

Spectral Simulation Methods

Numerical solution of partial differential equations

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Chapter 1

Introduction

Context: The term *simulation* refers to the numerical (computer-aided) solution of *models*. In this introductory chapter, we discuss how models of physical reality are built and present different classes of models. These models are usually described mathematically by means of *differential equations*, i.e. the simulation is often (but not always) the numerical solution of a set of ordinary or partial differential equations.

1.1 Models

Models are usually approximations for the behavior of the physical world at certain specific length scales. For example, a model that explicitly describes atoms may be appropriate for length scales $\sim \text{nm}$, but we would not want to describe a “macroscopic” system with dimensions $\sim \text{mm}$ with such a model. Key to carrying out simulations is therefore to match the physical phenomena we want to describe with the appropriate models and the mathematical methods required for their solution.

Note: While we could describe even macroscopic systems with atomic-scale models, this is typically prohibited by the computer resources available to us. In addition, the core question we want to answer may be hidden in such a fine-grained atomic-scale model like the legendary needle in a haystack.

Figure 1.1 shows the vertical arrangement of *length scales* and their assignment to different levels of description. On the shortest length scale, a quantum mechanical description is usually necessary. This means that if we

want to resolve the world with Å resolution, we find ourselves at the level of quantum mechanics and all underlying models are of a quantum mechanical nature. This typically means a solution of the *Schrödinger equation*, as implemented in various methods, such as *density functional theory*, a many-body description of the quantum mechanical electronic system. This type of many-body description in contrast to *molecular dynamics* as a method on a larger length scale. larger length scale, it is not a description of point particles, but coupled fields, which makes the effort compared to compared to pure point mechanics. In point mechanics, we have to deal with three position and three velocity variables for each of the n interacting particles, whereas in a quantum mechanical many-body description we are dealing with a field with three n position variables each, namely $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n; t)$.

Note:

- $1 \text{ Å} = 10^{-10} \text{ m}$
- Atoms in our environment are held together by quantum mechanical phenomena. Models based on quantum mechanical principles are also called *ab-initio* (“from the beginning”) models. In English, such models are also referred to as “first principles” models. The fundamental equation that describes quantum mechanical objects is the *Schrödinger equation*. This itself is in fact already an approximation!
- The single-particle Schrödinger equation is $i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \hat{H} \Psi(\vec{r}, t)$. This is a partial differential equation for the location- and time-dependent scalar matter field $\Psi(\vec{r}, t)$, with Planck’s constant \hbar and the Hamilton operator \hat{H} , which contains the details of the model. An equation of motion for many interacting particles, as given by $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n; t)$ is described, is incomparably more extensive.
- “Semiclassical“ means that the motion of the particles is calculated according to classical mechanics, but the interactions between the particles are derived from quantum mechanical laws. This is of course an approximation that needs to be justified.
- “Mesoscopic” means that the model has an internal length scale and/or thermal fluctuations are important. These models usually operate on length scales above the atomic scale ($\sim \text{nm}$) but below the scales of our perception of the environment ($\sim \text{mm}$).

