehat{A})_r^s$ converges towards M as $s \to 0$, such that its associated

PDE degenerates to a simple projection problem. Notice that in the limit this problem is not solvable due to the non-compatibility of f. Though, for all $s > 0$ the problem is solvable, forcing the solution to the utterly constant state possible in case of small exponents.

6 Error analysis

At some points of this thesis details have been spared for subsequent sections. We now have all the necessary tools to catch up this lack of accuracy. We will affirm that there exists a tuple of snapshots $t_1, ..., t_r$, naturally arising from convergence analysis, such that exponential decay in the error for both norm and operator action is obtained.

6.1 Error estimates for the reduced basis interpolation norm

Throughout the entire chapter let $V_h \subseteq H^1(\Omega)$ be a finite element space of dimension $N+1$ and $(z_k)_{k=0}^N$ the L_2-orthonormal basis of V_h, such that

$$\forall w \in V_h : \quad \langle z_k, w\rangle_{H^1} = \lambda_k^2 \langle z_k, w\rangle_{L_2}. \tag{6.1}$$

The goal of this section is to bound the error in the reduced basis norm, which reads as

$$\left| \|u\|_{B_r^s}^2 - \|u\|_{B^s}^2 \right| = \left| \int_0^\infty t^{-2s-1} \left(K_r^2(t,u) - K^2(t,u) \right) \, dt \right|. \tag{6.2}$$

As shown below, the reduced basis norm approximates $\|\cdot\|_{B^s}$ from above, such that absolute values can be spared.

Lemma 6.1. *Let $u \in V_h$ and $r \in \mathbb{N}$. Then there holds*

$$\forall t \in \mathbb{R}^+ : \quad K_r(t,u) \geq K(t,u).$$

Proof. The relation $\mathcal{V}_r \subseteq V_h$ immediately reveals

$$\begin{aligned} \forall t \in \mathbb{R}^+ : \quad K_r^2(t,u) &= \inf_{v_r \in \mathcal{V}_r} \|u - v_r\|_{L_2}^2 + t^2 \|v_r\|_{H^1}^2 \\ &\geq \inf_{v \in V_h} \|u - v\|_{L_2}^2 + t^2 \|v\|_{H^1}^2 = K^2(t,u), \end{aligned}$$

concluding the proof. ■

Theorem 6.2. *Let $u \in V_h$ and $r \in \mathbb{N}$. Then there holds*

$$\|u\|_{B_r^s} \geq \|u\|_{B^s}.$$

Proof. Due to Lemma 6.1 it follows

$$\|u\|_{B_r^s}^2 = \int_0^\infty t^{-2s-1} K_r^2(t,u) \, dt \geq \int_0^\infty t^{-2s-1} K^2(t,u) \, dt = \|u\|_{B^s}^2,$$

concluding the proof. ■

Estimates of (6.2) directly involve upper bounds for the reduced basis K-functional, justifying the further course of action.

6.1.1 Upper bounds for the reduced basis K-functional

We recap some important results. The reduced space is defined by $\mathcal{V}_r = [v^*(t_0), ..., v^*(t_r)]$ with

$$\forall w \in V_h : \quad \langle v^*(t_j), w\rangle_{L_2} + t_j^2 \langle v^*(t_j), w\rangle_{H^1} = \langle u, w\rangle_{L_2} \qquad j = 0, ..., r \tag{6.3}$$

and $t_0 = 0$, $t_1, ..., t_r \in \mathcal{I} \subseteq \mathbb{R}^+$. The minimizer $v^* \in V_h$ of $K^2(t, u)$ satisfies

$$\forall w \in V_h : \quad \langle v^*, w\rangle_{L_2} + t^2 \langle v^*, w\rangle_{H^1} = \langle u, w\rangle_{L_2}. \tag{6.4}$$

Its approximation $v_r^* \approx v^*$ in the reduced space satisfies

$$\forall w_r \in \mathcal{V}_r : \quad \langle v_r^*, w_r\rangle_{L_2} + t^2 \langle v_r^*, w_r\rangle_{H^1} = \langle u, w_r\rangle_{L_2}.$$

The orthonormal basis $(z_k)_{k=0}^N$ provides a beneficial representation for the minimizer v^*, which has already been referred to in former chapters.

Lemma 6.3. *Let v^* denote the solution of (6.4). Then there holds*

$$v^* = \sum_{k=0}^{N} \frac{u_k}{1 + t^2 \lambda_k^2} z_k.$$

Proof. Both v^* and $u \in V_h$ provide the Fourier expansion

$$v^* = \sum_{k=0}^{N} v_k^* z_k \qquad u = \sum_{k=0}^{N} u_k z_k.$$

It follows for all $j = 0, ..., N$

$$\begin{aligned}
& \langle v^*, z_j\rangle_{L_2} + t^2 \langle v^*, z_j\rangle_{H^1} = \langle u, z_j\rangle_{L_2} \\
\iff\quad & \langle \sum_{k=0}^{N} v_k^* z_k, z_j\rangle_{L_2} + t^2 \langle \sum_{k=0}^{N} v_k^* z_k, z_j\rangle_{H^1} = \langle \sum_{k=0}^{N} u_k z_k, z_j\rangle_{L_2} \\
\iff\quad & \sum_{k=0}^{N} v_k^* \langle z_k, z_j\rangle_{L_2} + t^2 \sum_{k=0}^{N} v_k^* \langle z_k, z_j\rangle_{H^1} = \sum_{k=0}^{N} u_k \langle z_k, z_j\rangle_{L_2} \\
\iff\quad & v_j^* + t^2 \lambda_j v_j^* = u_j \\
\iff\quad & v_j^* = \frac{u_j}{1 + t^2 \lambda_j^2}.
\end{aligned}$$

■

The following Lemma supplies us with the fundamental estimate on which further elaborations are based on.

Lemma 6.4. *Let $u \in V_h$ and $t \in \mathbb{R}^+$. Then there holds*

$$\forall w_r \in \mathcal{V}_r : \quad K_r^2(t, u) - K^2(t, u) \leq \|v^* - w_r\|_{L_2}^2 + t^2 \|v^* - w_r\|_{H_1}^2.$$

Proof. Due to the minimization property of v_r^* it follows for all $w_r \in \mathcal{V}_r$

$$K_r^2(t,u) - K^2(t,u) \leq \|u - w_r\|_{L_2}^2 + t^2\|w_r\|_{H^1}^2 - \|u - v^*\|_{L_2}^2 - t^2\|v^*\|_{H^1}^2. \tag{6.5}$$

One observes

$$\begin{aligned}\|u - w_r\|_{L_2}^2 - \|u - v^*\|_{L_2}^2 &= \langle u - w_r, u - w_r\rangle_{L_2} - \langle u - v^*, u - v^*\rangle_{L_2} \\ &= \|u\|_{L_2}^2 - 2\langle u, w_r\rangle_{L_2} + \|w_r\|_{L_2}^2 - \|u\|_{L_2}^2 + 2\langle u, v^*\rangle_{L_2} - \|v^*\|_{L_2}^2 \\ &= -2\langle u, w_r\rangle_{L_2} + \|w_r\|_{L_2}^2 + 2\langle u, v^*\rangle_{L_2} - \|v^*\|_{L_2}^2.\end{aligned}$$

We define the bilinear form

$$a(u,v) := \langle u, v\rangle_{L_2} + t^2\langle u, v\rangle_{H^1}.$$

Due to

$$\forall w \in V_h: \quad a(v^*, w) = \langle u, w\rangle_{L_2}$$

and $u \in V_h$ it follows

$$\|u - w_r\|_{L_2}^2 - \|u - v^*\|_{L_2}^2 = -2a(v^*, w_r) + \|w_r\|_{L_2}^2 + 2a(v^*, v^*) - \|v^*\|_{L_2}^2.$$

