

# ELLIPTIC EQUATIONS

Theory and Numerical Solution

(Lecture notes for AMa 204)

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# Contents of the Lecture Notes

## • Part 1: Classical Elliptic Theory and Finite Difference/Volume Methods

### 1. Overview of the theory and numerical treatment of elliptic equations

- (a) Classical PDE theory, finite difference methods, and Taylor series error analysis
- (b) The modern functional analytic approach to partial differential equations.
- (c) Finite element methods and abstract approximation theory
- (d) Solution of large sparse matrix equations
- (e) The failure of sparse Gaussian elimination techniques for discrete elliptic equations in 3D
- (f) The need for optimal complexity (multilevel) iterative methods for discrete elliptic equations

### 2. Review of classical elliptic partial differential equation (PDE) theory

- (a) Classification of second order PDEs into elliptic, parabolic, and hyperbolic type; examples
- (b) Summation convention, tensor notation, and multi-index notation
- (c) Classification of more general operators by the principle part
- (d) Side conditions to produce well-posedness for each class
- (e) Classification of PDEs in divergence form; the notion of “ellipticity”
- (f) The Poisson equation, potential theory, Green’s functions, and maximum principles
- (g) Additional comments on tensor notation; curved surfaces and covariant derivatives
- (h) Three difficult nonlinear elliptic equations to motivate the material in the course
- (i) **Extended Example:** Derivation of the Poisson-Boltzmann equation arising in biophysics

### 3. Finite difference (FD) and finite volume (FV) methods

- (a) Difference approximations; error bounds
- (b) FD discretization of 1D and 2D Poisson equations
- (c) Handling Dirichlet and Neumann boundary conditions: two examples
- (d) FD discretization of a general 3D linear elliptic equation; symmetry considerations
- (e) FV (box) methods in 1D; handling boundary conditions
- (f) FV discretization of a general 3D linear elliptic equation; automatic symmetries
- (g) **Extended example:** FV discretization of linear and nonlinear Poisson-Boltzmann equations
- (h) Error analysis ideas: norms, restrictions, consistency, stability, and convergence theorems
- (i) Consistency lemmas for the discrete Laplace operator
- (j) Review of matrix theory: irreducibility, diagonal dominance, positive definiteness, M-matrices
- (k) Stability lemmas and the spectra of the discrete Laplace operator
- (l) Some FD convergence theorems for the Laplace operator
- (m) Mehrstellen stencils; FD for more general operators

## • Part 2: Generalized Elliptic Theory and Finite Element Methods

### 1. Generalized elliptic PDE theory and a side-trip into functional analysis

- (a) The weak form of a one-dimensional example; integration by parts
- (b) How the Lebesgue space  $L^2$  and Sobolev space  $H^1$  arise naturally from the Schwarz inequality
- (c) Dirichlet conditions, linear spaces, the Trace Theorem, and the Sobolev spaces  $H_g^1$  and  $H_0^1$
- (d)  $L^2$  and  $H^1$  in more general settings; Riemann and Lebesgue integrals; completeness
- (e) The norms, semi-norms, and inner products in  $L^2$  and  $H^1$
- (f) The weak form of  $d$ -dimensional second order elliptic problems; the divergence theorem
- (g) The canonical problems P1 (weak form equations) and P2 (energy minimization problem)
- (h) Additional comments on the Trace Theorem and fractional order Sobolev spaces
- (i) Spaces  $H^k$  for  $k > 1$ , and spaces based on  $L^p$  for  $1 \leq p \leq \infty$ : the Sobolev spaces  $W^{k,p}$
- (j) Two subtleties we resolve later: equivalence classes of functions in  $L^p$  and “weak” derivatives

- (k) The role of functional analysis in elliptic theory
- (l) **WE TOOK A LONG SIDE-TRIP INTO FUNCTIONAL ANALYSIS HERE; REFER TO THE SUPPLEMENTARY FUNCTIONAL ANALYSIS NOTES**
- (m) Well-posedness of linear operator equations: existence, uniqueness, and a priori bounds
- (n) Problems P1 and P2 again as bilinear forms, linear functionals, and quadratic functionals
- (o) Problems P1 and P2 again: their precise connection via the Euler condition

