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# Least-Squares Finite Element Methods

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*To my mother and Biliana*

*To Janet*

# Preface

Since their emergence in the early 1950s, finite element methods have become one of the most versatile and powerful methodologies for the approximate numerical solution of partial differential equations. At the time of their inception, finite element methods were viewed primarily as a tool for solving problems in structural analysis. However, it did not take long to discover that finite element methods could be applied with equal success to problems in other engineering and scientific fields. Today, finite element methods are also in common use, and indeed are often the method of choice, for incompressible fluid flow, heat transfer, electromagnetics, and advection-diffusion-reaction problems, just to name a few. Given the early connection between finite element methods and problems engendered by energy minimization principles, it is not surprising that the first mathematical analyses of finite element methods were given in the environment of the classical Rayleigh–Ritz setting. Yet again, using the fertile soil provided by functional analysis in Hilbert spaces, it did not take long for the rigorous analysis of finite element methods to be extended to many other settings. Today, finite element methods are unsurpassed with respect to their level of theoretical maturity.

A finite element method is first and foremost a *quasi-projection scheme*.[1] This truly fundamental property establishes a link with sophisticated mathematical structures and has a tremendous impact on the algebraic problems generated by the method. The paradigm that describes and defines the key properties of what we refer to as a quasi-projection is the marriage of two ingredients: a *variational principle* and a *closed subspace.* Approximate solutions are then characterized as *quasi-projections of the exact* (*weak*) *solutions onto the closed subspace.* Finite element approximations are an example of this rule. Indeed, a finite element method and its properties are completely determined by specifying the variational principle and

[1] A projection in a Hilbert space is, of course, defined with respect to an inner product and a closed subspace. Finite element methods do not always involve a true projection because they are not always based on inner products; however, as we show, finite element approximations do, in general, possess many of the important properties of projections.

the approximation subspace.[2] The cornerstone of the great success of finite element methods is the remarkable fact that the combination of these two ingredients prove to be exceptionally well suited for the numerical solution of partial differential equations.

From a mathematical viewpoint, this success is rooted in the existence of strong intrinsic links between differential equations and variational principles; in fact, it is often the case that the latter serve as the primary mathematical model. On the other hand, the practical appeal of finite element methods and their wide acceptance in the engineering community results from the choice of approximating subspaces. These spaces are spanned by locally supported, piecewise polynomial functions defined over a subdivision of a domain into simple geometrical subdomains referred to as finite elements. Such spaces are not only simple to use, but allow for the almost automatic generation of high-order methods[3] with respect to arbitrary unstructured subdivisions, a trait that, if not outright impossible, is not easy to accomplish with other schemes. The popularity of finite element methods is also largely due to the small support of standard finite element basis functions. This property implies that the resulting algebraic problems involve banded and sparse matrices.

Although the choice of approximation space has, especially from a practical point of view, a tremendous influence on the attributes of the resulting discretized systems, all fundamental properties of finite element methods are ultimately governed by the variational principles from which they are defined. It is, therefore, a fortuitous coincidence that the variational foundations of the first finite element methods were provided by unconstrained, quadratic energy minimization principles, a setting that turned out to be, by far, the most attractive one for finite element methods. Such principles search for a point (in a suitable function space) that is the unconstrained minimizer of a convex quadratic functional and give rise to true inner-product projections in Hilbert spaces. This property, exemplified by the classical Rayleigh–Ritz principle, results in distinct, unique, and very desirable computational and analytic advantages for the resulting finite element methods. Most notably, true inner product projections allow for a wide and nonrestrictive choice for the approximating spaces and lead to symmetric and positive definite algebraic systems.

The connection between finite element methods and Rayleigh–Ritz principles was not immediately recognized as the fundamental cause for the remarkable success of the first finite element methods. As a result, some of the early attempts directed at extending finite element methods beyond the class of problems whose solutions can be characterized as global minimizers of convex quadratic functionals

[2] There exists a fundamental philosophical difference between finite difference and finite element methods. The former substitutes difference operators for differential operators and leads to approximations defined with respect to a discrete lattice, i.e., the fundamental discretization step is to *approximate operators*. Finite element methods, on the other hand, do not deal directly with the differential operators; instead, discretization is effected using alternative weak formulations of these equations posed over finite-dimensional function spaces. This leads to *functional* approximation as opposed to operator approximation. Finite volume methods occupy a middle ground as they exhibit features shared by both finite element and finite difference methods.

