

INTRODUCTION TO NUMERICAL METHODS FOR ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

LONG CHEN

CONTENTS

1. Outline of Topics	1
1.1. Finite Difference Methods	1
1.2. Finite Element Methods	1
1.3. Finite Volume Methods	2
1.4. Sobolev Spaces and Theory on Elliptic Equations	2
1.5. Iterative Methods: Conjugate Gradient and Multigrid Methods	2
1.6. Nonlinear Elliptic Equations	2
1.7. Adaptive Finite Element Methods	2
2. Poisson Equation	3
3. Physical Examples	4
3.1. Gauss' law and Newtonian gravity	4
3.2. Electrostatics	5
3.3. The heat equation	5
3.4. Poisson-Boltzmann equation	6

1. OUTLINE OF TOPICS

Computational PDE requires skills from different areas:

- *Calculus*: Taylor expansions.
- *PDE*: Sobolev spaces and weak formulations.
- *Approximation theory*: interpolation, quadrature.
- *Computational topology/geometry*: meshes.
- *Functional analysis*: stability.
- *Linear algebra*: solvers of linear algebraic systems.
- *Numerical analysis*: order of convergence.
- *Computer science*: data structure and programming.

1.1. Finite Difference Methods. The best known methods, finite difference, consists of replacing each derivative by a difference quotient in the classic formulation. It is simple to code and economic to compute. The drawback of the finite difference methods is accuracy and flexibility. Difficulties also arises in imposing boundary conditions.

Date: September 25, 2021.

1.2. Finite Element Methods. We start with simplex and triangulation. Based on a sequence of triangulations, we construct finite dimensional subspaces of Sobolev spaces and study Ritz-Galerkin methods for Poisson equation. We give error estimate of linear finite element approximation in H^1 and L^2 norm.

1.3. Finite Volume Methods. The finite volume method uses a volume integral formulation of the problem with a finite partitioning set of volumes to discretize the equations. Reasons for its popularity include its ability to be faithful to the physics in general and conservation. In a sense, finite volume methods lie in between the finite difference and finite element methods.

1.4. Sobolev Spaces and Theory on Elliptic Equations. Sobolev spaces are fundamental in the study of partial differential equations and their numerical approximations. The regularity theory for elliptic boundary value problems plays an important role in the numerical analysis.

1.5. Iterative Methods: Conjugate Gradient and Multigrid Methods. We shall discuss efficient iterative methods to solve the linear operator equation

$$(1) \quad Au = f,$$

posed on a finite dimensional Hilbert space \mathbb{V} equipped with an inner product (\cdot, \cdot) . Here $A : \mathbb{V} \mapsto \mathbb{V}$ is an symmetric positive definite (SPD) operator, $f \in \mathbb{V}$ is given, and we are looking for $u \in \mathbb{V}$ such that (1) holds.

1.6. Nonlinear Elliptic Equations. We first introduce Picard and Newton iteration for solving nonlinear elliptic equations. We then combine the multilevel technique to design more efficient nonlinear solver. This includes a two-grid method which uses the coarse grid approximation as an initial guess in the Newton method and a nonlinear multigrid (FAS) which in contrast use Newton methods as a smoother.

1.7. Adaptive Finite Element Methods. Adaptive methods are now widely used in the scientific computation to achieve better accuracy with minimum degree of freedom. We shall discuss the programming and convergence analysis of adaptive finite element methods (AFEMs) for second order elliptic partial differential equations.

2. POISSON EQUATION

We shall focus on the Poisson equation, one of the most important and frequently encountered equations in many mathematical models of physical phenomena, and its variants in this course. Just as an example, the solution of the Poisson equation gives the electrostatic potential for a given charge distribution. The Poisson equation is

$$(2) \quad -\Delta u = f, \quad x \in \Omega.$$

Here Δ is the Laplacian operator given by

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \dots + \frac{\partial^2}{\partial x_d^2}$$

and Ω is a d -dimensional domain (e.g., a rod in 1d, a plate in 2d and a volume in 3d). The unknown function u represents the electrostatic potential and the given data is the charge distribution f . If the charge distribution vanishes, this equation is known as Laplace's equation and the solution to the Laplace equation is called harmonic function.

The Poisson equation also frequently appears in structural mechanics, theoretical physics, and many other areas of science and engineering. It is named after the French mathematician Siméon-Denis Poisson. When the equation is posed on a bounded domain with boundary, boundary conditions should be included as an essential part of the equation.