## 2. The mechanics of the finite element method

- (a) Galerkin methods, convergence, and Cea's Lemma
- (b) The canonical problem: a general second order  $d$ -dimensional linear elliptic equation
- (c) Weak formulation (our familiar problem P1) and the five linear and bilinear forms: I1–I5
- (d) Axiomatic definition of a conforming finite element method: FEM1, FEM2, and FEM3
- (e) Finite element discretization of problem P1 with simplicial elements
- (f) Discretization of the five forms I1–I5; the stiffness matrix and the load vector
- (g) Representation via element stiffness matrices and element load vectors
- (h) Affine mappings and their inverses over 2D/3D simplices; affine-equivalent elements
- (i) Simplices in 2D/3D: master element, basis functions, affine transformations, quadrature
- (j) Implementation details: the 2D/3D bilinear form I1 (stiffness matrix entries)
- (k) A second example: the various linear and bilinear forms in  $d$ -dimensional linear elasticity
- (l) Implementation details: the modified 2D/3D linear form I1 for the linear elasticity equations
- (m) Implementation details: the 2D/3D linear form I3 (load vector entries)
- (n) Implementation details: the 2D/3D linear forms I2, I4 (Neumann condition surface integrals)
- (o) Some comments about the remaining form I5 (Dirichlet condition)
- (p) Some 2D triangular meshes: how to efficiently represent an arbitrary polygonal mesh
- (q) Some 3D tetrahedral meshes: tetrahedral orientations, maintaining correct face orientations
- (r) Refinements of simplicial meshes: regular, bisection; uniform, adaptive
- (s) The problem of 3D: Zhang's shortest interior edge rule for tetrahedra
- (t) The FEM MATLAB package (listing in Appendix A)

## 3. Finite element approximation theory

- (a) The canonical problem P1 again, and the Galerkin solution
- (b) Cea's Lemma about the quality of the Galerkin solution; proof of Cea's Lemma
- (c) The energy norm, orthogonality in a Hilbert space, and best approximation in a subspace
- (d) An improved Cea's Lemma (and its proof) under a symmetry assumption
- (e) An overview of the basic finite element error analysis framework
- (f) Nodal basis functions and the finite element interpolant
- (g) Why Cea's Lemma allows one to work with the interpolant rather than the Galerkin solution
- (h) The idea of a "homogeneity argument" and affine transformations to/from a master element
- (i) Bounding the global interpolant error in  $H^k$  norms ( $k \geq 0$ ) by local affine transformations
- (j) Getting an  $L^2$  error estimate for the Galerkin solution using the Aubin-Nitsche technique
- (k) Shorthand notation for the  $L^2$  and  $H^k$  norms and semi-norms
- (l) Setup for the error analysis of linear basis functions over triangles in 2D
- (m) Lemma 1: Mesh geometry effect via affine mappings and 4 geometrical results for triangles
- (n) Lemma 2: Master element interpolant error estimation based on the Bramble-Hilbert Lemma
- (o) Theorem 1: Finite element interpolation error on 2D triangles (proof via Lemmas 1 and 2)
- (p) Setup for the error analysis of bilinear basis functions over axi-parallel rectangles in 2D
- (q) Lemma 1': Mesh geometry effect via affine mappings and 4 geometrical results for rectangles
- (r) Theorem 1': Finite element interpolation error on 2D rectangles (proof via Lemmas 1' and 2)
- (s) More general  $d$ -dimensional forms of Lemma 1 via inscribing and circumscribing spheres
- (t) Proof of the Bramble-Hilbert Lemma; the Sobolev "Imbedding Theorems"

- (u) The Aubin-Nitsche “ $L^2$ -lifting” trick: the adjoint problem and elliptic regularity inequalities
- (v) Summary of the string of inequalities which yield the rigorous finite element error estimates

• **Part 3: Fundamentals of Iterative Methods for Discrete Elliptic Equations**

**1. Introduction and some background material on linear equations operators**

- (a) An example showing the need for optimal complexity methods for discrete elliptic equations
- (b) Abstract finite element operator equations from the Bounded Operator and Riesz Theorems
- (c) Finite element and finite difference matrix equations and their common essential structure
- (d) The underlying abstract operator equation  $Au = f$  in a finite-dimensional Hilbert space  $\mathcal{H}$
- (e) The “native” inner-product and induced norm in  $\mathcal{H}$
- (f) Linear operators: boundedness, positivity, the adjoint, self-adjoint operators, SPD operators
- (g) The  $A$ -inner-product and induced norm in  $\mathcal{H}$  based on an arbitrary SPD operator  $A$
- (h) The  $A$ -adjoint of an operator and relation to the normal Hilbert adjoint
- (i) Cauchy-Schwarz inequalities in the native and  $A$ -inner-products
- (j) The spectral theory of self-adjoint linear operators; eigenvalues and Raleigh quotients
- (k) The norm and spectral radius of an operator and their relationship