Hence

$$\begin{aligned}\|u - w_r\|_{L_2}^2 + t^2\|w_r\|_{H^1}^2 - \|u - v^*\|_{L_2}^2 - t^2\|v^*\|_{H^1}^2 &= -2a(v^*, w_r) + a(w_r, w_r) + 2a(v^*, v^*) - a(v^*, v^*) \\ &= a(w_r, w_r) - 2a(v^*, w_r) + a(v^*, v^*) \\ &= \|w_r - v^*\|_{L_2}^2 + t^2\|w_r - v^*\|_{H^1}^2,\end{aligned}$$

which concludes the proof. ∎

Remark 6.5. *Along with the choice $w_r = v_r^*$ we can replace "$\leq$" in* (6.5) *by "$=$" to obtain*

$$K_r^2(t,u) - K^2(t,u) = \|v_r^* - v^*\|_{L_2}^2 + t^2\|v_r^* - v^*\|_{H^1}^2.$$

Theorem 6.6. *Let $u \in V_h$ and $t \in \mathbb{R}^+$. Then for all $\alpha_0, ..., \alpha_r \in \mathbb{R}$ there holds*

$$K_r^2(t,u) - K^2(t,u) \leq \sum_{k=0}^{N}(1 + t^2\lambda_k^2)\left(\frac{1}{1 + t^2\lambda_k^2} - \sum_{j=0}^{r}\alpha_j\frac{1}{1 + t_j^2\lambda_k^2}\right)^2 u_k^2.$$

Proof. According to Lemma 6.4 it holds for any $w_r = \sum_{j=0}^{r}\alpha_j v^*(t_j) \in \mathcal{V}_r$

$$K_r^2(t,u) - K^2(t,u) \leq \|v^* - w_r\|_{L_2}^2 + t^2\|v^* - w_r\|_{H_1}^2.$$

Spectral decomposition gives

$$\begin{aligned}\|v^* - w_r\|_{H^1}^2 &= \|v^* - \sum_{j=0}^{r}\alpha_j v^*(t_j)\|_{H^1}^2 \\ &= \|\sum_{k=0}^{N}v_k^* z_k - \sum_{j=0}^{r}\alpha_j\sum_{k=0}^{N}(v^*(t_j))_k z_k\|_{H^1}^2.\end{aligned}$$

Lemma 6.3 reveals

$$\begin{aligned}
\|v^* - w_r\|_{H^1}^2 &= \|\sum_{k=0}^{N} \frac{u_k}{1+t^2\lambda_k^2} z_k - \sum_{j=0}^{r} \alpha_j \sum_{k=0}^{N} \frac{u_k}{1+t_j^2\lambda_k^2} z_k\|_{H^1}^2 \\
&= \|\sum_{k=0}^{N} \left(\frac{1}{1+t^2\lambda_k^2} - \sum_{j=0}^{r} \alpha_j \frac{1}{1+t_j^2\lambda_k^2} \right) u_k z_k\|_{H^1}^2 \\
&= \sum_{k=0}^{N} \| \left(\frac{1}{1+t^2\lambda_k^2} - \sum_{j=0}^{r} \alpha_j \frac{1}{1+t_j^2\lambda_k^2} \right) u_k z_k\|_{H^1}^2 \\
&= \sum_{k=0}^{N} \lambda_k^2 \left(\frac{1}{1+t^2\lambda_k^2} - \sum_{j=0}^{r} \alpha_j \frac{1}{1+t_j^2\lambda_k^2} \right)^2 u_k^2.
\end{aligned}$$

Computations in the L_2-norm can be concluded analogously, proofing the claim. ■

In the following, similar techniques we are familiar with from finite element error estimations are applied. Since Theorem 6.6 holds for any arbitrary choice of $\alpha_0, ..., \alpha_r \in \mathbb{R}$, we aim to choose those coefficients in a way, such that

$$\forall \lambda \in [\sqrt{\lambda_{min}}, \sqrt{\lambda_{max}}] : \quad \left(\frac{1}{1+t^2\lambda^2} - \sum_{j=0}^{r} \alpha_j \frac{1}{1+t_j^2\lambda^2} \right) \tag{6.6}$$

becomes small, whereas $\lambda_{min} := \lambda_{min}(M^{-1}A)$ and $\lambda_{max} := \lambda_{max}(M^{-1}A)$. In order to simplify this problem we make the rather unrestrictive assumption that $\lambda_{min} \geq 1$ and consider (6.6) for $\lambda \in \hat{\sigma} := [1, \sqrt{\lambda_{max}}] \supseteq [\sqrt{\lambda_{min}}, \sqrt{\lambda_{max}}]$ instead. Any possible bound of (6.6) on $\hat{\sigma}$ then trivially also holds on $[\sqrt{\lambda_{min}}, \sqrt{\lambda_{max}}]$.

In the further course of action we will derive two different choices for the coefficients $(\alpha_j)_{j=0}^r$ in dependency of $t \in \mathbb{R}^+$. The first one ensures that (6.6) becomes small for $t \geq 1$ whereas the second achieves the same for $t < 1$.

To this extent we make a first ansatz and set $\alpha_0 = 0$ (the justification for this will become clear in the following). The latter coefficients are determined by means of a rational interpolation problem, being inquired in the subsequent Lemma.

Lemma 6.7. *Let $a > 1$, $J_l = [a^{-1}, 1]$ and $J_r = [1, a]$. Assume that $\kappa, \kappa_1, ..., \kappa_r \in J_l$, such that $\kappa_i \neq \kappa_j$ for $i \neq j$. Further define $g_\kappa(x) := \frac{1}{1+\kappa x}$ and the rational function space*

$$\mathcal{R} := \left[\left\{ f(x) = \frac{1}{1+\kappa_j x} \,\middle|\, j = 1, ..., r \right\} \right].$$

Then the solution q of the rational interpolation problem: Find $q \in \mathcal{R}$, such that

$$\forall j \in \{1, ..., r\} : \quad q\left(\frac{1}{\kappa_j}\right) = g_\kappa\left(\frac{1}{\kappa_j}\right) \tag{6.7}$$

satisfies the error estimate

$$\forall x \in J_r : \quad |g_\kappa(x) - q(x)| \leq \frac{1}{1+\kappa x} \prod_{j=1}^{r} \left| \frac{(1-\kappa_j x)}{(1+\kappa_j x)} \right|. \tag{6.8}$$

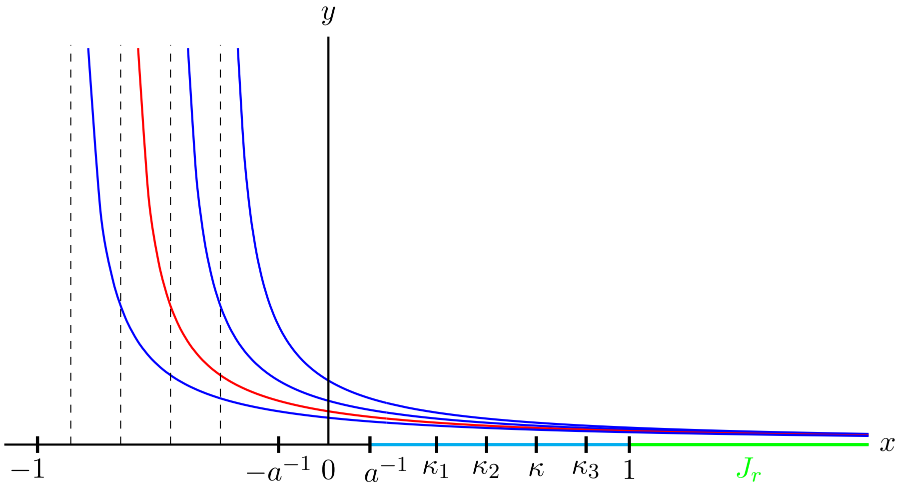


Figure 5: Illustration of the rational interpolation problem: Intervals J_l (cyan), J_r (green) together with $g_\kappa(x)$ (red) and its approximating rational functions (blue) in $\mathcal{R}$.