[3] This is due to the possibility of using internal degrees of freedom that enrich the finite element space inside each element.

led to disappointing results and a reluctance (by some) to apply the methods outside the field of structural analysis. However, with the rapid development of the mathematical theory of finite element methods and the rapid accumulation of a wealth of practical experience in applying the methods, there came the understanding for what were the reasons behind these early setbacks. It was realized that differential equations not associated with unconstrained minimization principles lead to two other classes of variational principles with strikingly different properties. In one of them, the quasi-projection is induced by a search for a stationary point of an indefinite functional; constrained minimization problems provide an example of this class. The other type offers even less mathematical structure and defines the quasi-projection by a formal *residual orthogonalization* process. In both cases, the variational principle does not lead to a true inner-product projection; this causes the associated finite element methods to operate in a much less favorable setting as compared to those based on Rayleigh–Ritz principles. The computation of stationary points that is the paradigm of *mixed-Galerkin methods* demands strict compatibility conditions on the discrete spaces, if stable and accurate approximations are desired. Likewise, the formal residual orthogonalization process that provides the template for *Galerkin methods* may require onerous stability conditions on the approximation spaces. In both cases, one is confronted by the problem of solving indefinite and/or non-symmetric algebraic equations.

Not surprisingly, there have been many efforts aimed at developing finite element methods that, for problems not connected to unconstrained energy principles, share some, if not all, of the attractive mathematical and algorithmic properties of the Rayleigh–Ritz setting. Broadly speaking, there are two different ways to approach the construction of better projections or quasi-projections than those afforded by the original problem. The first one improves the quasi-projection by penalization or regularization of the original variational principle. In this approach, the principal role of the naturally occurring variational principle[4] is retained, but the principle itself is modified so as to behave more like a true inner-product projection.[5] Galerkin least-squares, stabilized Galerkin, penalized Lagrangian methods, artificial diffusion, and upwind Petrov–Galerkin methods are all examples of finite element methods resulting from this approach.

A second approach that leads to better quasi-projections, indeed to true projections, is to abandon completely the naturally occurring variational principle and to devise a Rayleigh–Ritz-like environment by *formulating an artificial, externally defined energy-type principle.* This energy principle most often takes the form of *residual minimization* in a suitable Hilbert space; thus, there arises the commonly used adjective *least-squares* to denote the resulting finite element methods. Residual

[4] "Naturally occurring" variational principles include Galerkin principles that are based on residual orthogonalization and may or may not have any physical interpretation.

[5] Often the same effect can be achieved by posing the original variational principle on a *modified* finite element space. One example is the SUPG method which can be viewed both as resulting from the use of a modified test space or a modified variational principle. Another example is finite element spaces "enriched" by bubble functions. In many cases, enriched spaces lead to exactly the same formulations as modified Galerkin principles posed on conventional finite element spaces.

minimization is as universal as residual orthogonalization so that, in principle, least-squares finite element methods have the same wide range of applicability as do Galerkin finite element methods, i.e., they are both applicable to virtually any partial differential equation problem. However, residual minimization differs fundamentally from other variational settings, including modified and formal Galerkin principles. Unlike the case for other settings, *least-squares finite element methods are consistently capable of recovering almost all of the advantages of the Rayleigh–Ritz setting* over a wide range of problems and, with some additional effort, they can often create a completely analogous variational environment for finite element methods. This is what makes least-squares finite element methods stand apart from the rest of the methods in the finite element universe.

Mostly over the last ten to fifteen years, efforts focused on least-squares finite element methods have achieved tremendous success in making the methods viable alternatives to existing schemes. There is a wealth of theoretical and practical experience with the methods and they are steadily gaining a solid reputation and popularity among researchers and practitioners for providing robust, efficient, and practical computational tools. Nevertheless, compared with established finite element techniques, such as mixed-Galerkin methods, the theory for least-squares finite element methods remains much less unified and is not always well understood. Because such methods are based on inner-product projections, they tend to be exceptionally robust and stable. As a result, one is often tempted to forego analyses and proceed with the seemingly most natural and simple least-squares formulations. This sometimes leads to unsatisfactory results and methods that cannot fully exploit the advantages of the least-squares approach.