**2. Classical linear iterative methods**

- (a) Richardson, Jacobi, Gauss-Seidel, and SOR methods for matrix equations
- (b) The usual and natural point-wise implementation view of Jacobi and Gauss-Seidel
- (c) The matrix (operator) view of Jacobi and Gauss-Seidel
- (d) The abstract underlying basic linear method:  $u^{n+1} = (I - BA)u^n + Bf$
- (e) The approximate inverse  $B \approx A^{-1}$  and conditions on the error propagator  $E = I - BA$
- (f) Properties of the error propagation operator and some simple but useful results
- (g) The number of required iterations as a function of the norm of the error propagator
- (h) The number of required iterations as a function of the  $A$ -condition number  $\kappa_A(BA)$

**3. The conjugate gradient (CG) method**

- (a) The Cayley-Hamilton Theorem; characteristic and minimum polynomials
- (b) The matrix inverse as a matrix polynomial; (shifted) Krylov spaces
- (c) Building an orthogonal basis for a Krylov space; three-term recursions due to  $A$ -symmetry
- (d) Construction of an orthogonal error method; choice of the step-length  $\alpha$
- (e) The resulting “CG” method and its relationship to the classical (Hestenes-Stiefel) algorithm
- (f) The error propagation operator of CG; derivation of the mini-max problem
- (g) Solution of the mini-max problem by scaled and shifted Chebyshev polynomials
- (h) The CG error propagator and the appearance of the  $A$ -condition number  $\kappa_A(BA)$  again
- (i) Some relationships between linear methods and CG; linear methods are preconditioners
- (j) Why CG always “accelerates” any linear method
- (k) The number of required iterations as a function of the  $A$ -condition number  $\kappa_A(BA)$
- (l) Spectrally equivalent operators

**4. Discrete elliptic equations and some classical convergence results for linear methods**

- (a) Discrete elliptic equations, quasi-uniform meshes, and shape-regular elements
- (b) The number of mesh points as a function of the mesh-size and spatial dimension
- (c) Derivation of the condition number of general finite element operators and matrices
- (d) The role of abstraction: the finite element spaces  $\mathcal{M}_k$  and the grid-function spaces  $\mathcal{U}_k$
- (e) Convergence of Richardson, Jacobi, Gauss-Seidel, and SOR for the Poisson equation
- (f) Resulting total solution complexities under the shape-regular, quasi-uniform assumptions

**5. Multilevel and multigrid (MG) iterative methods**

- (a) Introduction and referral to classical (Fourier) materials on MG; a simple illustrative picture

- (b) Nested sequences of spaces, prolongation and its “restriction” adjoint, Galerkin conditions
- (c) Two-level methods as simply two-step composite linear methods
- (d) Symmetrizing the two-level method; why this is important
- (e) Variational (Galerkin) conditions and  $A$ -orthogonal projection
- (f) Multilevel methods as recursive two-level methods; the implicit approximate inverse  $B$
- (g) Recursive and product forms of the error propagation operator  $E$
- (h) The complexity of a single multilevel iteration and necessary limitations in the algorithm
- (i) Total solution complexities of classical, CG, and MG methods for Poisson equation

#### 6. Domain decomposition (DD) iterative methods

- (a) Overlapping subdomains built from finite difference and finite element meshes
- (b) Solution method 1: simple successive solution of the overlapping subdomain problems
- (c) Solution method 2: simple parallel solution of the overlapping subdomain problems
- (d) Reformulating Method 1 to employ the error equation – the multiplicative Schwarz iteration
- (e) Reformulating Method 2 to employ the error equation – the additive Schwarz iteration
- (f) Equivalence of the solution and error formulations: an example showing boundary updates
- (g) Non-overlapping subdomains built from finite difference and finite element meshes
- (h) Block Gaussian-elimination, the Schur complement, and non-overlapping Schwarz
- (i) CG and applying the Schur complement operator via subdomain solves

### • Part 4: A Framework for Analyzing MG and DD Methods

#### 1. Linear operator equations

- (a) Linear operators and spectral theory
- (b) The basic linear method
- (c) Properties of the error propagation operator
- (d) Conjugate gradient acceleration of linear methods

