Algebraic Error in Matrix Computations in the Context of Numerical Solution of Partial Differential Equations

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This thesis presents an investigation of the role played by the algebraic error in the numerical solution of partial differential equations, that is, the error which arises from the solution of the underlying algebraic equations (as distinct from discretisation errors incurred by transferring from the continuous PDE to a finite-dimensional grid-based representation). The role of algebraic errors in the solution of PDEs is a topic which has been gaining increasing attention from researchers in recent years and this thesis makes a valuable contribution to current developments. The ideas discussed are of practical importance in this area and will certainly be of interest to those working on developing efficient algorithms, with particular reference to adaptive grid generation.

After a brief introduction, the bulk of Chapter 2 is formed by a paper entitled "Distribution of discretization and algebraic error in numerical solution of partial differential equations" which has been published in the journal *Linear Algebra and its Applications.* In the past, it has largely been assumed that algebraic and discretisation errors will have a similar spatial profile, with the latter dominating the overall error. Here the authors present some examples which show that this is not always the case and that, in fact, the algebraic error can have large local components which affect the final error profile significantly. This is supported by some additional results in the subsequent sections in Chapter 2 (using more complicated test problems representing inhomogeneous tensors). The third chapter focusses on a particular interpretation of the algebraic error relating to traditional backward error analysis from numerical linear algebra. The transformations of the discrete basis functions are investigated in this context, and there is a discussion for the implications in terms of discrete Green's functions. There is also a discussion of how Fréchet derivatives can be used to estimate the algebraic error, and the chapter concludes with some numerical experiments to support these ideas. Chapter 4 consists largely of a paper submitted to the *IMA Journal of Numerical Analysis* entitled "Galerkin orthogonality and the multiplicative factors in the residual-based a posteriori error estimator for total error". This looks at algebraic error in the context of residual-based a posteriori error estimators, which play an important role in adaptive grid generation. The key result shows that removing the usual assumption on Galerkin orthogonality can significantly change the situation, leading to improved bounds. Some additional numerical experiments concerning adaptive mesh refinement are reported on in Section 4.2. The fifth chapter contains the text of a paper submitted to *Numerische Mathematik* entitled "Estimating and localizing the algebraic and total numerical errors using flux reconstructions". Here, several bounds are derived for these errors when using conforming finite element methods and standard iterative solvers. There is also a discussion of the relevance of this for stopping criteria for iterative methods. The focus of the last scientific chapter is the relevance of these ideas to algebraic preconditioning, which is an integral part of any modern iterative solver. Finally, Chapter 7 contains a brief conclusion and some idea of future work.

Nowadays, mathematical models play a key role in many branches of science, engineering and business, being used to represent diverse processes such as cancer growth, chemical doping, liquid crystal displays, queuing systems, weather prediction, financial option pricing and many more. Almost inevitably, numerical models for solving partial differential equations lead to a very large set of algebraic equations whose solution causes a significant bottleneck in the overall computational process. Research into how these problems can be solved more efficiently and effectively clearly has the potential to be of significant importance across a wide range of disciplines. In particular, the area of designing appropriate grids, usually those which adapt to the development of a problem in a time-dependent setting, is crucial to the reduction of computing times and memory resources. Although the problems in this thesis are mainly discussed in terms of more academic problems, it is clear that the issues highlighted here will almost certainly be important (indeed, even more so) in realistic application settings. In addition, although - as the author himself indicates - the more theoretical results in Chapter 3 at the moment are less practical from a computational viewpoint due to the implementation costs involved, there are examples in the literature where focussing on the theory of Green's functions has led to very practical preconditioners (such as Fp preconditioners for Stokes problems), so there is certainly potential for these clever ideas to be developed further. I therefore have no doubt about the potential relevance and application of this thesis. It contains a great deal of novel scientific material, as evidenced by the published paper and two others already submitted to top journals in the field.

Overall, the thesis is of the correct form and length. It is very well written and, in general, the grammar and spelling is excellent. The subject matter is important and should be of interest to practitioners using these types of method across many application areas. There is certainly sufficient novel material to form a basis for several high-quality publications, and I am confident that the overall standard is commensurate with the award of the PhD. degree.

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