This book is motivated by the premise that there exists a real need to put least-squares finite element methods on a common, mathematically sound foundation and also to discuss important implementation issues that are critical to their success in practice. It is intended to give both the researcher and the practitioner a guide to the theory and practice of least-squares finite element methods, their strengths and weaknesses, caveats to be followed, and established successes.

The factors that set least-squares finite element methods apart from other finite element methods also call for a different approach in the algorithmic development of these methods, if truly reliable, efficient, and accurate schemes are desired. Most notably, reliance of a least-squares method on externally defined variational principles makes the choice of this principle the single most important step in the design of a method. Unlike traditional finite element methods for which the variational principle is almost always dictated by the given problem, least-squares finite element methods dictate the variational principle and then fit the problem into the principle. Thus, the flexibility afforded by the freedom to choose the variational principle places the principal responsibility for the success of the method on the "fitting" process. There are two, often opposing, forces that affect this process. One is the desire to keep the method as simple as possible so as to develop a scheme that is easy to implement. The other is the need to adhere to the basic premises of a Rayleigh–Ritz-like framework, namely, to work with projections defined by inner products that are equivalent to the natural inner products in suitable Hilbert spaces. The interaction between these two competing forces is, in our opinion, the key to understanding least-squares finite element methods; we make it the central theme of this book. Indeed, we show over and over again that the choices made in reconciling ease of implementation with adherence to the Rayleigh–Ritz framework affect all aspects of least-squares finite element methods, from condition numbers of the algebraic problems and their efficient preconditioning to the existence of quasioptimal asymptotic error estimates.

## An overview of the book

Throughout the book, careful attention is paid to not only the rigorous analysis of least-squares finite element methods, but also to practical issues that arise in their implementation.

For those who wish to gain a full understanding of the mathematical analyses connected with least-squares finite element methods, space limitations necessitate the requirement of certain prerequisites. In particular, a basic familiarity with functional analysis in Hilbert spaces and with the theory and implementation of standard finite element methods is assumed at the level of, e.g., [250] and [76, 123, 188], respectively. More advanced background material on functional analysis, partial differential equations, and finite element methods is contained within the book, especially in the appendices. Those who merely wish to learn about least-squares finite element algorithms and their implementation can still use the book by focusing on those sections that consider these topics. In this case, space limitations necessitate familiarity with the algorithmic and implementation aspects of standard finite element methods.

The book is organized into parts, each containing several chapters. In Part I of the book, we provide a necessarily brief review of the finite element universe. It is not meant to give a comprehensive treatment, but rather to provide a context for understanding where least-squares finite element methods fit into that universe. In Chapter 1, "classical" finite element methods, i.e., those based on Rayleigh–Ritz, mixed-Galerkin, and Galerkin variational principles, are discussed. Then, in Chapter 2, a discussion is provided about several of the attempts that have been made to try to recover some of the advantageous features of finite element methods in the Rayleigh–Ritz setting through the definition of modifications to the "classical" principles. Along the way, the strengths and weaknesses of the specific finite element methods encountered are pointed out. At that point, one is ready for the discussion provided in the latter part of Chapter 2 about why and how least-squares finite element methods are meant to improve on the three "classical" approaches and their modifications.

In Part II, we provide the theoretical core of the book that is repeatedly referred to in the rest of the book. Chapter 3 is devoted to an abstract theory of least-squares finite element methods for systems of elliptic partial differential equations. The abstract framework can itself be divided into three classes of least-squares finite element methods that are characterized by discrete least-squares principles having different derivations and properties. The first is defined by simply restricting the minimization of a continuous least-squares functional for the partial differential equations to a finite element space. The other two classes additionally involve a discretization of the least-squares functional itself and differ from each other by the type of equivalence relations that exist (or do not exist) between least-squares functionals and the norms used to measure the size of the solution and the data for the problem. All the possible scenarios emanating from this classification of least-squares finite element methods are analyzed. For a specific problem, one can usually define several different realizations of least-squares finite element methods. Most of these can be viewed as particular applications of one or another of the different scenarios covered by the abstract framework. In addition, several additional basic ingredients needed to define and analyze least-squares finite element methods but which transcend the specific context to which those methods are applied are also discussed. In Chapter 4, the Agmon–Douglis–Nirenberg theory for elliptic partial differential equations is exploited to provide "automated" mechanisms for using solution and data spaces and norms for the definition of least-squares variational principles.