Denote by $\partial\Omega$ the boundary of Ω , and with $\mathbf{n} = (n_1, \dots, n_d)^T$ the unit normal vector to $\partial\Omega$ pointing outside of Ω . For the Poisson equation, the following types of boundary conditions are often used. These are:

- Dirichlet (or first type) boundary condition:

$$(3) \quad u|_{\partial\Omega} = g_D$$

- Neumann (or second type) boundary condition:

$$(4) \quad \frac{\partial u}{\partial \mathbf{n}} = \nabla u \cdot \mathbf{n}|_{\partial\Omega} = g_N$$

- Mixed boundary condition:

$$(5) \quad u|_{\Gamma_D} = g_D, \quad \text{and} \quad \nabla u \cdot \mathbf{n}|_{\Gamma_N} = g_N$$

where $\Gamma_D \cup \Gamma_N = \partial\Omega$ and Γ_D is closed.

- Robin (or third type) boundary condition:

$$(6) \quad (\alpha u + \beta \nabla u \cdot \mathbf{n})|_{\partial\Omega} = g_R.$$

Dirichlet and Neumann boundary conditions are two special cases of the mixed boundary condition by taking $\Gamma_D = \partial\Omega$ or $\Gamma_N = \partial\Omega$, respectively. Mixed boundary condition itself is a special example of Robin boundary condition by taking the coefficient $\alpha = \chi_{\Gamma_D}$ and $\beta = \chi_{\Gamma_N}$, where χ is the characteristic function defined as usual. When the boundary data is zero, we call it homogenous.

For convenience of exposition, we shall mainly consider the following Poisson equation with homogeneous mixed boundary condition:

$$(7) \quad \begin{cases} -\Delta u = f, & x \in \Omega \\ u = 0, & x \in \Gamma_D \\ \frac{\partial u}{\partial \mathbf{n}} = 0, & x \in \Gamma_N. \end{cases}$$

Remark 2.1. For the Poisson equation with Neumann boundary condition

$$(8) \quad -\Delta u = f \text{ in } \Omega, \quad \frac{\partial u}{\partial \mathbf{n}} = g \text{ on } \partial\Omega,$$

there is a compatible condition for f and g :

$$(9) \quad \int_{\Omega} f \, dx = - \int_{\Omega} \Delta u \, dx = \int_{\partial\Omega} \frac{\partial u}{\partial \mathbf{n}} \, dS = \int_{\partial\Omega} g \, dS.$$

The solution is unique up to a constant. Namely if u is a solution to (8), so is $u + c$.

Equation (2) together with one of the boundary conditions given in (3)-(6), is called well-posed, if the solution exists and is unique, and moreover, depends continuously on the given data (f, g_D, g_N, g_R) . In other words, the differential equation above is well posed if its solution is unique and “small” perturbations in data lead to “small” perturbations in the solution u . The perturbation will be measured precisely in terms of various norm of functions.

The problem of solving the Poisson equation, together with the boundary conditions is called a second order *boundary value problem*. Second order is to indicate that the highest order of the differentiation of u which appears in the equation is 2.

3. PHYSICAL EXAMPLES

3.1. Gauss’ law and Newtonian gravity. The gravitational field \mathbf{g} (also called gravitational acceleration) is a vector field so that the gravitational force \mathbf{F}_g experienced by a particle is

$$\mathbf{F}_g(\mathbf{r}) = m\mathbf{g}(\mathbf{r})$$

where m is the mass of a particle and \mathbf{r} is the position vector of the particle. The gravity is a conservative force, i.e., when an object moves from one location to another, the force changes the potential energy of the object by an amount that does not depend on the path taken. Or equivalently $\nabla \times \mathbf{g} = 0$. So it can be written as the gradient of a scalar potential u , called the gravitational potential:

$$(10) \quad \mathbf{g} = -\nabla u.$$

The Gauss’ law for gravity states:

$$(11) \quad \int_{\partial V} \mathbf{g} \cdot \mathbf{n} \, dS = -4\pi G M_V$$

where ∂V is any closed surface, $\int_{\partial V} dS$ is the surface integral with the outward-pointing surface normal \mathbf{n} , G is the universal gravitational constant, and M_V is the total mass of V – a closed region bounded by ∂V .