Proof. Let

$$q(x) = \sum_{j=1}^{r} \alpha_j \frac{1}{1+\kappa_j x}$$

denote the unique solution of (6.7). Then

$$g_\kappa(x) - q(x) = \frac{1}{1+\kappa x} - \sum_{j=1}^{r} \alpha_j \frac{1}{1+\kappa_j x} = \frac{p(x)}{(1+\kappa x)\prod_{j=1}^{r}(1+\kappa_j x)} \tag{6.9}$$

for some $p \in \Pi_r$. Due to the interpolation property there holds

$$\forall j \in \{1, ..., r\}: \quad p\left(\frac{1}{\kappa_j}\right) = 0.$$

The fundamental Theorem of algebra claims the existence of a constant $\tilde{C} = \tilde{C}(\kappa) \in \mathbb{R}$, such that

$$p(x) = \tilde{C} \prod_{j=1}^{r}\left(x - \frac{1}{\kappa_j}\right) = \tilde{C} \prod_{j=1}^{r}\left(\frac{x\kappa_j - 1}{\kappa_j}\right) = \underbrace{-\frac{\tilde{C}}{\prod_{j=1}^{r}\kappa_j}}_{=:C} \prod_{j=1}^{r}(1-\kappa_j x).$$

$C = C(\kappa)$ can be further specified. Multiplying (6.9) by $(1+\kappa x)$ and setting $x = -\frac{1}{\kappa}$ yields

$$1 = \frac{C\prod_{j=1}^{r}(1+\frac{\kappa_j}{\kappa})}{\prod_{j=1}^{r}(1-\frac{\kappa_j}{\kappa})} \quad \Longleftrightarrow \quad C = \prod_{j=1}^{r}\frac{(1-\frac{\kappa_j}{\kappa})}{(1+\frac{\kappa_j}{\kappa})} = \prod_{j=1}^{r}\frac{(\kappa-\kappa_j)}{(\kappa+\kappa_j)}.$$

All together we obtain for all $x \in J_r$

$$|g_\kappa(x) - q(x)| = \frac{1}{1+\kappa x} \prod_{j=1}^{r} \left| \frac{(\kappa - \kappa_j)}{(\kappa + \kappa_j)} \frac{(1-\kappa_j x)}{(1+\kappa_j x)} \right| \leq \frac{1}{1+\kappa x} \prod_{j=1}^{r} \left| \frac{(1-\kappa_j x)}{(1+\kappa_j x)} \right|.$$

■

Remark 6.8. *Notice that the interpolation takes place remote from the function's singularities, which are all accumulated on* $\mathbb{R}^-$.

Minimizing the maximal deviation of the interpolation error (6.8) leads to a min-max problem resembling error estimations with Chebyshev polynomials: Find $\kappa_1, ..., \kappa_r \in J_l$, such that

$$\min_{\theta_1,...,\theta_r \in J_l} \max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{(1-\theta_j x)}{(1+\theta_j x)} \right| = \max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{(1-\kappa_j x)}{(1+\kappa_j x)} \right|. \tag{6.10}$$

Closely related problems have been discussed in [9], [10], [11], [18] and [21]. We summarize the most important results.

Zolotarëv Points

Definition 6.9. *Let* $k \in (0,1)$ *and*

$$z(\phi; k) = \int_0^\phi \frac{1}{\sqrt{1-k^2\sin^2(\theta)}}\, d\theta.$$

The elliptic function

$$\mathrm{dn}(z; k) = \sqrt{1-k^2\sin^2(\phi)}$$

is called delta amplitudinis. The parameter k *is being referred to as elliptic modul.* $k' := 1-k$ *defines the complimentary elliptic modul. The functions*

$$\bar{K}(k) = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1-k^2\sin^2(\phi)}}\, d\phi \qquad \text{and} \qquad \bar{K}'(k) = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1+k^2\cos^2(\phi)}}\, d\phi$$

are called elliptic integrals.

Remark 6.10. dn *denotes one out of 12 so-called Jacobi elliptic functions, whose names come from their application in differential geometry.*

The solution of (6.10) is closely related to a slightly different min-max problem, giving rise to the following Theorem.

Theorem 6.11. *Assume that* $\delta \in (0,1)$ *and* $m \in \mathbb{N}$. *Then the solution of the problem: Find* $\kappa_1, ..., \kappa_r \in [\delta, 1]$, *such that*

$$\min_{\theta_1,...,\theta_r \in [\delta,1]} \max_{x \in [\delta,1]} \prod_{j=1}^{r} \left| \frac{(x-\theta_j)}{(x+\theta_j)} \right| = \max_{x \in [\delta,1]} \prod_{j=1}^{r} \left| \frac{(x-\kappa_j)}{(x+\kappa_j)} \right| \tag{6.11}$$

is given by the Zolotarëv points

$$\mathcal{Z}_j := \mathrm{dn}\left(\frac{2(r-j)+1}{2r} \bar{K}(\delta'), \delta' \right) \qquad j = 1, ..., r \tag{6.12}$$

with $\delta' := 1-\delta^2$.

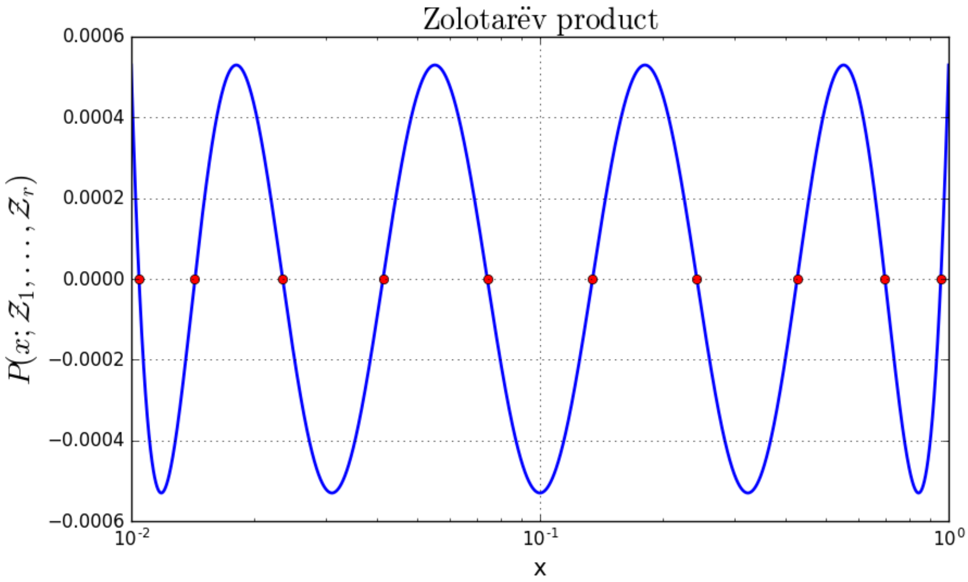


Figure 6: Zolotarëv points (red) with $r = 10$, $\delta = \frac{1}{100}$ and its associated Zolotarëv product (blue).

Proof. See [9] and [21]. ■

The Zolotarëv points cause the least deviation from zero on $[\delta, 1]$ among all functions of the form

$$P(x; \theta_1, ..., \theta_r) := \prod_{j=1}^{r} \frac{(x - \theta_j)}{(x + \theta_j)}.$$

As illustrated in figure 6 they are roughly geometrically distributed across the interior of the interval, getting denser at the boundary and cause a similar behavior we are familiar with from Chebyshev polynomials. The *Zolotarëv product* $P(x; \mathcal{Z}_1, ..., \mathcal{Z}_r)$ has exactly r roots and $r - 1$ local extrema in $[\delta, 1]$.

We are now interested in the value

$$E_r(\delta) := \max_{x \in [\delta, 1]} \prod_{j=1}^{r} \left| \frac{(x - \mathcal{Z}_j)}{(x + \mathcal{Z}_j)} \right|.$$

Theorem 6.12. *Let* $\delta \in (0, 1)$ *and define*

$$\mu = \left(\frac{1 - \sqrt{\delta}}{1 + \sqrt{\delta}} \right)^2 \qquad \mu_1 = \sqrt{1 - \mu^2} \qquad \rho = \exp\left(-\pi \frac{\bar{K}(\mu_1)}{\bar{K}(\mu)} \right).$$

Then the product

$$\prod_{n=1}^{\infty} (1 + \rho^{rn})^{(-1)^n}$$

converges for all $r \in \mathbb{N}$ *and*

$$E_r(\delta) = 2\rho^{\frac{r}{4}} \prod_{n=1}^{\infty} (1 + \rho^{rn})^{(-1)^n} \leq 2\rho^{\frac{r}{4}}.$$

Proof. See [10]. ■

Theorem 6.12 immediately provides an exponential decay of the error in r.

