TECHNISCHE UNIVERSITÄT CHEMNITZ

Faculty of Mathematics
Research Group Numerical Mathematics
(Partial Differential Equations)

TU Chemnitz · Faculty of Mathematics · 09107 Chemnitz, Germany

Building: Reichenhainer Straße 41
Room: 41/604
Phone: +49 371 531-22530
Fax: +49 371 531-836538
E-Mail: roland.herzog@mathematik.tu-chemnitz.de
Internet: http://www.tu-chemnitz.de/mathematik/part_dgl

Place, Date: Chemnitz, 18/8/2020

Report on the Dissertation

Krylov Subspace Methods – Analysis and Application

by Tomáš Gergelits

Summary and Main Contributions

The thesis submitted by Tomáš Gergelits considers the solution of linear second-order partial differential equations governed by the differential operators $-\operatorname{div}(k \operatorname{grad})$ and $-\operatorname{div}(K \operatorname{grad})$ with homogeneous Dirichlet boundary conditions. These operators are ubiquitous in computational science and their study is a fundamental problem in partial differential equations and numerical analysis.

Usually k and K are positive, essentially bounded scalar or symmetric matrix-valued coefficient functions on the domain of interest. These differential operators generate norms which are equivalent to the norm induced by the standard Laplace problem obtained by setting $k \equiv 1$ and $K \equiv \operatorname{id}$, respectively. The same is true for Galerkin approximations, such as those arising from conforming finite element discretizations. It is therefore straightforward to obtain bounds in the spectrum of the Poisson-preconditioned operators, both in the continuous and discrete settings.

That said, the author is the first to analyze *precisely* the spectrum of the Poisson-preconditioned operators, both in the infinite dimensional and discrete settings. The results obtained are truly remarkable and serve as the basis for further investigations by the author, such as the convergence behavior of the preconditioned Krylov subspace methods for self-adjoint problems, notably the conjugate gradient method.

Detailed Report

The dissertation thesis consists of five chapters and is accompanied by two scientific papers [1, 2], both published in the prestigious SIAM Journal on Numerical Analysis. Chapter 1 gives a brief introduction into the topic and provides an overview over the content of the dissertation. Chapter 2 reviews the conjugate gradient Krylov subspace method for self-adjoint, positive definite systems $\mathcal{A}x = b$ in general Hilbert spaces with an emphasis on the highly non-trivial implications of finite precision arithmetic. In particular, Section 2.5 focuses on a third paper co-authored by the candidate, which relates quantities of the conjugate gradient and minimal residual methods in finite precision computation.

Chapter 3 reviews the results of [1], where the problem $-\operatorname{div}(k \operatorname{grad})$ with diffusion coefficient k essentially bounded and bounded away from zero is considered, preconditioned by the Laplace operator. The focus in this chapter is on discrete problems, with an emphasis on discretizations whose basis functions have local support, as it is the case for finite element discretizations. The main result is that the eigenvalues of the discrete, preconditioned operator are in one-to-one correspondence with the range of values of the coefficient function k, restricted to the support to one of the local basis functions (Theorem 3.1.1). The result can be further strengthened (Theorem 3.1.4) in case of piecewise linear basis functions. The proofs are based on a clever combination of perturbation theory for symmetric eigenvalue problems and Hall's theorem for bipartite graphs. As an extension to the results in [1], the author provides further improvements and an alternative proof of Theorem 3.1.4 in Section 3.3.

Chapter 4 reviews the results of [2], which is devoted to the operator $-\operatorname{div}(K \operatorname{grad})$ where K is an essentially bounded, symmetric matrix-valued diffusion coefficient. The Laplacian serves as preconditioner also here. In the continuous setting, it turns out that the spectrum of the preconditioned operator is *equal* to the interval formed by the maximum respectively minimum of the extremal eigenvalues of K across the domain (Theorem 4.1.1). An assumption of positive definiteness of K is not required. An interesting consequence of Theorem 4.1.1 is that the spectrum is unaffected by pointwise orthogonal transformation of the diffusion matrix function K. A number of open problems related to this observation is formulated. An extension of Theorem 3.1.1 studying the discrete setting in the case of a matrix-valued coefficient is provided in Theorem 4.1.3. The proof follows the same steps as the proof of Theorem 3.1.1 but it is technically more involved. Interestingly, this matrix-valued case allows a much less accurate localization of the discrete eigenvalues.

Conclusions are drawn in Chapter 5 and a number of open questions are raised, which provide directions to areas of possible further research.

Summary and Evaluation

The dissertation submitted by Tomáš Gergelits is primarily based on two peer-reviewed publications in the top-tier SIAM Journal on Numerical Analysis. The results obtained in those articles are groundbreaking since they provide, for the first time, an analysis of the entire spectrum of an important class of infinite dimensional partial differential operators, as well as their discretized, finite element counterparts. It is the reviewer's belief that these results will open up a whole new field of investigation in the active research area on the preconditioned solution of partial differential equations by Krylov subspace methods in the near future.

Altogether, Tomáš Gergelits demonstrates in his thesis his ability for creative scientific work of the highest quality. The thesis as well as the articles accompanying it are very well written, nicely illustrated and I found only very few possibilities for improvements of the presentation.

I therefore strongly recommend acceptance of the thesis.

Roland Herzog

References

[1] Tomáš Gergelits, Kent-André Mardal, Bjørn Fredrik Nielsen, and Zdeněk Strakoš. Laplacian preconditioning of elliptic PDEs: localization of the eigenvalues of the discretized operator. *SIAM Journal on Numerical Analysis*, 57(3):1369–1394, 2019.

[2] Tomáš Gergelits, Bjørn Fredrik Nielsen, and Zdeněk Strakoš. Generalized Spectrum of Second Order Differential Operators. *SIAM Journal on Numerical Analysis*, 58(4):2193–2211, 2020.