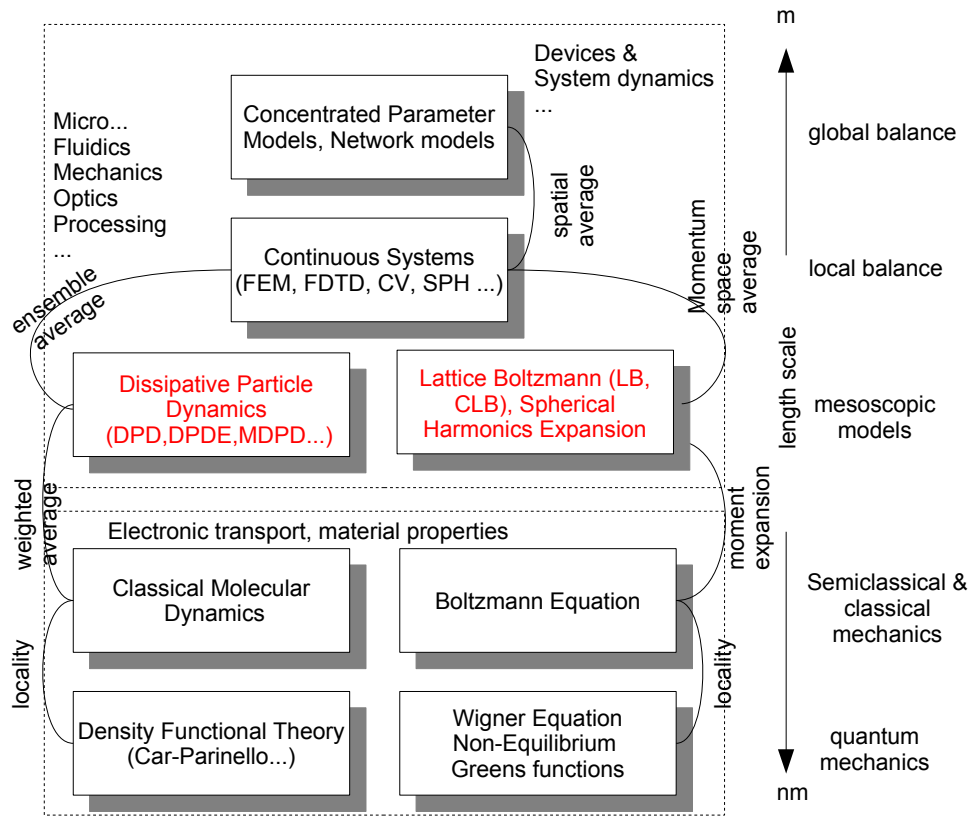


Figure 1.1: The vertical arrangement of the boxes represents the length scale, which is shown on the right. The boxes themselves contain simulation methods that are used on these scales. In this course we deal with the discretization of fields and choose a specific use case that falls into the *local balance*.

- “balance” means that the core of the description is a *conservation quantity* that can be easily counted. Preserved are e.g. particle numbers. A *balance equation* or balancing then simply counts the particles that flow into, out of or are produced in a volume over a certain time interval. Other conservation variables that can be balanced are momentum and energy. The balance equation is also called the *continuity equation*.

At the level of semiclassical and classical mechanics, also referred to as the kinetic level, the models are either described by molecular dynamics or by the equation of motion of the single-particle probability density in phase space $f(\vec{r}, \vec{p})$ - with the independent variables location \vec{r} and momentum \vec{p} . In the second case, we have a function $f(\vec{r}(t), \vec{p}(t), t)$ which of location, momentum and time both explicitly and implicitly via $\vec{r}(t)$ and $\vec{p}(t)$ depends. Let's assume that we need $f(\vec{r}(t), \vec{p}(t), t)$ must be interpolated by discrete sampling points. With a low resolution of 10 points per variable, this is already already 10,000,000 interpolation points. This may be manageable, but the resolution is not particularly good. And therefore this undertaking is rather useless. We do not want to conceal the fact that there are methods for the numerical solution to the two problems described above, but these will not be discussed in detail in this will not be discussed in detail in this course.

1.2 Particles

We can therefore roughly distinguish between two types of models: Models that have individual discrete elements, for example particles (atoms, molecules, grains, etc.), as the central element and models that have continuous fields (electrostatic potential, ion concentrations, mechanical stresses and strains) as the central element. In the first type of model, evolution equations are formulated for discrete properties defined on the particles, such as their positions \vec{r}_i and velocities \vec{v}_i .

For example, to describe the kinetics of these particles, we could solve Newton's equations of motion. This means that for each of the n particles we have to formulate 6 ordinary differential equations, which are still coupled to each other, namely:

$$\dot{\vec{r}}_i(t) = \vec{v}_i(t) = \frac{\vec{p}_i(t)}{m_i} \quad (1.1)$$

This is the equation for the trajectory of the particle i in space. Since \vec{r} is a vector, Eq. (1.1) is a system of 3 ordinary differential equations. The velocity \vec{v}_i of the particle i at time t is also subject to a system of differential equations due to the momentum \vec{p}_i system of differential equations:

$$\dot{\vec{p}}_i(t) = \sum_j \vec{F}_{ij}(t) \quad (1.2)$$

Equation (1.2) describes the temporal development of the momentum of the particle i . Equation (1.1) and (1.2) are each $3 \times n$ coupled ordinary differential equations. If, for example, we want to describe the movement of all molecules in a liter of water by a simulation, this is impossible due to the large number of equations and we must switch to a description using balance equations and fields.