Corollary 6.13. *Let $\delta \in (0,1)$ and $r \in \mathbb{N}$. Then there holds*

$$\exists C \in \mathbb{R}^+ : \quad E_r(\delta) \preccurlyeq e^{-Cr},$$

whereas the involved constants only depend on δ.

Proof. Follows directly from Theorem 6.12. ■

Since we are now familiar with the solution of (6.11), results can be set in correspondence with the original min-max problem (6.10).

Lemma 6.14. *Let $r \in \mathbb{N}$, $\mathcal{Z}_j$, $j = 1, ..., r$, the Zolotarëv points (6.12) on $J_l = [a^{-1}, 1]$ for some $a > 1$ and further $J_r = [1, a]$. Then there holds*

$$\min_{\theta_1,\dots,\theta_r \in J_l} \max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{1-\theta_j x}{1+\theta_j x} \right| = \max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{1-\mathcal{Z}_j x}{1+\mathcal{Z}_j x} \right|.$$

Proof. Direct computations reveal

$$\begin{aligned} \max_{x \in J_l} \prod_{j=1}^{r} \left| \frac{x-\theta_j}{x+\theta_j} \right| &= \max_{x \in J_l} \prod_{j=1}^{r} \left| \frac{\frac{1}{x}(x-\theta_j)}{\frac{1}{x}(x+\theta_j)} \right| \\ &= \max_{x \in J_l} \prod_{j=1}^{r} \left| \frac{1-\theta_j \frac{1}{x}}{1+\theta_j \frac{1}{x}} \right| = \max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{1-\theta_j x}{1+\theta_j x} \right|. \end{aligned}$$

It follows that $\theta_1, .., \theta_r \in J_l$ minimize

$$\max_{x \in J_l} \prod_{j=1}^{r} \left| \frac{x-\theta_j}{x+\theta_j} \right|$$

if and only if they minimize

$$\max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{1-\theta_j x}{1+\theta_j x} \right|.$$

Theorem 6.11 concludes the proof. ■

Corollary 6.15. *Let $r \in \mathbb{N}$ and $\mathcal{Z}_j$, $j = 1, ..., r$, the Zolotarëv points (6.12) on J_l. Then*

$$\exists C \in \mathbb{R}^+ : \quad \max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{1-\mathcal{Z}_j x}{1+\mathcal{Z}_j x} \right| \preccurlyeq e^{-Cr},$$

whereas the involved constants only depend on $\lambda_{max}(M^{-1}A)$.

Proof. Combining the proof of Lemma 6.14 with Corollary 6.13 one obtains

$$\max_{x \in J_r} \prod_{j=1}^{r} \left| \frac{1-\mathcal{Z}_j x}{1+\mathcal{Z}_j x} \right| = \max_{x \in J_l} \prod_{j=1}^{r} \left| \frac{x-\mathcal{Z}_j}{x+\mathcal{Z}_j} \right| \preccurlyeq e^{-Cr}.$$

■

Optimal choice of $\mathcal{V}_r$

We return from the abstract setting to the original problem, finding an upper bound for (6.6). Define $\kappa := t^2$, $\kappa_j := t_j^2$, $x := \lambda^2$ and further $J_l := [\lambda_{max}^{-1}, 1]$, $J_r := [1, \lambda_{max}]$ in order to apply Lemma 6.7 to obtain

$$\forall \lambda \in \hat{\sigma}: \quad \left(\frac{1}{1+t^2\lambda^2} - \sum_{j=1}^{r} \hat{\alpha}_j \frac{1}{1+t_j^2\lambda^2} \right) \leq \frac{1}{1+t^2\lambda^2} \prod_{j=1}^{r} \left| \frac{(1-t_j^2\lambda^2)}{(1+t_j^2\lambda^2)} \right| . \tag{6.13}$$

At this point it becomes clear why the snapshots $t_1, ..., t_r$ have to be chosen with respect to the interval $\mathcal{I} = [\sqrt{\lambda_{max}^{-1}}, 1]$. In order to minimize deviation of the error product in (6.13) we need $1 - t_j^2\lambda^2 \approx 0$ and therefore $\frac{1}{t_j} \approx \lambda \in \hat{\sigma} = [1, \sqrt{\lambda_{max}}]$.

Lemma 6.14 suggests the choice of optimal sampling points t_j with the property $t_j^2 = \mathcal{Z}_j$. Along with this choice Corollary 6.15 guarantees

$$\exists C \in \mathbb{R}: \quad \prod_{j=1}^{r} \left| \frac{(1-t_j^2\lambda^2)}{(1+t_j^2\lambda^2)} \right| \preccurlyeq e^{-Cr} =: \Theta(r)$$

and therefore

$$\forall \lambda \in \hat{\sigma}: \quad \left(\frac{1}{1+t^2\lambda^2} - \sum_{j=1}^{r} \hat{\alpha}_j \frac{1}{1+t_j^2\lambda^2} \right) \preccurlyeq \frac{\Theta(r)}{1+t^2\lambda^2}. \tag{6.14}$$

Motivated by its induced (asymptotically) optimal convergence rate we define:

Definition 6.16. *A reduced space $\mathcal{V}_r = [v^*(t_0), ..., v^*(t_r)] \subseteq V_h$ is called optimal if and only if its snapshots $t_0, ..., t_r \in \mathcal{I}$ satisfy*

- $t_0 = 0$,
- $\forall j \in \{1, ..., r\}: \quad t_j^2 = \mathcal{Z}_j$ *with Zolotarëv points* $\mathcal{Z}_j$ *on* $[\lambda_{max}^{-1}, 1]$.

Summarizing the outcomes from above leads to the main result of this section.

Theorem 6.17. *Let $u \in V_h$, $t \in \mathbb{R}^+$ and $\mathcal{V}_r \subseteq V_h$ optimal. Then*

$$\forall r \in \mathbb{N}: \quad K_r^2(t,u) - K^2(t,u) \preccurlyeq \sum_{k=0}^{N} \frac{u_k^2}{1+t^2\lambda_k^2} \Theta^2(r), \tag{6.15}$$

whereas the involved constants only depend on $\lambda_{max}(M^{-1}A)$.

Proof. Theorem 6.6 together with (6.14) yields

$$\begin{aligned} K_r^2(t,u) - K^2(t,u) &\preccurlyeq \sum_{k=0}^{N} (1+t^2\lambda_k^2) \left(\frac{1}{1+t^2\lambda_k^2} \right)^2 \Theta^2(r) u_k^2 \\ &= \sum_{k=0}^{N} \frac{u_k^2}{1+t^2\lambda_k^2} \Theta^2(r). \end{aligned}$$

■

6.1.2 Error estimates with optimal sampling points

Section 6.1.1 procures an upper bound for the error in the reduced basis K-functional. It immediately follows

$$\begin{aligned} 0 \leq \|u\|_{B_r^s}^2 - \|u\|_{B^s}^2 &= \int_0^\infty t^{-2s-1}(K_r^2(t,u) - K^2(t,u))\,dt \\ &\preccurlyeq \sum_{k=0}^{N} \Theta^2(r) u_k^2 \int_0^\infty t^{-2s-1} \frac{1}{1+t^2\lambda_k^2}\,dt. \end{aligned}$$

The problem is that for any $s \in (0,1)$

$$\forall t \in (0,1]: \quad \frac{t^{-2s-1}}{1+t^2\lambda_k^2} = \frac{1}{t^{2s+1}(1+t^2\lambda_k^2)} \geq \frac{1}{t(1+t^2\lambda_k^2)},$$

such that

$$\lim_{\varepsilon\to 0} \int_\varepsilon^1 t^{-2s-1} \frac{1}{1+t^2\lambda_k^2}\,dt \geq \lim_{\varepsilon\to 0} \int_\varepsilon^1 \frac{1}{t(1+t^2\lambda_k)}\,dt = \infty.$$

It follows that the integral

$$\int_0^1 t^{-2s-1} \frac{1}{1+t^2\lambda_k^2}\,dt$$

does not exist, while

$$\int_1^\infty \frac{1}{t^{2s+1}(1+t^2\lambda_k^2)}\,dt \leq \int_1^\infty \frac{1}{t(1+t^2\lambda_k^2)}\,dt \leq \frac{1}{\lambda_k^2} \int_1^\infty \frac{1}{t^3}\,dt < \infty.$$

We conclude that estimate (6.15) is sharp enough for $t \in [1,\infty)$ but not for the case $t < 1$. This issue can be overwhelmed by taking $v^*(t_0)$ in the rational interpolation problem from Lemma 6.7 into account. By similar techniques we derive another interpolant to gain convergence on $(0,1)$.

