

Chapter 2

Basic Theory of Partial Differential Equations and Their Discretization

In this chapter we present some basic elements of the analysis of partial differential equations, and of their numerical discretization by finite differences. Our aim is to introduce some notions that enable the reader to follow the material developed in the subsequent chapters. Both the analysis and the numerical solution of partial differential equations (PDEs) are research areas by themselves, with a large amount of related literature. We refer, for instance, to the books [9, 19] for the analysis of PDEs and to, e.g., [23, 52] for their numerical approximation.

2.1 Notation and Lebesgue Spaces

Let X be a Banach space and let $\|\cdot\|_X$ be the associated norm. The topological dual of X is denoted by X' and the duality pair is written as $\langle \cdot, \cdot \rangle_{X', X}$. If X is, in addition, a Hilbert space, we denote by $(\cdot, \cdot)_X$ its inner product.

The set of bounded linear operators from X to Y is denoted by $\mathcal{L}(X, Y)$ or by $\mathcal{L}(X)$ if $X = Y$. The norm of a bounded linear operator $T : X \rightarrow Y$ is given by

$$\|T\|_{\mathcal{L}(X, Y)} := \sup_{v \in X, \|v\|_X=1} \|Tv\|_Y.$$

For $T \in \mathcal{L}(X, Y)$ we can also define an operator $T^* \in \mathcal{L}(Y', X')$, called the adjoint operator of T , such that

$$\langle w, Tv \rangle_{Y', Y} = \langle T^* w, v \rangle_{X', X}, \text{ for all } v \in X, w \in Y'$$

and $\|T\|_{\mathcal{L}(X, Y)} = \|T^*\|_{\mathcal{L}(Y', X')}.$

Definition 2.1. Let Ω be an open subset of \mathbb{R}^N and $1 \leq p < \infty$. The set of p -integrable functions is defined by

$$L^p(\Omega) = \{u : \Omega \rightarrow \mathbb{R}; u \text{ is measurable and } \int_{\Omega} |u|^p dx < \infty\},$$

and the following norm is used: $\|u\|_{L^p} = (\int_{\Omega} |u(x)|^p dx)^{\frac{1}{p}}$.

Moreover, we also define the space

$$L^\infty(\Omega) = \{u : \Omega \rightarrow \mathbb{R}; u \text{ is measurable and } |u(x)| \leq C \text{ a.e. in } \Omega \text{ for some } C > 0\}$$

and endow it with the norm $\|u\|_{L^\infty} = \inf\{C : |u(x)| \leq C \text{ a.e. in } \Omega\}$.

Theorem 2.1 (Hölder). Let $u \in L^p(\Omega)$ and $v \in L^q(\Omega)$ with $\frac{1}{p} + \frac{1}{q} = 1$. Then $uv \in L^1(\Omega)$ and

$$\int_{\Omega} |uv| dx \leq \|u\|_{L^p} \|v\|_{L^q}.$$

The spaces $L^p(\Omega)$ are Banach spaces for $1 \leq p \leq \infty$ and reflexive for $1 < p < \infty$. For $L^2(\Omega)$, a scalar product can be defined by

$$(u, v)_{L^2} = \int_{\Omega} uv dx$$

and a Hilbert space structure is also obtained.

2.2 Weak Derivatives and Sobolev Spaces

Next, we study a weak differentiability notion which is crucial for the definition of Sobolev function spaces and for the variational study of PDEs.