Using the divergence theorem

$$\int_{\partial V} \mathbf{g} \cdot \mathbf{n} \, dS = \int_V \nabla \cdot \mathbf{g} \, dx \, dy \, dz,$$

and the formula for mass $M = \int_V \rho \, dV$ where ρ is the mass density, we obtain the differential form of Gauss’ law for gravity

$$(12) \quad \nabla \cdot \mathbf{g} = -4\pi G \rho.$$

Combining with the relation (10) from conservation property of the potential, we arrive at the Poisson equation:

$$\Delta u = 4\pi G \rho.$$

3.2. Electrostatics. The derivation of Poisson's equation in electrostatics follows. We start from Gauss' law, also known as Gauss' flux theorem, which is a law relating the distribution of electric charge to the resulting electric field. In its integral form, the law states that, for any volume V in space, with boundary surface ∂V , the following equation holds:

$$(13) \quad \int_{\partial V} \mathbf{E} \cdot \mathbf{n} \, dS = \frac{Q_V}{\varepsilon}$$

where the left hand side of (13) is called the "electric flux through ∂V ", \mathbf{E} is the electric field, $\int_{\partial V} \mathbf{n} \, dS$ is a surface integral with an outward facing surface normal orientation. The surface ∂V is the surface bounding the volume V , $Q_V = \int_V \rho \, dv$ is the total electric charge in the volume V , and ε is the electric constant - a fundamental physical constant.

Again using divergence theorem, the differential form the Gauss' law is:

$$(14) \quad \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon},$$

where ρ is the charge density.

In the absence of a changing magnetic field, \mathbf{B} , Faraday's law of induction gives:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} = 0.$$

Since the curl of the electric field is zero, it is defined by a scalar electric potential field

$$\mathbf{E} = -\nabla u$$

Eliminating by substitution, we have a form of the Poisson equation:

$$(15) \quad \Delta u = -\frac{\rho}{\varepsilon}.$$

Remark 3.1. The left-hand side of (11) is called the flux of the gravitational field. Note that it is always negative (or zero), and never positive. This can be contrasted with Gauss' law for electricity, where the flux can be either positive or negative. The difference is because charge can be either positive or negative, while mass can only be positive.

3.3. The heat equation. We consider a solid material that occupies a region $\Omega \subset \mathbb{R}^3$ with the boundary $\partial\Omega$. Denote the temperature at point $x \in \mathbb{R}^3$ at the time instant t by $u(x, t)$. Suppose r is the heat received per unit volume by radiation. For any domain $D \subset \Omega$, the heat energy Q contained in the material is

$$(16) \quad Q = \int_D \rho \kappa_s u(x, t) \, dx,$$

where ρ is the density of the material and κ_s a physical characteristic of the material called the specific heat capacity. By Fourier's law, the flow rate of heat energy through a surface is proportional to the negative temperature gradient across the surface, i.e. $-\sigma \nabla u$, where σ is the thermal conductivity. Then the heat transfer in whole D will be governed by

$$(17) \quad \frac{\partial Q}{\partial t} = \int_{\partial D} \sigma \mathbf{n} \cdot \nabla u \, ds + \int_D r \, dx.$$

Suppose the material is isotropic, that means the physical parameters ρ, κ_s, σ are constants. Together with (16) and (17), it holds

$$\int_D \rho \kappa_s \frac{\partial u}{\partial t} \, dx = \int_{\partial D} \sigma \mathbf{n} \cdot \nabla u \, ds + \int_D r \, dx.$$

Using integration by part, we have

$$\int_D \rho \kappa_s \frac{\partial u}{\partial t} dx = \int_D \sigma \Delta u ds + \int_D r dx.$$

Because of the arbitrariness of D , the last equality equal to

$$\rho \kappa_s \frac{\partial u}{\partial t} = \sigma \Delta u + r \quad \text{in } \Omega \times (0, +\infty).$$

Now let $\kappa = \frac{\sigma}{\rho \kappa_s}$ and $f = \frac{r}{\rho \kappa_s}$. Therefore we get the heat equation as follows.

$$\frac{\partial u}{\partial t} - \kappa \Delta u = f \quad \text{in } \Omega \times (0, +\infty).$$

3.4. Poisson-Boltzmann equation. Solving Poisson's equation (15) for the potential requires knowing the charge density distribution. If the charge density is zero, then Laplace's equation results. If the charge density follows a Boltzmann distribution, then the Poisson-Boltzmann equation results. The Poisson-Boltzmann equation plays a role in the development of the Debye-Hückel theory of dilute electrolyte solutions.