Newton's equations of motion (1.1) and (1.2) are by their nature *physical basic principles*. They apply to atoms or planets. The nature of the force itself, \vec{F}_{ij} in the equations above, is of course based on physically describable effects, but is not necessarily a principle of nature. A simple example is the Lennard-Jones interaction, for which the interaction energy

$$V_{ij} = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (1.3)$$

and thus the force

$$\vec{F}_{ij} = -4\varepsilon \left[12 \left(\frac{\sigma^{12}}{r_{ij}^{13}} \right) - 6 \left(\frac{\sigma^6}{r_{ij}^7} \right) \right] \hat{r}_{ij} \quad (1.4)$$

where r_{ij} is the distance between the particles (here atoms or molecules) i and j . The term $\propto r^{-13}$ describes the repulsion of the atoms due to the Pauli exclusion principle and the term $\propto r^{-7}$ describes the attraction of the atoms due to the London dispersion interaction. Both interactions are based on fundamental physical principles, but the formulation Eq. (1.4) reduces these complex phenomena to a simple constituent law. Such laws are often called *constitutive laws*. The numerical solution of Newton's equations of motion for atoms is called *molecular dynamics simulation*.

Note: The term constitutive law often appears in the context of field theories. For the Lennard-Jones potential, this term is rather unusual, but this law is nevertheless of a constitutive nature.

Another example of models with discrete elements are network models for electrical circuits. Here, an element links a potential difference (energy difference) with a flowing current, for example describes

$$i = u/R \tag{1.5}$$

describes the current i that flows through a resistor R across which the voltage u drops. Kirchhoff's rules for current and voltage are also used. Such models are often referred to as "lumped-element models". Equation (1.5) naturally also has the quality of a *constitutive law*, as complex electronic processes are behind the individual parameter R . Kirchhoff's rules, on the other hand, have the quality of a *balance equation*. In Fig. 1.1, these models are therefore referred to as *global balance*. "Lumped-element models" also lead to systems of ordinary differential equations, which are often solved numerically by explicit time propagation. Well-known representatives of this type of simulation software are, for example *SPICE* or *MATLAB Simulink*.

This global image level is characterized by a lack of interest in local resolution. We are not interested not in densities, but only in total masses, not in current densities but only for currents. This is best illustrated by the above-mentioned resistor whose contacts are at different potentials. This results in a current flow in the simplest case. We do not ask ourselves how the current is distributed in the resistor. We do not even ask whether the resistor is homogeneous or inhomogeneous, we take it as a total value, as a black box to which we assign a parameter value. This approach has already been discussed in detail in electrical engineering and systems theory.

1.3 Fields

However, if we now realize that the black box is only insufficiently described with one parameter, then we start replace it with a more complex equivalent circuit with details that resolve the internal state of the component. This in turn can be taken so far, that a continuum is created at the end - we have arrived at the *local image level*. For this, we need parameters such as conductivity, viscosity or diffusivity. viscosity or diffusivity, which in turn cannot be derived as models from the continuous continuous description of the local balance. For example, experiments or *ab-initio* simulations are needed to determine these parameters.

Local balance means that we can assign a density, concentration, temperature or similar quantity to the system at each point in space. can be assigned. However, this means that the temporal changes in the local degrees of freedom - i.e. the momentum or velocity - are determined in their distribution by a

local, thermodynamic equilibrium condition determined. (In thermodynamic equilibrium, the momentum satisfies a Maxwell-Boltzmann distribution). This local equilibrium does not mean that we no longer have dynamics. But if we think of a swarm of gas or liquid particles, then their individual velocities follow an equilibrium individual velocities follow an equilibrium distribution function, but their mean follows the balance equation. The dynamics are therefore averaged over over a huge number of these particles. Local balance also does not mean that different temperatures or densities cannot exist at different locations. densities at different locations. The differences in these parameters are then the driving forces of the dynamics - temperature gradient, density gradient, etc.