Let $\Omega \subset \mathbb{R}^N$, $N = 2, 3$, be a bounded Lipschitz domain and consider functions $y, v \in C^1(\overline{\Omega})$. Utilizing Green's formula, we obtain the equivalence

$$\int_{\Omega} v(x) D_i y(x) dx = \int_{\Gamma} v(x) y(x) n_i(x) ds - \int_{\Omega} y(x) D_i v(x) dx,$$

where $n_i(x)$ denotes the i -th component of the exterior normal vector to Ω at the point $x \in \Gamma$ and ds stands for the Lebesgue surface measure at the boundary Γ . If, in addition, $v = 0$ on Γ , then

$$\int_{\Omega} y(x) D_i v(x) dx = - \int_{\Omega} v(x) D_i y(x) dx.$$

More generally, if higher order derivatives are involved, we obtain the following formula:

$$\int_{\Omega} y(x) D^{\alpha} v(x) dx = (-1)^{|\alpha|} \int_{\Omega} v(x) D^{\alpha} y(x) dx,$$

where $\alpha = (\alpha_1, \dots, \alpha_N)$ is a multi-index and D^{α} denotes the differentiation operator with respect to the multi-index, i.e., $D^{\alpha} = \frac{\partial^{|\alpha|}}{\partial x^{\alpha_1} \dots \partial x^{\alpha_N}}$, with $|\alpha| = \sum_{i=1}^N \alpha_i$. The last equation is the starting point for the definition of a weaker notion of differentiable function, which takes advantage of the presence of the integral and the accompanying regular function $v(x)$.

Definition 2.2. Let $L^1_{\text{loc}}(\Omega)$ denote the set of locally integrable functions on Ω , i.e., integrable on any compact subset of Ω . Let $y \in L^1_{\text{loc}}(\Omega)$ and α be a given multi-index. If there exists a function $w \in L^1_{\text{loc}}(\Omega)$ such that

$$\int_{\Omega} y(x) D^{\alpha} v(x) dx = (-1)^{|\alpha|} \int_{\Omega} w(x) v(x) dx,$$

for all $v \in C_0^{\infty}(\Omega)$, then w is called the derivative of y in the weak sense (or weak derivative), associated with α , and is denoted by $w = D^{\alpha} y$.

Example 2.1. $y(x) = |x|$ in $\Omega = (-1, 1)$. The weak derivative of $y(x)$ is given by

$$y'(x) = w(x) = \begin{cases} -1 & \text{if } x \in (-1, 0), \\ 1 & \text{if } x \in [0, 1). \end{cases}$$

Indeed, for $v \in C_0^{\infty}(-1, 1)$,

$$\begin{aligned} \int_{-1}^1 |x| v'(x) dx &= \int_{-1}^0 (-x) v'(x) dx + \int_0^1 x v'(x) dx \\ &= -x v(x) \Big|_{-1}^0 - \int_{-1}^0 (-1) v(x) dx + x v(x) \Big|_0^1 - \int_0^1 v(x) dx \\ &= - \int_{-1}^1 w(x) v(x) dx. \end{aligned}$$

Note that the value of y' at the point $x = 0$ is not important since the set $\{x = 0\}$ has zero measure.

Definition 2.3. Let $1 \leq p < \infty$ and $k \in \mathbb{N}$. The space of functions $y \in L^p(\Omega)$ whose weak derivatives $D^{\alpha} y$, for $\alpha : |\alpha| \leq k$, exist and belong to $L^p(\Omega)$ is denoted by $W^{k,p}(\Omega)$ and

is called Sobolev space. This space is endowed with the norm

$$\|y\|_{W^{k,p}} = \left(\sum_{|\alpha| \leq k} \int_{\Omega} |D^{\alpha} y|^p dx \right)^{1/p}.$$

If $p = \infty$, the space $W^{k,\infty}(\Omega)$ is defined in a similar way, but endowed with the norm

$$\|y\|_{W^{k,\infty}} = \max_{|\alpha| \leq k} \|D^{\alpha} y\|_{L^{\infty}}.$$

The spaces $W^{k,p}(\Omega)$ constitute Banach spaces, reflexive for $1 < p < +\infty$. In the special case $p = 2$ the Sobolev spaces are denoted by $H^k(\Omega) := W^{k,2}(\Omega)$.