#### 2. The theory of products and sums of operators

- (a) Basic product and sum operator theory
- (b) The interaction hypothesis
- (c) Allowing for a global operator
- (d) Main results of the theory

#### 3. Abstract Schwarz theory

- (a) The Schwarz methods
- (b) Subspace splitting theory
- (c) Product and sum splitting theory for non-nested Schwarz methods
- (d) Product and sum splitting theory for nested Schwarz methods

#### 4. Applications to domain decomposition

- (a) Variational formulation and subdomain-based subspaces
- (b) The multiplicative and additive Schwarz methods
- (c) Algebraic domain decomposition methods
- (d) Convergence theory for the algebraic case
- (e) Improved results through finite element theory

#### 5. Applications to multigrid

- (a) Recursive multigrid and nested subspaces
- (b) Variational multigrid as a multiplicative Schwarz method
- (c) Algebraic multigrid methods
- (d) Convergence theory for the algebraic case
- (e) Improved results through finite element theory

## • Appendix A – Listing of the MATLAB 2D Finite Element Multigrid Package

1. `README` → package description
2. `go.m` → main driver; defines mesh, refines, discretizes, solves.
3. `mesh.m` → mesh and domain definition routine
4. `mesh_dir.m` → example "mesh.m" file for purely dirichlet bc's
5. `mesh_neu.m` → example "mesh.m" file for mix of dirichlet and neumann bc's
6. `refin.m` → uniform mesh refinement routine
7. `edgtp.m` → a mesh search algorithm used by the refinement procedure
8. `isnod.m` → a mesh search algorithm used by the refinement procedure
9. `mastr.m` → master element information definitions
10. `assem.m` → assembly routine (currently a copy of "assem.f.m")
11. `assem.a.m` → matrix assembly following very closely Axelsson and Barker
12. `assem.f.m` → much faster matrix assembly routine with loops rearranged
13. `aa.m` → function "a" in linear elliptic equation
14. `bb.m` → function "b" in linear elliptic equation
15. `ff.m` → function "f" in linear elliptic equation
16. `gg.m` → function "g" in linear elliptic equation
17. `hh.m` → function "h" in linear elliptic equation
18. `uu.m` → function "u" in linear elliptic equation (analytical solution)
19. `draw.m` → draws a finite element mesh
20. `drawf.m` → draws a function defined over a finite element mesh
21. `mypaus.m` → pauses and displays a message
22. `mg.m` → recursive linear multilevel iterative method
23. `mgdrv.m` → iteration driver for the recursive multilevel method
24. `smooth.m` → some classical smoothing iteration for multilevel

## • Appendix B – Problem Sets

1. Homework #1
2. Homework #2
3. Homework #3
4. Homework #4
5. Homework #5
6. Homework #6
7. Homework #7
8. Homework #8

# AMa 204abc

## Numerical Methods for Differential and Integral Equations

Term: Fall 1995 (AMa 204a: Theory and numerical treatment of elliptic equations)  
Place & Time: Firestone 308, 1:00pm-2:00pm, MWF  
Instructor: Michael Holst (holst@ama.caltech.edu), 313 Firestone, Caltech, x4549  
TA: Helen Si (si@ama.caltech.edu)

This course will cover mainly finite element methods and finite element approximation theory for general  $d$ -dimensional linear and nonlinear elliptic equations on polyhedral domains. Since even a basic understanding of finite element approximation theory requires at least a familiarity with the fundamental ideas of variational elliptic theory and functional analysis, the subject of this course can be seen as lying at the intersection of the following three general areas of mathematics:

**Differential Equations:** The branch of mathematics concerned with the study of ordinary and partial differential equations which arise in all areas of mathematics and science. Analysis of differential equations, especially partial differential equations, often involves the tools of **functional analysis**. Most differential equations can be solved analytically only in very special situations, and as a result the algorithms developed in **numerical analysis** must often be employed in mathematics, science, and engineering.

**Numerical Analysis:** The branch of mathematics concerned with the study of computation and of its accuracy, stability, and often its implementation on a computer. One central concern is the determination of appropriate numerical models for applied problems. Another is the construction and analysis of robust and efficient algorithms for various mathematical problems such as those of numerical integration and differentiation, and combinatorial and constrained optimization problems. One area of numerical analysis which finds use in many other areas of science and engineering is the construction and analysis of methods for the numerical solution of ordinary and partial **differential equations** of all kinds. The analysis of such differential equations as well as the analysis of the appropriate numerical algorithms often requires tools from **functional analysis**. (Adapted with much liberty from the Harper Collins Mathematics Dictionary.)