Theorem 6.18. *Under the same assumptions of Theorem 6.17 there holds*

$$\forall r \in \mathbb{N}: \quad K_r^2(t,u) - K^2(t,u) \preccurlyeq \sum_{k=0}^{N} \frac{t^4\lambda_k^4}{1+t^2\lambda_k^2} \Theta^2(r) u_k^2,$$

whereas the involved constants only depend on $\lambda_{max}(M^{-1}A)$.

Proof. The proof follows the outline of section 6.1.1. Once more we aim to find an interpolant, such that (6.6) becomes small, but this time with respect to a slightly adapted interpolation problem without requiring $\alpha_0 = 0$. The problem reads as: For $\kappa_0 = 0$ and given $\kappa, \kappa_1, ..., \kappa_r \in J_l$ find $q \in \hat{\mathcal{R}}$ with

$$\hat{\mathcal{R}} := \left[\left\{ f(x) = \frac{1}{1+\kappa_j x} \,\middle|\, j = 0, ..., r \right\}\right],$$

such that

$$\begin{aligned} \forall i \in \{1, ..., r\}: \quad q\left(\frac{1}{\kappa_i}\right) &= g_\kappa\left(\frac{1}{\kappa_i}\right), \\ q(0) &= g_\kappa(0). \end{aligned}$$

The solution

$$q(x) = \sum_{j=0}^{r} \alpha_j \frac{1}{1+\kappa_j x} \in \hat{\mathcal{R}}$$

satisfies

$$g_\kappa(x) - q(x) = \frac{1}{1+\kappa x} - \alpha_0 - \sum_{j=1}^{r} \alpha_j \frac{1}{1+\kappa_j x} = \frac{\hat{p}(x)}{(1+\kappa x)\prod_{j=1}^{r}(1+\kappa_j x)}$$

for some $\hat{p} \in \Pi_{r+1}$. One ascertains that

$$\hat{p}(x) = C(\kappa)x \prod_{j=1}^{r}(1-\kappa_j x) \qquad \text{with} \qquad C(\kappa) = \kappa \prod_{j=1}^{r} \frac{\kappa - \kappa_j}{\kappa + \kappa_j}.$$

It follows for all $x \in J_r$

$$|g_\kappa(x) - q(x)| = \frac{\kappa x}{1+\kappa x} \prod_{j=1}^{r} \left| \frac{(\kappa - \kappa_j)}{(\kappa + \kappa_j)} \frac{(1-\kappa_j x)}{(1+\kappa_j x)} \right| \leq \frac{\kappa x}{1+\kappa x} \prod_{j=1}^{r} \left| \frac{(1-\kappa_j x)}{(1+\kappa_j x)} \right|.$$

The rest follows analogously to the previous case. ■

This time we obtain

$$\begin{aligned}
\|u\|^2_{B^s_r} - \|u\|^2_{B^s} &\preccurlyeq \sum_{k=0}^{N} \Theta^2(r) u_k^2 \int_0^\infty t^{-2s-1} \frac{t^4 \lambda_k^4}{1+t^2\lambda_k^2}\, dt \\
&= \sum_{k=0}^{N} \Theta^2(r) u_k^2 \int_0^\infty \frac{t^{3-2s}\lambda_k^4}{1+t^2\lambda_k^2}\, dt.
\end{aligned}$$

Even though the integral

$$\int_0^\infty \frac{t^{3-2s}\lambda_k^4}{1+t^2\lambda_k^2}\, dt$$

does not exist, we gain convergence for $t < 1$, since

$$\begin{aligned}
\int_0^1 \frac{t^{3-2s}\lambda_k^4}{1+t^2\lambda_k^2}\, dt &\leq \int_0^1 \frac{t^3\lambda_k^4}{1+t^2\lambda_k^2}\, dt \\
&\leq \int_0^1 \frac{t^3\lambda_k^4}{t^2\lambda_k^2}\, dt = \lambda_k^2 \int_0^1 t\, dt < \infty.
\end{aligned}$$

In conclusion we have aimed to establish two different interpolants in order to bound the error in K_r^2 on $(0,1)$ and $[1,\infty)$ separately, finally guaranteeing exponential convergence for the reduced basis interpolation norm.

Theorem 6.19. *Let $u \in V_h$ and $\mathcal{V}_r \subseteq V_h$ optimal. Then*

$$\forall r \in \mathbb{N}\, \exists C \in \mathbb{R}^+ : \quad \|u\|^2_{B^s_r} - \|u\|^2_{B^s} \preccurlyeq \|u\|^2_{H^1} e^{-Cr},$$

whereas the involved constants only depend on $\lambda_{max}(M^{-1}A)$.

Proof. Theorems 6.17 and 6.18 conclude

$$\|u\|_{H_r^s}^2 - \|u\|_{H^s}^2 \preccurlyeq \sum_{k=0}^{N} \left(\int_0^1 \frac{t^{3-2s}\lambda_k^4}{1+t^2\lambda_k^2} \Theta^2(r)\, dt\, u_k^2 + \int_1^\infty \frac{t^{-2s-1}}{1+t^2\lambda_k^2} \Theta^2(r)\, dt\, u_k^2 \right).$$

Substituting with $\tau = t\lambda_k$ we obtain

$$\begin{aligned}
\|u\|_{H_r^s}^2 - \|u\|_{H^s}^2 &\preccurlyeq \sum_{k=0}^{N} u_k^2 \left(\int_0^{\lambda_k} \frac{\tau^{3-2s}\lambda_k^{2s-3}\lambda_k^4}{1+\tau^2} \Theta^2(r) \frac{d\tau}{\lambda_k} + \int_{\lambda_k}^\infty \frac{\tau^{-2s-1}\lambda^{2s+1}}{1+\tau^2} \Theta^2(r) \frac{d\tau}{\lambda_k} \right) \\
&= \sum_{k=0}^{N} \lambda_k^{2s}\Theta^2(r) u_k^2 \int_0^{\lambda_k} \frac{\tau^{3-2s}}{1+\tau^2}\, d\tau + \lambda_k^{2s}\Theta^2(r) u_k^2 \int_{\lambda_k}^\infty \frac{\tau^{-2s-1}}{1+\tau^2}\, d\tau \\
&\le \sum_{k=0}^{N} \lambda_k^{2s}\Theta^2(r) u_k^2 \left(\int_0^{\lambda_k} \frac{\tau^{3-2s}}{\tau^2}\, d\tau + \int_{\lambda_k}^\infty \frac{\tau^{-2s-1}}{\tau^2}\, d\tau \right) \\
&= \sum_{k=0}^{N} \lambda_k^{2s}\Theta^2(r) u_k^2 \left(\int_0^{\lambda_k} \tau^{1-2s}\, d\tau + \int_{\lambda_k}^\infty \tau^{-2s-3}\, d\tau \right) \\
&= \sum_{k=0}^{N} \lambda_k^{2s}\Theta^2(r) u_k^2 \left(\lambda_k^{2-2s} - \lambda_k^{-2s-2} \right) \\
&= \sum_{k=0}^{N} \Theta^2(r) u_k^2 \left(\lambda_k^{2} - \lambda_k^{-2} \right) \\
&\le \sum_{k=0}^{N} \Theta^2(r) u_k^2 \lambda_k^2 = \Theta^2(r)\|u\|_{H^1}^2.
\end{aligned}$$