Such models fall into the field of field theories, and their mathematical description is based on *partial* differential equations. differential equations. (This is in contrast to the ordinary differential equations of discrete models). A field theory based on the balancing of mass, momentum or energy always requires constitutive laws for the description of the material behavior. These constitutive laws contain *transport parameters* such as the viscosity or diffusion constant. There are also field theories that have the character of a basic physical principle. This is, for example, the Schrödinger equation mentioned above or the Maxwell equations of electrodynamics. In this course we want to concentrate on such continuous systems that are formulated as field theory with the help of partial differential equations.

1.4 Which model is the right one?

Mind you, we have not assigned any of the levels of description on different length scales with any value. Just because it is called quantum mechanics and leaves one or the other in awe at its complexity, it does not awe at its complexity, it does not necessarily offer the solution. On the contrary On the contrary, it can even be a hindrance to want to resolve too much detail and we must constantly ask ourselves how much detail is necessary in the simulation. is necessary. Even more, we always ask ourselves before we start a simulation: “Is a simulation of this complexity really necessary, or can I simplify the problem?” The simulation should be seen as a tool and not as an end in itself, according to the American mathematician American mathematician Richard Wesley Hamming (*1915, †1998): *The purpose of computing is insight, not numbers.*

Chapter 2

Differential equations

Context: Most of the phenomena we encounter in engineering are very well described by differential equations. We remember the discrete network models from electrical engineering and systems theory. They are, for example, by a system of linear ordinary differential equations with time as an independent variable. We also remember the diffusion process, such as the heat transport in a component on a heat sink that is exposed to a heat source. This phenomenon is best explained using a partial differential equation (partial differential equation). In this chapter we deal with an abstract classification of differential equations. The diffusion process will be repeated in more detail in the next chapter.

2.1 Ordinary differential equations

We recall the classification (properties) of *ordinary* differential equations (GDGLs) and recognize the different types of differential equations. For all these differential equations, we are always interested in a solution for a certain initial value (or boundary value), e.g. $x(t=0) = x_0$ etc. This initial value is always part of the definition of the differential equation.

2.1.1 Linearity

A linear differential equation is, for example

$$m\ddot{x}(t) + c\dot{x}(t) + kx = f(t) \tag{2.1}$$

which describes the damped and driven harmonic oscillator, while

$$\frac{d^2 x}{dt^2} + \mu(x^2 - 1)\frac{dx}{dt} + x = 0 \quad (2.2)$$

is a non-linear equation of motion for x . It describes the so-called van der Pol oscillator. The non-linearity can be recognized here by the fact that x^2 multiplies the derivative dx/dt .

Note: The first or higher order derivative is a linear operation, since

$$\frac{d^n}{dx^n} \lambda f(x) = \lambda \frac{d^n}{dx^n} f(x) \quad (2.3)$$

for a constant λ and

$$\frac{d^n}{dx^n} [f(x) + g(x)] = \frac{d^n}{dx^n} f(x) + \frac{d^n}{dx^n} g(x). \quad (2.4)$$

Time derivatives are displayed with a dot,

$$\dot{x}(t) = \frac{d}{dt} x(t). \quad (2.5)$$

For functions of a variable, the derivative is often displayed with a dash,

$$f'(x) = \frac{d}{dx} f(x). \quad (2.6)$$

This is no longer possible for functions with several variables. We will therefore always explicitly use the differential operator here.

2.1.2 Order

The order of a differential equation is given by the highest derivative that appears in the equation. Eq. (2.1) and Eq. (2.2) are examples of second-order differential equations.

2.1.3 Systems

A system of first-order differential equations is formed, for example, by the equations

$$\frac{dx}{dt} = x(m - ny), \quad (2.7)$$

$$\frac{dy}{dt} = -y(\gamma - \delta x), \quad (2.8)$$

the well-known Räuber-Beute equations or Lotka-Volterra equations. Equations (2.7) and (2.8) are still non-linear.