The abstract frameworks developed and analyzed in Part II can be used to define and analyze many least-squares finite element methods for a number of specific settings. In these cases, one need only show how the setting fits into the abstract frameworks and that the hypotheses invoked in those frameworks hold. Thus, there is no need to repeat over and over again proofs specialized to each setting. Using this approach, Part III of the book is devoted to the application of the abstract framework developed in Part II to concrete elliptic partial differential equations.[6] In Chapters 5 and 6, least-squares finite element methods for scalar and vector elliptic partial differential equations are considered, respectively, and, in Chapter 7, least-squares finite element methods for the Stokes equations are considered.

In Part IV, least-squares finite element methods in contexts that do not fit into the abstract theory of Part II, but nevertheless rely on some aspects of that theory, are examined. In Chapter 8, the nonlinear stationary Navier–Stokes equations are considered. In addition to the intrinsic interest engendered by the Navier–Stokes equations, this setting provides an example of how least-squares finite element methods can be used for nonlinear problems. In Chapters 9 and 10, parabolic and hyperbolic (time-dependent) partial differential equations are considered, respectively. The application of least-squares finite element methods to optimization and control problems for systems governed by elliptic partial differential equations is treated in Chapter 11.

Then, in Chapter 12, other settings to which least-squares finite element methods have been applied, but that are not discussed in Chapters 5 through 11, are briefly considered.[7] In that chapter, some variations on the least-squares finite element

[6] There are a few settings considered in Part III that do not fit into the abstract frameworks of Part II; these are treated directly on a case-by-case basis.

[7] Providing a full treatment of all the topics discussed in Chapter 12 would have easily doubled the length of the book. However, we believe these topics should be included in the book, even in a somewhat cursory manner, not only because they are important, but because they serve to further

methods are also briefly discussed; these are methods that have a least-squares character or that use least-squares principles in different ways or for different purposes than those discussed in the rest of the book. Included in Chapter 12 are discussions of boundary condition treatments, $LL^*$ least-squares methods, mimetic reformulations of least-squares methods, least-squares collocation methods, restricted least-squares methods, optimization-based least-squares methods, advection–diffusion–reaction problems, higher-order problems, div–grad–curl systems, domain decomposition least-squares methods, multi-physics problems, problems with singular solution, Treffetz least-squares methods, a posteriori error estimation and mesh refinement, least-squares wavelet methods, and meshless least-squares methods.

In the four Appendices, results from functional analysis, partial differential equations, and finite element theory that are used in various places in the rest of the book are provided. In particular, we define a consistent and unified notational system that does not vary from setting to setting, even though much of the source material used for the book is not consistent in this regard. This not only greatly reduces the notational definitions introduced, but, more important, facilitates making connections between the different settings treated in the book. We also include, in addition to the expected index, a list of often used acronyms and a glossary of often used notations.

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This book is dedicated, by Pavel Bochev, to his wife, Biliana, for her unyielding support, kindness and exceptional patience, and for nurturing his resolve in those moments when the sheer magnitude of this endeavor made its success seem distant and unattainable. A special debt of gratitude is owed by Pavel to his mother Dora for believing in his dreams and making the many sacrifices that helped turn these dreams into reality.

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illustrate the very significant progress that has recently been made in algorithmic, theoretical, and application aspects of least-squares finite element methods.

took to the completion of the book, but for the constant and enduring patience she has shown, support and help she has provided, sacrifices she has made, and love she has given that have been instrumental to his success, not only in his professional life, but, more important, in his personal life.

*Pavel Bochev and Max Gunzburger*
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