We shall derive a Poisson-Boltzmann equation in the application of biomolecular modeling.

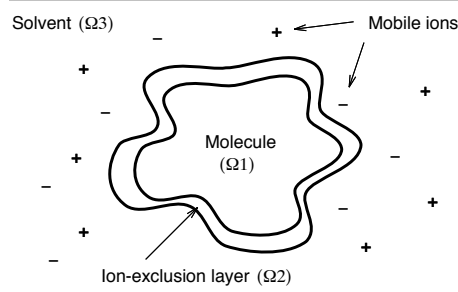


FIGURE 1. A charged biological structure immersed in a salt solution. The molecular (solute) region is Ω_m with dielectric constant ε_m , the solvent region is Ω_s with dielectric constant ε_s , the ion-exclusion layer is Ω_2 , and the mobile ions denoted by plus and minus signs.

The Poisson equation (15), which relates the electrostatic potential Φ in a dielectric to the charge density ρ , now takes the form

$$-\nabla \cdot (\varepsilon \nabla \Phi) = \rho,$$

where ε is dielectric constant of the medium, and here is typically piecewise constant. Usually it jumps by one or two orders of magnitude at the interface between the charged structure (a biological molecular or membrane) and the solvent (a salt solution).

The charge density ρ consist of two components: $\rho = \rho_{\text{macro}} + \rho_{\text{ion}}$. For the macromolecule, the charge density is a summation of δ -distributions at N_m point charges, i.e.,

$$\rho_{\text{macro}}(x) = \sum_{i=1}^{N_m} q_i \delta(x - x_i), \quad q_i = \frac{4\pi e_c^2}{\kappa_B T} z_i,$$

where $\kappa_B > 0$ is the Boltzmann constant, T is the temperature, e_c is the unit of charge, and z_i is the amount of charge.

For the mobile ions in the solvent, the charge density ρ_{ion} cannot be given in a deterministic way. Instead it will be given by the Boltzmann distribution. If the solvent contains N types of ions, of valence Z_i , and of bulk concentration c_i , then a Boltzmann assumption about the equilibrium distribution of the ions leads to

$$\rho_{\text{ion}} = \sum_{i=1}^N c_i Z_i e_c \exp\left(-Z_i \frac{e_c \Phi}{\kappa_B T}\right).$$

For a symmetric 1 : 1 electrolyte, $N = 2$, $c_i = c_0$, and $Z_i = (-1)^i$, which yields

$$\rho_{\text{ion}} = -2c_0 e_c \sinh\left(\frac{e_c \Phi}{\kappa_B T}\right).$$

We can now write out the PBE for modeling the electrostatic potential of a solvated biological structure. Let us denote the molecule region by $\Omega_m \subset \mathbb{R}^d$ and consider the solvent region $\Omega_s = \mathbb{R}^d \setminus \Omega_m$. We use u to denote the dimensionless potential and $\bar{\kappa}^2$ to denote the modified Debye-Hückel parameter (which is a function of the ionic strength of the solvent). The nonlinear Poisson-Boltzmann equation is then:

$$(18) \quad -\nabla \cdot (\varepsilon \nabla u) + \bar{\kappa}^2 \sinh(u) = \sum_{i=1}^{N_m} q_i \delta_i, \quad \text{in } \mathbb{R}^d$$

$$(19) \quad u(\infty) = 0,$$

where

$$\varepsilon = \begin{cases} \varepsilon_m & \text{if } x \in \Omega_m \\ \varepsilon_s & \text{if } x \in \Omega_s \end{cases}, \quad \text{and} \quad \bar{\kappa} = \begin{cases} 0 & \text{if } x \in \Omega_m \\ \sqrt{\varepsilon_s} \kappa > 0 & \text{if } x \in \Omega_s. \end{cases}$$

It has been determined empirically that $\varepsilon_m \approx 2$ and $\varepsilon_s \approx 80$. The structure itself (e.g., a biological molecule, or a membrane) is represented implicitly by ε and $\bar{\kappa}$, as well as explicitly by the N_m point charges $q_i = z_i e_c$ at the positions x_i . The charge positions are located in the strict interior of the molecular region Ω_m .