A frequently used space is

$$H^1(\Omega) = \{y \in L^2(\Omega) : D_i y \in L^2(\Omega), \forall i = 1, \dots, N\}$$

endowed with the norm

$$\|y\|_{H^1} = \left(\int_{\Omega} (y^2 + |\nabla y|^2) dx \right)^{1/2},$$

and the scalar product

$$(u, v)_{H^1} = \int_{\Omega} u \cdot v dx + \int_{\Omega} \nabla u \cdot \nabla v dx.$$

The space $H^1(\Omega)$ constitutes a Hilbert space with the provided scalar product.

Definition 2.4. The closure of $C_0^{\infty}(\Omega)$ in $W^{k,p}(\Omega)$ is denoted by $W_0^{k,p}(\Omega)$. The resulting space is endowed with the $W^{k,p}$ -norm and constitutes a closed subspace of $W^{k,p}(\Omega)$.

Next, we summarize some important Sobolev spaces embedding results (see [12, Sect. 6.6] for further details).

Theorem 2.2. *Let $\Omega \subset \mathbb{R}^N$ be an open bounded set with Lipschitz continuous boundary. Then the following continuous embeddings hold:*

1. If $p < N$, $W^{1,p}(\Omega) \hookrightarrow L^{p^*}(\Omega)$, for $\frac{1}{p^*} = \frac{1}{p} - \frac{1}{N}$,
2. If $p = N$, $W^{1,p}(\Omega) \hookrightarrow L^q(\Omega)$, for $1 \leq q < +\infty$,
3. If $p > N$, $W^{1,p}(\Omega) \hookrightarrow C^{0,1-N/p}(\overline{\Omega})$.

Theorem 2.3 (Rellich–Kondrachov). *Let $\Omega \subset \mathbb{R}^N$ be an open bounded set with Lipschitz continuous boundary. Then the following compact embeddings hold:*

1. If $p < N$, $W^{1,p}(\Omega) \hookrightarrow L^q(\Omega)$, for all $1 \leq q < p^*$ with $\frac{1}{p^*} = \frac{1}{p} - \frac{1}{N}$,
2. If $p = N$, $W^{1,p}(\Omega) \hookrightarrow L^q(\Omega)$, for all $1 \leq q < +\infty$,
3. If $p > N$, $W^{1,p}(\Omega) \hookrightarrow C(\overline{\Omega})$.

An important issue in PDEs is the value that the solution function takes at the boundary. If the function is continuous on Ω , then its boundary value can be determined by continuous extension. However, if the function is defined in an almost everywhere sense, then its boundary value has no specific sense, since the boundary has zero measure. The following result clarifies in which sense such a boundary value may hold (see [9, p. 315] for further details).

Theorem 2.4. *Let Ω be a bounded Lipschitz domain. There exists a bounded linear operator $\tau: W^{1,p}(\Omega) \longrightarrow L^p(\Gamma)$ such that*

$$(\tau y)(x) = y(x) \quad \text{a.e. on } \Gamma,$$

for each $y \in C(\overline{\Omega})$.

Definition 2.5. The function τy is called the trace of y on Γ and τ is called the trace operator.

If Ω is a bounded Lipschitz domain, then it holds that

$$W_0^{1,p}(\Omega) = \{y \in W^{1,p}(\Omega) : \tau y = 0 \text{ a.e. on } \Gamma\}.$$

In particular, $H_0^1(\Omega) = \{y \in H^1(\Omega) : \tau y = 0 \text{ a.e. on } \Gamma\}$, which, thanks to the Poincaré inequality, can be endowed with the norm

$$\|y\|_{H_0^1} := \left(\int_{\Omega} |\nabla y|^2 dx \right)^{1/2}.$$

2.3 Elliptic Problems

2.3.1 Poisson Equation

Consider the following classical PDE:

$$\begin{cases} -\Delta y = f & \text{in } \Omega, \\ y = 0 & \text{on } \Gamma. \end{cases} \quad (2.1)$$

Existence of a unique solution $y \in C^2(\bar{\Omega})$ can be obtained by classical methods (see [19, Chap. 2]), under the assumption that the right hand side belongs to the space of continuous functions. In practice, however, it usually happens that the function on the right hand side has less regularity. To cope with that situation, an alternative (and weaker) notion of solution may be introduced.