Differential equations of higher order can be rewritten into a system of 1st order equations. In the example of the damped harmonic oscillator,

$$m\ddot{x}(t) + c\dot{x}(t) + kx = f(t), \quad (2.9)$$

we replace $\dot{x} = y$ and thus obtain two first-order equations order instead of the original second-order equation, namely

$$\dot{x} = y \quad (2.10)$$

$$m\dot{y} = -cy - kx + f(t) \quad (2.11)$$

2.2 Partial differential equations

Partial differential equations (PDGLs) are differential equations with more than one independent variable. As an example, we imagine a time-dependent arm transport problem in one dimension. one dimension. This is represented by a diffusion equation for the local temperature temperature of the system. The temperature is therefore represented as a function of two independent variables, the time t and the spatial position x , is represented: $T(x, t)$. The time evolution of the temperature is given by

$$\frac{\partial T(x, t)}{\partial t} = \kappa \frac{\partial^2 T(x, t)}{\partial x^2}, \quad (2.12)$$

where κ denotes the Wärm conduction coefficient. This equation was developed by Joseph Fourier (*1768, †1830), whom we will encounter again during this course.

Note: In Eq. (2.12) $\partial/\partial t$ denotes the *partial derivative*. This is the derivative with respect to one of the arguments (here t), i.e. the variation of the function if all other arguments are kept constant. With GDGLs, in contrast to PDGLs, only derivatives with respect to one variable (usually the time t) occur, which are then denoted by the differential operator d/dt .

2.2.1 First order

Quasilinear PDGLs of the first order, i.e. equations of the form

$$P(x, t; u) \frac{\partial u(x, t)}{\partial x} + Q(x, t; u) \frac{\partial u(x, t)}{\partial t} = R(x, t; u), \quad (2.13)$$

for an (unknown) function $u(x, t)$ and the initial condition $u(x, t = 0) = u_0(x)$ can be systematically traced back to a system of coupled first-order GDGLs. We want to investigate this important property.

Note: In Eq. (2.13) a representation with two variables x and t was chosen for illustration. In general, we can write

$$\sum_i P_i(\{x_i\}; u) \frac{\partial u(\{x_i\})}{\partial x_i} = R(\{x_i\}; u) \quad (2.14)$$

The notation used here is $u(\{x_i\}) = u(x_0, x_1, x_2, \dots)$, i.e. the curly brackets denote all degrees of freedom x_i .

Equation (2.13) can be transformed to a system of GDGLs. This is called the method of characteristics. We can then apply the formalisms (analytical or numerical) for solving systems of GDGLs that we learned about in the lecture “Differential Equations”.

We proceed as follows:

1. First, we parameterize the independent variables in Eq. (2.13) with a parameter s according to $x(s)$ and $t(s)$.
2. We then form the *total derivative* of $u(x(s), t(s))$ to s

$$\frac{du(x(s), t(s))}{ds} = \frac{\partial u(x(s), t(s))}{\partial x} \frac{dx(s)}{ds} + \frac{\partial u(x(s), t(s))}{\partial t} \frac{dt(s)}{ds}. \quad (2.15)$$

3. By comparing the coefficients of the total derivative (2.15) with the PDGL (2.13), you can see that this DGL is solved exactly when

$$\frac{dx(s)}{ds} = P(x, t, u), \quad (2.16)$$

$$\frac{dt(s)}{ds} = Q(x, t, u) \quad \text{und} \quad (2.17)$$

$$\frac{du(s)}{ds} = R(u(s)). \quad (2.18)$$

is fulfilled. This describes the solution along certain curves in the (x, t) -plane.

We have thus converted the PDGL into a set of coupled first-order GDGLs, Eq. (2.21)-(2.23).

Example: The transport equation

$$\frac{\partial u(x, t)}{\partial t} + c \frac{\partial u(x, t)}{\partial x} = 0 \quad (2.19)$$

with the initial condition $u(x, t = 0) = u_0(x)$ is to be solved. We proceed according to the recipe above:

1. We parameterize the variables x and t with the help of a new variable s , i.e. $x(s)$ and $t(s)$. We are now looking for an expression with which we can determine $x(s)$ and $t(s)$.
2. We now ask how the function $u(x(s), t(s))$ behaves. This function describes the change in an initial value $u(x(0), t(0))$ with the variable s . The total derivative becomes

$$\frac{du(x(s), t(s))}{ds} = \frac{\partial u}{\partial t} \frac{dt(s)}{ds} + \frac{\partial u}{\partial x} \frac{dx(s)}{ds}. \quad (2.20)$$