■

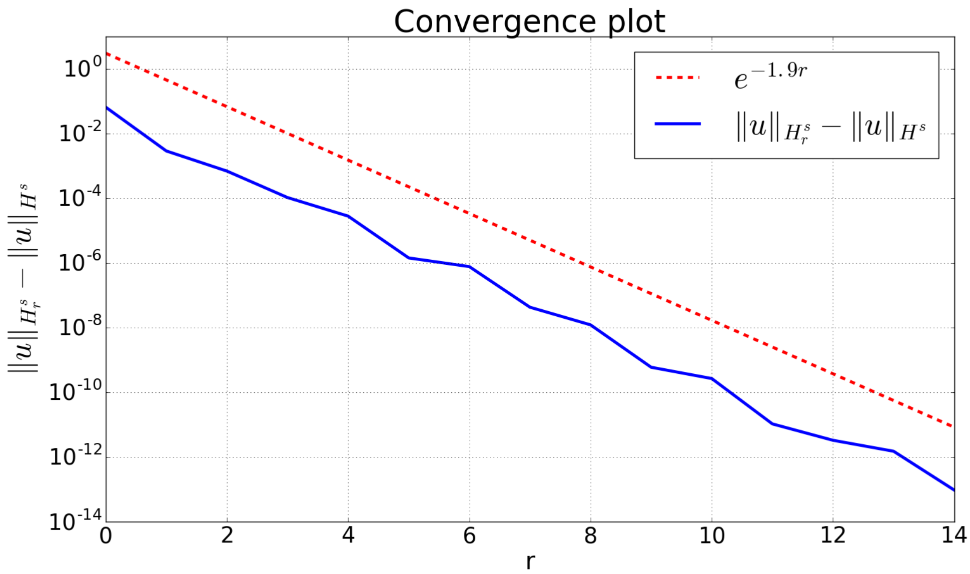


Figure 7: Convergence plot of the error in the reduced basis norm.

A numerical example is performed in order to testify analytical results. Consider the function

$$u = \sum_{k=0}^{m} z_k$$

for some $m < N$ and eigenfunctions $(z_k)_{k=0}^m$ of (6.1). We study the convergence rate of $\|u\|_{H_r^s}$ for increasing r. Due to Theorem 4.17 the value $\|u\|_{H_m^s}$ can be taken as exact reference. As illustrated in figure 7, exponential convergence is confirmed.

6.2 Error estimates for fractional operators

The reduced basis norm satisfies exponential convergence rates in r, granting good chances that the same holds for the induced operator. Indeed, convergence behavior for the operator directly follows from the previous section.

Theorem 6.20. *Let $u \in V_h$ and $\mathcal{V}_r \subseteq V_h$ optimal. Then for all $r \in \mathbb{N}$ there exists a constant $C \in \mathbb{R}^+$, such that*

$$\forall w \in V_h\colon \quad |\langle w, u\rangle_{B^s_{r(u)}} - \langle w, u\rangle_{B^s}| \preccurlyeq \|w\|_{H^1}\|u\|^2_{H^1} e^{-Cr},$$

whereas the involved constants only depend on $\lambda_{max}(M^{-1}A)$.

Proof. Due to Lemma 5.3 the operator error $\langle w, u\rangle_{B^s_{r(u)}} - \langle w, u\rangle_{B^s}$ has the following form

$$\underline{w}^T M \left(\int_0^\infty t^{-2s-1} \left[V_r(I_r - (I_r + t^2 A_r)^{-1}) V_r^T - M^{-1} + (M + t^2 A)^{-1} \right] dt \right) M\underline{u}.$$

One ascertains that the first term cancels out the third.

$$\begin{aligned} \underline{w}^T M \left(V_r V_r^T - M^{-1} \right) M\underline{u} &= \underline{w}^T \left(M V_r V_r^T M V_r \underline{\underline{u}} - M\underline{u} \right) \\ &= \underline{w}^T (M V_r \underline{\underline{u}} - M\underline{u}) = \underline{w}^T (M\underline{u} - M\underline{u}) = 0. \end{aligned}$$

Computations of the remaining terms reveal

$$\underline{w}^T \left[-M V_r (I_r + t^2 A_r)^{-1} V_r^T M \underline{u} + M (M + t^2 A)^{-1} M \underline{u} \right] = \underline{w}^T \left[-M \underline{v}_r^* + M \underline{v}^* \right].$$

All together this yields

$$\begin{aligned} \langle w, u\rangle_{B^s_{r(u)}} - \langle w, u\rangle_{B^s} &= \underline{w}^T \left(\int_0^\infty t^{-2s-1} \left(M\underline{v}^*(t) - M\underline{v}_r^*(t) \right) dt \right) \\ &= \int_0^\infty t^{-2s-1} \underline{w}^T M \left(\underline{v}^*(t) - \underline{v}_r^*(t) \right) dt \\ &= \int_0^\infty t^{-2s-1} \langle w, v^*(t) - v_r^*(t)\rangle_{L_2} \, dt. \end{aligned}$$

Together with the Cauchy-Schwarz inequality one obtains

$$\begin{aligned} |\langle w, u\rangle_{B^s_{r(u)}} - \langle w, u\rangle_{B^s}| &\leq \int_0^\infty t^{-2s-1} |\langle w, v^*(t) - v_r^*(t)\rangle_{L_2}| \, dt \\ &\leq \int_0^\infty t^{-2s-1} \|w\|_{L_2} \|v^*(t) - v_r^*(t)\|_{L_2} \, dt. \end{aligned}$$

Due to remark 6.5 there holds for all $t \in \mathbb{R}^+$

$$\|v^*(t) - v_r^*(t)\|_{L_2} \leq \|v^*(t) - v_r^*(t)\|_{L_2} + t^2\|v^*(t) - v_r^*(t)\|_{H^1} = K_r^2(t,u) - K^2(t,u)$$

and thus

$$\begin{aligned} |\langle w, u\rangle_{B^s_{r(u)}} - \langle w, u\rangle_{B^s}| &\leq \|w\|_{L_2} \int_0^\infty t^{-2s-1} \left(K_r^2(t,u) - K^2(t,u)\right) dt \\ &= \|w\|_{L_2}(\|u\|^2_{B^s_r} - \|u\|^2_{B^s}) \\ &\preccurlyeq \|w\|_{H^1}\|u\|^2_{H^1} e^{-Cr}. \end{aligned}$$

■

Remark 6.21. *Due to equivalence of the norms, convergence analysis from above also holds for the Hilbert case.*

7 Numerical examples

In the subsequent, tools provided in previous chapters are examined and testified by means of the open source finite element packages Netgen and NGSolve, see [14] and [15]. Consider the Fractional Cahn-Hilliard Equation from chapter 2 on $\Omega = [-\pi, \pi]^2$:

$$\begin{aligned}
\forall (x,t) \in \Omega \times (0,T]: \quad & \frac{\partial u}{\partial t}(x,t) + (-\Delta)^s(-\varepsilon^2 \Delta u(x,t) + f(u(x,t))) = 0, \\
\forall t \in (0,T]: \quad & u(.,t) \text{ is } 2\pi\text{-periodic}, \\
\forall x \in \Omega: \quad & u(x,0) = u_0(x),
\end{aligned}$$

with $f(u) = u^3 - u$ and its weak formulation: Find $u \in L_2([0,T], H^{1+s}_{per}(\Omega))$, satisfying

$$\forall v \in H^{1+s}_{per}(\Omega): \quad \langle \frac{\partial u}{\partial t}, v\rangle_{L_2} + \langle \varepsilon^2 (-\Delta)^{\frac{1+s}{2}} u, (-\Delta)^{\frac{1+s}{2}} v\rangle_{L_2} + \langle f(u), (-\Delta)^s v\rangle_{L_2} = 0, \tag{7.1}$$

such that initial conditions are satisfied. Finite element discretization results in the system of ODEs

$$\begin{aligned}
& M\underline{u}' + \varepsilon^2 M(M^{-1}\widehat{A})^{1+s}\underline{u} + M(M^{-1}\widehat{A})^s F(\underline{u}) = 0 \\
\iff \quad & \underline{u}' + \varepsilon(M^{-1}\widehat{A})^{1+s}\underline{u} + (M^{-1}\widehat{A})^s F(\underline{u}) = 0.
\end{aligned} \tag{7.2}$$

This system can be solved efficiently by so called splitting methods in which the non-linear operator is decoupled from the regular Laplacian. The linear parabolic equation is solved directly on the low dimensional reduced space, while the nonlinear equation is treated with an explicit time stepping method.