Assuming enough regularity of y and multiplying (2.1) with a test function $v \in C_0^\infty(\Omega)$, we obtain the integral relation

$$-\int_{\Omega} \Delta y \, v \, dx = \int_{\Omega} f v \, dx,$$

which, using integration by parts, yields

$$\int_{\Omega} \nabla y \cdot \nabla v \, dx - \int_{\Gamma} v \, \partial_{\mathbf{n}} y \, ds = \int_{\Omega} f v \, dx,$$

where $\partial_{\mathbf{n}} y = \nabla y \cdot \mathbf{n} = \frac{\partial y}{\partial \mathbf{n}}$. Since $v = 0$ on Γ , it follows that

$$\int_{\Omega} \nabla y \cdot \nabla v \, dx = \int_{\Omega} f v \, dx.$$

Since $C_0^\infty(\Omega)$ is dense in $H_0^1(\Omega)$ and both terms in the previous equation are continuous with respect to the $H_0^1(\Omega)$ -norm, then the equation holds for all $v \in H_0^1(\Omega)$.

Definition 2.6. A function $y \in H_0^1(\Omega)$ is called a weak solution for problem (2.1) if it satisfies the following variational formulation:

$$\int_{\Omega} \nabla y \cdot \nabla v \, dx = \int_{\Omega} f v \, dx, \quad \forall v \in H_0^1(\Omega). \quad (2.2)$$

Existence of a unique solution to (2.2) can be proved by using the well-known Lax–Milgram theorem, which is stated next.

Theorem 2.5 (Lax–Milgram). *Let V be a Hilbert space and let $a(\cdot, \cdot)$ be a bilinear form such that, for all $y, v \in V$,*

$$|a(y, v)| \leq C \|y\|_V \|v\|_V, \quad (2.3)$$

$$a(y, y) \geq \kappa \|y\|_V^2, \quad (2.4)$$

for some positive constants C and κ . Then, for every $\ell \in V'$, there exists a unique solution $y \in V$ to the variational equation

$$a(y, v) = \langle \ell, v \rangle_{V', V}, \text{ for all } v \in V. \quad (2.5)$$

Moreover, there exists a constant \tilde{c} , independent of ℓ , such that

$$\|y\|_V \leq \tilde{c} \|\ell\|_{V'}. \quad (2.6)$$

2.3.2 A General Linear Elliptic Problem

We consider the following general linear elliptic problem:

$$\begin{aligned} Ay + c_0 y &= f && \text{in } \Omega, \\ \partial_{n_A} y + \alpha y &= g && \text{on } \Gamma_1, \\ y &= 0 && \text{on } \Gamma_0, \end{aligned} \quad (2.7)$$

where A is an elliptic operator in divergence form:

$$Ay(x) = - \sum_{i,j=1}^N D_j(a_{ij}(x) D_i y(x)). \quad (2.8)$$

The coefficients $a_{ij} \in L^\infty(\Omega)$ satisfy the symmetry condition $a_{ij}(x) = a_{ji}(x)$ and the following ellipticity condition: $\exists \kappa > 0$ such that

$$\sum_{i,j=1}^N a_{ij}(x) \xi_i \xi_j \geq \kappa |\xi|^2, \quad \forall \xi \in \mathbb{R}^n, \text{ for a.a. } x \in \Omega. \quad (2.9)$$

The operator ∂_{n_A} stands for the conormal derivative, i.e.,

$$\partial_{n_A} y(x) = \nabla y(x)^T n_A(x),$$

with $(n_A)_i(x) = \sum_{j=1}^N a_{ij}(x) n_j(x)$. Additionally $\Gamma = \Gamma_0 \uplus \Gamma_1$ and $c_0 \in L^\infty(\Omega)$, $\alpha \in L^\infty(\Gamma_1)$, $f \in L^2(\Omega)$, $g \in L^2(\Gamma_1)$.