**Functional Analysis:** The branch of mathematics concerned with the modern abstract study of linear and non-linear functions in terms of the underlying linear (topological, normed, Banach, Hilbert, ...) spaces on which the functions are defined and the duals of those spaces. This perspective, growing out of the study of linear operators and functionals, aims at producing a unifying corpus of results and techniques for linear spaces and linear operators. This is applicable to the study of such diverse areas of mathematics as algebra, real analysis, **numerical analysis**, calculus of variations, and **differential equations**, through the application of general theorems such as the Hahn-Banach Theorem, the Uniform Boundedness Principle, the Open Mapping Theorem, and the Riesz Representation Theorem. (Twisted somewhat from the Harper Collins Mathematics Dictionary.)

## General Outline

Of course, we will only have time to touch on a small number of key topics in the above areas. In this course, we will attempt to present the fundamental ideas of the following interrelated topics:

- The modern functional analytic approach to the theory of elliptic partial differential equations.
- Finite element methods, their use and implementation.
- Approximation theory and finite element error analysis.
- Optimal complexity (multilevel) iterative methods for solving discretized elliptic equations.

We will begin with a brief general overview of the theory and numerical treatment of elliptic equations. Following the overview will be a review of classical elliptic theory and finite difference theory, before coming to the core material on variational elliptic theory and the finite element method.

While we will spend some time on iterative methods (such as multilevel and domain decomposition methods) for discrete elliptic equations towards the end of the course, there will be no material on sparse Gaussian elimination and related techniques due to their complexity problems in 3D.

## Requirements, Homework, Exams, etc

- The main requirement is to attend class.
- There will be a final exam.
- Homeworks will be assigned every one or two weeks.
- Machine problems will be assigned two or three times (we will try to use MATLAB).

The basic approach in this course will be to present the theory in the lectures, proving some of the more important results. We will then work together on the homeworks and machine problems to apply the theoretical guidelines to solve some interesting problems. We will also prove some results in the homeworks to “hammer home” some of the fundamental concepts.

## Books and Reference Material

A book is not really required; hopefully the lecture notes will be complete enough. In general, the two books of Hackbusch [18, 19] cover most of the material in the course.

Below is a list of what I feel are some of the more important reference books for this “intersection” area of elliptic equations, numerical analysis, and functional analysis. The list is a little excessive but you can use it as a guide. For particular topics, I’ll supplement material from a few of these books (for example, I’ll present some material from [3, 9, 6, 37] at different points). I have all of books on the list below in my office (with the exception of [25]) so feel free to come by and browse my library.

- General numerical analysis: [10, 11, 22, 40, 48]
- General numerical treatment of elliptic equations: [18, 20, 43]
- Finite element theory: [3, 4, 6, 9, 18, 39, 42]
- Finite element implementation: [3, 5, 23]
- Iterative methods for linear problems: [19, 49, 50, 52]
- Iterative methods for nonlinear problems: [13, 25, 35, 41]
- Multigrid and domain decomposition methods: [8, 17, 46]
- Linear elliptic equations: [2, 15, 18, 34, 37, 44, 47]
- Nonlinear elliptic equations: [14, 15, 38]
- Real analysis: [24, 28, 36, 45]
- Functional analysis: [7, 12, 25, 27, 33, 51]
- Operator and matrix theory [16, 19, 21, 26, 29, 49]
- Sobolev and Besov spaces: [1, 30, 31, 32]

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## Additional *A Posteriori* Remarks For My Class

The Table of Contents for the notes is simply an expanded form of the original outline I handed out at the beginning of the course; I just filled out the details following what we did in class. Recall that we also took a long side-trip into functional analysis, operator theory, and Sobolev spaces, between our discussions of generalized elliptic theory and the finite element method. This supplementary material can be found in the functional analysis notes (“FAN”); this is the second bound set of notes that I passed out at the beginning of class. You’ll have to refer to the two bound sets of notes together for the complete picture. For example, the detailed proofs of the Contraction Mapping Theorem and the Lax-Milgram Theorem that we went through in the lectures are in FAN rather than in this set of notes. A few of the sections in both sets of notes are only sketched out, but hopefully these sections will get filled in as I teach this material a few more times.

While we touched on nearly every topic in the Table of Contents at some point in the lectures, in roughly the same order as they appear in the Table of Contents, we only had time to discuss many of the topics briefly; perhaps we can examine things in more detail in a future course.