7.1 Splitting methods

We give a short introduction to fundamental concepts of splitting methods, justifying the further course of action. Consider the ordinary differential equation

$$u' + Au + Bu = 0 \tag{7.3}$$

with initial condition $u'(0) = u_0$ and linear operators A and B. By means of the matrix exponential function the solution of (7.3) is given by

$$u(t) = e^{-t(A+B)}u_0.$$

The concept of splitting methods is based on the consideration

$$e^{-t(A+B)}u_0 \approx e^{-tA}e^{-tB}u_0,$$

referring to the combined evolution of the simpler equations

$$u' + Au = 0 \qquad u' + Bu = 0.$$

Only for commutating operators this leads to the exact evolution of (7.3), otherwise one can show that

$$e^{-\tau(A+B)}u_0 - e^{-\tau A}e^{-\tau B}u_0 = \mathcal{O}(\tau^2)$$

for general bounded operators A and B. Theory becomes more difficult as soon as nonlinear or rather unbounded operators are included, nevertheless basic concepts remain the same.

7.1.1 Lie-Trotter splitting for FCHE

We apply the approach from above to (7.2) in its simplest form by means of Lie-Trotter splitting techniques. Decoupling of the equations leads to the linear, parabolic ODE

$$\underline{u}' + \varepsilon^2 (M^{-1}\widehat{A})^{1+s}\underline{u} = 0$$

and its nonlinear pendant

$$\underline{u}' + (M^{-1}\widehat{A})^{s} F(\underline{u}) = 0.$$

We establish the reduced basis approximations

$$\underline{u}' + \varepsilon^2 (M^{-1}\widehat{A})_r^{1+s}\underline{u} = 0, \tag{7.4a}$$

$$\underline{u}' + (M^{-1}\widehat{A})_r^{s} F(\underline{u}) = 0. \tag{7.4b}$$

The solution $\underline{u}(t)$ of (7.4a) is given by the matrix exponential function

$$\underline{u}(t) = \exp(-t\varepsilon^2 (M^{-1}\widehat{A})_r^{1+s})\underline{u}_0$$

and can be computed exactly on the low dimensional space $\mathcal{V}_r$. One observes

$$\begin{aligned} \underline{u}' + \varepsilon^2 (M^{-1}\widehat{A})_r^{1+s}\underline{u} = 0 \iff & \underline{u}' + \varepsilon^2 V_r \widehat{A}_r^{1+s} V_r^T M \underline{u} = 0 \\ \iff & V_r \underline{\underline{u}}' + \varepsilon^2 V_r \widehat{A}_r^{1+s} V_r^T M V_r \underline{\underline{u}} = 0. \end{aligned}$$

Multiplication $V_r^T M$ form the left together with $M_r = V_r^T M V_r = I_r$ yields

$$\begin{aligned} \underline{u}' + \varepsilon^2 (M^{-1}\widehat{A})_r^{1+s}\underline{u} = 0 \iff & \underline{\underline{u}}' + \varepsilon^2 \widehat{A}_r^{1+s} \underline{\underline{u}} = 0 \\ \iff & \underline{\underline{u}}' + \varepsilon^2 Z_r \Lambda_r^{1+s} Z_r^T \underline{\underline{u}} = 0. \end{aligned}$$

The exact flow of this ODE on $\mathcal{V}_r$ is given by

$$\underline{\underline{u}}(t) = \exp(-t\varepsilon^2 Z_r \Lambda_r^{1+s} Z_r^T)\underline{\underline{u}}_0 = Z_r \exp(-t\varepsilon^2 \Lambda_r^{1+s}) Z_r^T \underline{\underline{u}}_0.$$

There is now need to apply time stepping methods: The reduced basis operator projects the entire ODE to the low dimensional space where the exact evolution can be determined by means of the small eigen-system on $\mathcal{V}_r$.

For the nonlinear ODE (7.4b) time stepping methods are required, giving rise to the question whether explicit or implicit techniques should be deployed. The fractional Laplacian suggests an implicit procedure, requiring the solutions of nonlinear equations or rather an explicit representation of the matrix

$$(M^{-1}\widehat{A})_{r(\cdot)}^{s}$$

independent of its input argument. This can not be provided by the tools established in previous chapters. In order to overcome this inconvenience as well as the non-linearity of the operator $F(\cdot)$ we will consider explicit schemes only. The most simple procedure to do so is given by the explicit Euler method

$$\frac{\underline{u}_{n+1} - \underline{u}_n}{\tau} + (M^{-1}\widehat{A})_r^{s} F(\underline{u}_n) = 0 \iff \underline{u}_{n+1} = \underline{u}_n - \tau (M^{-1}\widehat{A})_r^{s} F(\underline{u}_n).$$

The approach from above is summarized in the following way. For given $\underline{u}_n \approx \underline{u}(t_n)$ and time step $\tau > 0$ generate $\underline{u}_{n+1}$ by

- computing
$$\underline{\tilde{u}}_{n+1} = V_r Z_r \exp(-\tau\varepsilon^2 \Lambda^{1+s}) Z_r^T V_r^T M \underline{u}_n,$$
- applying an explicit Euler step to obtain
$$\underline{u}_{n+1} = \underline{\tilde{u}}_{n+1} - \tau (M^{-1}\widehat{A})_r^{s} F(\underline{\tilde{u}}_{n+1}).$$

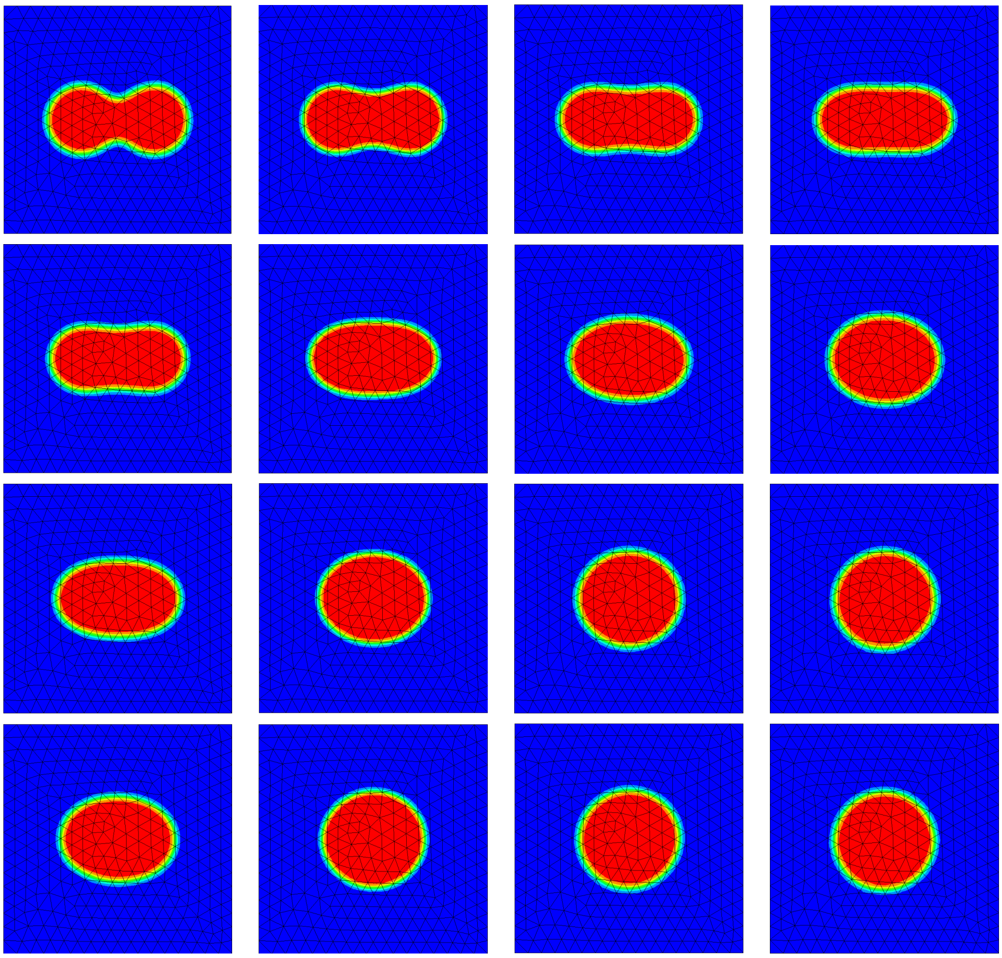
7.2 Mass preservation on the reduced space

Before the first experiment is performed, some further theoretical considerations need to be taken into account. Analogously to Lemma 2.3 mass conservation is also valid for the finite element setting. The choice $v \equiv 1 \in V_h \subseteq H^1_{per}(\Omega)$ ensures that the solution $u \in V_h$ satisfies

$$\frac{\partial}{\partial t} \int_{\Omega} u(x,t)\, dx = 0.$$

In general this does not hold for the reduced space case. If constant functions are not contained, the choice $v \equiv 1$ is not feasible, yielding that the Fractional Cahn-Hilliard Equation does not preserve mass on $\mathcal{V}_r$. Problems of this kind can be easily dispatched by extending the reduced basis by a constant function, ensuring that mass conservation is obtained.