By introducing the Hilbert space

$$V = \left\{ y \in H^1(\Omega) : y|_{\Gamma_0} = 0 \right\}$$

and the bilinear form

$$a(y, v) := \int_{\Omega} \sum_{i,j=1}^N a_{ij} D_i y D_j v \, dx + \int_{\Omega} c_0 y v \, dx + \int_{\Gamma_1} \alpha y v \, ds, \quad (2.10)$$

the variational formulation of problem (2.7) is given in the following form: Find $y \in V$ such that

$$a(y, v) = (f, v)_{L^2(\Omega)} + (g, v)_{L^2(\Gamma_1)}, \quad \forall v \in V.$$

Theorem 2.6. *Let Ω be a bounded Lipschitz domain and $c_0 \in L^\infty(\Omega)$, $\alpha \in L^\infty(\Gamma_1)$ given functions such that $c_0(x) \geq 0$ a.e. in Ω and $\alpha(x) \geq 0$ a.e. on Γ_1 , respectively. If one of the following conditions holds:*

- i) $|\Gamma_0| > 0$,
- ii) $\Gamma_1 = \Gamma$ and $\int_{\Omega} c_0^2(x) dx + \int_{\Gamma} \alpha^2(x) ds > 0$,

then there exist a unique weak solution $y \in V$ to problem (2.7). Additionally, there exists a constant $c_A > 0$ such that

$$\|y\|_{H^1} \leq c_A \left(\|f\|_{L^2(\Omega)} + \|g\|_{L^2(\Gamma_1)} \right).$$

Proof. The proof makes use of the Lax–Milgram theorem and Friedrichs’ inequality, and is left as an exercise for the reader. \square

2.3.3 Nonlinear Equations of Monotone Type

An important class of nonlinear PDEs involve differential operators of monotone type. Such is the case, for instance, of equations that arise as necessary conditions in the minimization of energy functionals.

Let V be a separable, reflexive Banach space and consider the variational equation

$$\langle A(y), v \rangle_{V', V} = \langle \ell, v \rangle_{V', V}, \quad \text{for all } v \in V, \quad (2.11)$$

where $\ell \in V'$ and the operator $A : V \rightarrow V'$ satisfies the following properties.

Assumption 2.1.

- i) A is monotone, i.e., for all $u, v \in V$,

$$\langle A(u) - A(v), u - v \rangle_{V', V} \geq 0. \quad (2.12)$$

- ii) A is hemicontinuous, i.e., the function

$$t \rightarrow \langle A(u + tv), w \rangle_{V', V}$$

is continuous on the interval $[0, 1]$, for all $u, v, w \in V$.

iii) A is coercive, i.e.,

$$\lim_{\|u\|_V \rightarrow \infty} \frac{\langle A(u), u \rangle_{V', V}}{\|u\|_V} = +\infty. \quad (2.13)$$

Theorem 2.7 (Minty–Browder). *Let $\ell \in V'$ and $A : V \rightarrow V'$ be an operator satisfying Assumption 2.1. Then there exists a solution to the variational equation (2.11). If A is strictly monotone, then the solution is unique.*

Proof. Since V is separable, there exists a basis $\{v_i\}_{i=1}^\infty$ of linearly independent vectors, dense in V . Introducing

$$V_n = \text{span}\{v_1, \dots, v_n\},$$

we consider a solution $y_n \in V_n$ of the equation

$$\langle A(y_n), v_j \rangle_{V', V} = \langle \ell, v_j \rangle_{V', V}, \text{ for } j = 1, \dots, n. \quad (2.14)$$

By using the expression $y_n = \sum_{i=1}^n c_i v_i$, problem (2.14) can be formulated as a system of nonlinear equations in \mathbb{R}^n .

