REDUCED BASIS METHOD FOR PARAMETER FUNCTIONS WITH APPLICATION IN QUANTUM MECHANICS

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Often Quantum systems are studied under isolated conditions. However, the influence of external potentials on quantum systems are of major interest, both for quantum physics and quantum chemisty. For instance, controlling chemical reactions leads to a PDE constrained bilinear optimal control problem, where the the external potential arises in the time-dependent linear Schrödinger equation as a reaction term, or more precisely: Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary, $\mathscr{I} := (0,T)$ a time interval and $\mu_d \in L_2(\Omega,\mathbb{C})$ a desired state. Then, following [1], for suitable seperable Hilbert spaces $\mathscr{X}$ and $\mathscr{P}$, the PDE constrained bilinear optimal control problem reads:

$$\min_{(\psi,\mu)\in(\mathscr{X},\mathscr{P})} J(\psi,\mu) = \frac{1}{2}\|\psi(T,x)-\mu_d\|^2_{L_2(\Omega,\mathbb{C})} + \frac{\alpha}{2}\|\mu\|^2_{\mathscr{P}}$$

such that $(\psi,\mu) \in (\mathscr{X},\mathscr{P})$ solves

$$\mathrm{i}\,\partial_t\psi(t,x) = -\frac{1}{2}\Delta_x\psi(t,x) + \mu(t,x)\psi(t,x) + g(t,x), \qquad (t,x) \in \mathscr{I}\times\Omega$$

together with suitable boundary conditions. Aim of this project is to solve the PDE constrained bilinear optimal control problem in a real-time context by reducing the so called *control-to-state operator* within the *Reduced Basis Method* (RBM), where the external potential is interpreted as a variable reaction coefficient and therefore - in the language of the RB theory - as a parameter function. Typically, in the theory of the RBM the parameter space $\mathscr{P}$ is given by a finite-dimensional subset of $\mathbb{R}^P$, $P \in \mathbb{N}$. However, in our case it holds $\dim(\mathscr{P}) = \infty$. While finite-dimensional parameter spaces have been extendively studied in recent decades, there has been done little work on the infinite-dimensional setting so far. First progress in this direction has been made by [3], where the initial condition of a parabolic partial differential equation is interpreted as a parameter function. The main idea used in [3] is to split the problem into two subproblems and dealing with this subproblems by using a so called *Two-Step-Greedy-Algorithm*. However, since the parameter function arises in the reaction term this approach is not employable in our case.

It is well-known that if the constrained equation is well-posed according to the Banach-Nĕcas theorem we get both, the existence of an optimal control and the existence of a control-to-state operator. In our work we want to consider a space-time variational formulation of the constrained equation. Although there are existing many well-posedness results for the Schrödinger equation in the literature, see e.g. [2], all results, known to us, provide no basis to construct a well-posed space-time variational formulation according to the Banach-Nĕcas theorem. In this talk we want to present a well-posedness result, which provides a basis for a well-posed space-time variational formulation, along with the theory of dealing with parameter function arising as coefficient varaibles. Numerical experiments according to a stable space-time finite element discretization will be also presented.

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References

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