We are finally able to conduct a first numerical example in order to verify considerations from above and test the reliability of our implementation.



(a) $s = 0.1$ (b) $s = 0.3$ (c) $s = 0.5$ (d) $s = 0.7$

Figure 8: Evolution of the solution of FCHE for different fractional powers s with $\dim(\mathcal{V}_r) = 9$, including constant functions, and initial condition u_0. Configurations from top to bottom at $t = 5, 20, 50, 80$.

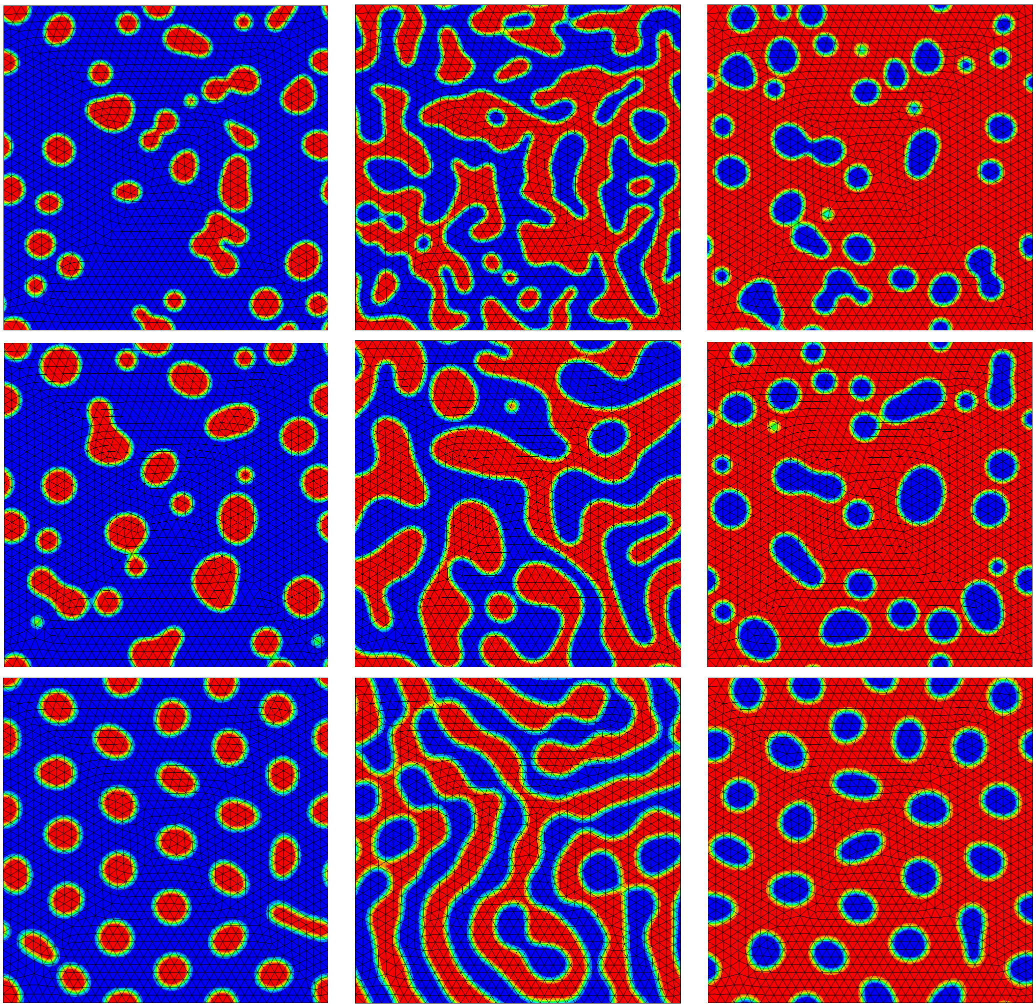
Example: We simulate the fusion of two tangential bubbles, represented by the initial condition

$$u_0(x) = \begin{cases} 1, & \text{if } (x+1)^2 + y^2 \leq 1 \quad \text{or} \quad (x-1)^2 + y^2 \leq 1 \\ -1, & \text{else} \end{cases}$$

with $\varepsilon = \frac{1}{10}$. The impact of changing fractional powers on the solution's characteristic is illustrated in figure 8. For all $s \in (0, 1]$ mass conservation can be observed. In all conducted tests both bubbles merge to one large circular shape, such that a steady state is obtained. The rate at which this stationary state is achieved differs in the value of s. The larger s the faster transition takes place. This phenomenon is plausible since the proof of Lemma 2.6 suggests that the rate of change in the energy increases for raising fractional orders.

7.3 Coarsening dynamics of FCHE

Phase separation of a perturbed binary mixture, such as oil droplets in water, is simulated.



(a) $\phi = 0.25$ (b) $\phi = 0.5$ (c) $\phi = 0.75$

Figure 9: Solutions of FCHE for various configurations ϕ and fractional orders s at $T = 5$ with the same random initial perturbation and $\varepsilon = \frac{4}{100}$. Top to bottom: $s = 0.2, 0.5, 0.8$.

Example: Consider a binary alloy set to a constant state $\bar{u} = 1 - 2\phi$ endued with a uniform disturbance in $[-0.2, 0.2]$. The coarsening dynamics is surveyed with respect to the exponent s and the composition ϕ in figure 9.

Similar behaviors can be observed for $\phi = 0.25$ and $\phi = 0.75$. The respective components tend to form circular shaped droplets while in the case of equally composed mixtures an even behavior is studied. Small fractional powers refer to rather subtle formations, whereas large s come along with more connected and structured forms. Similar results have been observed in [1].

8 Conclusion and outlook

Summary

In this thesis an alternative approach for fractional diffusion operators has been established. We have considered two different approaches for space interpolation with respect to the Hilbert interpolation couple $(L_2(\Omega), H^1(\Omega))$ in a finite element setting. The Banach setting gives rise to a natural choice of a reduced space $\mathcal{V}_r$, providing all the essential information in order to introduce the reduced basis norm. Along with an optimal choice of the sampling points exponential convergence in $\dim(\mathcal{V}_r)$ has been proofed. Computations are carried out in the Hilbert space setting, such that only a small eigen-system has to be determined.

The reduced basis interpolation norms induce fractional operators, providing computationally appealing approximations for the associated fractional operator actions. Again, exponential convergence rates are confirmed. An efficient interaction between reduced basis operators and the matrix exponential function has been deployed. This enables us to project arising linear, parabolic ODEs to the low dimensional space $\mathcal{V}_r$, where they are solved exactly.

Outlook

The present construction of the reduced space involves the choice of sampling points $t_j \in \mathcal{I}$ by means of the Zolotarëv points. This approach does not respect any hierarchical structures, making manipulations of both r and mesh-size h computationally costly. One could aim to derive an adapted selection procedure which provides successive composition of the reduced basis, granting that computations can be spared as dimension of $\mathcal{V}_r$ increases or substantial manipulations in h are performed.

Moreover, it is desirable to examine our approach in context with other differential operators, equations and higher dimensions. All of this requires the coupling of the deployed reduced basis method with feasible preconditioners, being of great interest for further experiments.

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