Thanks to the properties of A , we may use Brouwer's fixed point theorem (see, e.g., [12, p. 723]) and get existence of a solution to (2.14), with the additional bound:

$$\|y_n\|_V \leq C,$$

with $C > 0$ a constant independent of n .

From Assumption 2.1 it follows that A is locally bounded [12, p. 740], which implies that there exist constants $r > 0$ and $\rho > 0$ such that

$$\|v\|_V \leq r \quad \Rightarrow \quad \|A(v)\|_V \leq \rho.$$

Consequently, it follows that

$$\begin{aligned} \langle A(y_n), v \rangle_{V', V} &\leq \langle A(y_n), y_n \rangle_{V', V} - \langle A(v), y_n \rangle_{V', V} + \langle A(v), v \rangle_{V', V} \\ &= \langle \ell, y_n \rangle_{V', V} - \langle A(v), y_n \rangle_{V', V} + \langle A(v), v \rangle_{V', V} \\ &\leq \|\ell\|_{V'} C + \rho C + \rho r, \end{aligned}$$

for all $n \geq 1$ and all $\|v\|_V \leq r$, and, therefore, the sequence $\{A(y_n)\}$ is bounded in V' .

Thanks to the reflexivity of the spaces and the boundedness of the sequences, there exists a subsequence $\{y_m\}_{m \in \mathbb{N}}$ and limit points $y \in V$ and $g \in V'$ such that

$$y_m \rightharpoonup y \text{ weakly in } V \quad \text{and} \quad A(y_m) \rightharpoonup g \text{ weakly in } V'.$$

For any $k \geq 1$, we know that

$$\langle A(y_m), v_k \rangle_{V', V} = \langle \ell, v_k \rangle_{V', V}, \text{ for all } m \geq k.$$

Consequently,

$$\langle g, v_k \rangle_{V', V} = \lim_{m \rightarrow \infty} \langle A(y_m), v_k \rangle_{V', V} = \langle \ell, v_k \rangle_{V', V}$$

and, since the latter holds for all $k \geq 1$, we get that

$$\langle g, v \rangle_{V', V} = \langle \ell, v \rangle_{V', V}, \text{ for all } v \in V.$$

Therefore, $g = \ell$ in V' . Additionally,

$$\langle A(y_m), y_m \rangle_{V', V} = \langle \ell, y_m \rangle_{V', V} \rightarrow \langle \ell, y \rangle_{V', V}, \quad \text{as } m \rightarrow \infty.$$

From the monotonicity of A ,

$$\langle A(y_m) - A(v), y_m - v \rangle_{V', V} \geq 0, \forall v \in V.$$

By passing to the limit, we then get that

$$\langle \ell - A(v), y - v \rangle_{V', V} \geq 0, \forall v \in V.$$

Taking $v = y - tw$, with $t > 0$ and $w \in V$, it then follows that

$$\langle \ell - A(y - tw), w \rangle_{V', V} \geq 0, \forall w \in V.$$

Thanks to the hemicontinuity of A and taking the limit as $t \rightarrow 0$, we finally get that

$$A(y) = \ell \text{ in } V'.$$

□

Example 2.2 (A semilinear equation). Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain, $u \in L^2(\Omega)$ and consider the following nonlinear boundary value problem:

$$-\Delta y + y^3 = u \quad \text{in } \Omega, \quad (2.15a)$$

$$y = 0 \quad \text{on } \Gamma. \quad (2.15b)$$

Weak formulation of the PDE. Multiplying the state equation by a test function $v \in C_0^\infty(\Omega)$ and integrating yields

$$\int_{\Omega} -\Delta y v \, dx + \int_{\Omega} y^3 v \, dx = \int_{\Omega} uv \, dx.$$

<http://www.springer.com/978-3-319-13394-2>

Numerical PDE-Constrained Optimization

De los Reyes, J.C.

2015, X, 123 p. 13 illus., 2 illus. in color., Softcover

ISBN: 978-3-319-13394-2