3. The total derivative is identical to the partial differential equation that we want to solve if

$$\frac{dx(s)}{ds} = c \quad \text{and} \quad (2.21)$$

$$\frac{dt(s)}{ds} = 1. \quad (2.22)$$

In this case, the following applies

$$\frac{du(s)}{ds} = 0. \quad (2.23)$$

4. The general solutions for the three ordinary differential equations (2.21)-(2.23) are given by

$$x(s) = cs + \text{const.}, \quad (2.24)$$

$$t(s) = s + \text{const.} \quad \text{and} \quad (2.25)$$

$$u(s) = \text{const.} \quad (2.26)$$

5. With the initial conditions $t(0) = 0$, $x(0) = \xi$ and $u(x, t = 0) = f(\xi)$ you get $t = s$, $x = ct + \xi$ and $u = f(\xi) = f(x - ct)$,

The initial condition $f(\xi)$ is transported with the speed c in the positive x -direction. The solution for u remains constant, as the derivative of u is zero, so u retains the value given by the initial condition. The field $u(x, 0)$ is therefore shifted at a constant speed c : $u(x, t) = u(x - ct, 0)$.

2.2.2 Second order

Examples of second-order PDGLs are the...

- ...wave equation:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0 \quad (2.27)$$

- ...diffusion equation (which we will look at in more detail here):

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0 \quad (2.28)$$

- ...Laplace equation (which we will also get to know better):

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad (2.29)$$

The second order here refers to the second derivative. These examples are formulated for two variables, but these differential equations can also be written down for more degrees of freedom.

For two variables, the general form of second-order linear PDGLs is

$$a(x, y) \frac{\partial^2 u}{\partial x^2} + b(x, y) \frac{\partial^2 u}{\partial x \partial y} + c(x, y) \frac{\partial^2 u}{\partial y^2} = F \left(x, y; u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \right), \quad (2.30)$$

where F itself must of course also be linear in the arguments if the entire equation is to be linear. We now classify 2nd order PDGLs, but note that this classification is not exhaustive and that it only applies pointwise. The latter means that the PDGL can fall into a different classification at different points in space.

We first assume that $F = 0$ and a, b, c are constant. Then we get:

$$a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2} = 0. \quad (2.31)$$

We rewrite this equation as the quadratic form

$$\begin{pmatrix} \partial/\partial x \\ \partial/\partial y \end{pmatrix} \cdot \begin{pmatrix} a & b/2 \\ b/2 & c \end{pmatrix} \cdot \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \end{pmatrix} u = \nabla \cdot \underline{C} \cdot \nabla u = 0 \quad (2.32)$$

We can now diagonalize the coefficient matrix \underline{C} . This for to

$$\underline{C} = \underline{U} \cdot \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \cdot \underline{U}^T, \quad (2.33)$$

where \underline{U} is unitary due to the symmetry of \underline{C} , $\underline{U}^T \cdot \underline{U} = \underline{1}$. The geometric interpretation of the operation \underline{U} is a rotation. We now introduce transformed coordinates x' and y' so that

$$\nabla = \underline{U} \cdot \nabla' \quad (2.34)$$

with $\nabla' = (\partial/\partial x', \partial/\partial y')$. In other words, the transformation matrix is given as

$$\underline{U} = \begin{pmatrix} \partial x'/\partial x & \partial y'/\partial x \\ \partial x'/\partial y & \partial y'/\partial y \end{pmatrix}. \quad (2.35)$$

Equation (2.31) becomes

$$\lambda_1 \frac{\partial^2 u}{\partial x'^2} + \lambda_2 \frac{\partial^2 u}{\partial y'^2} = 0. \quad (2.36)$$

We have diagonalized the coefficients of the differential equation. For any twice differentiable function $f(z)$, is

$$u(x', y') = f\left(\sqrt{\lambda_2} x' + i\sqrt{\lambda_1} y'\right) \quad (2.37)$$

a solution of Eq. (2.36).

The analytical expression for the eigenvalues is:

We now distinguish three cases:

- The case $\det \underline{C} = \lambda_1 \lambda_2 = ac - b^2/4 = 0$ with $b \neq 0$ and $a \neq 0$ leads to a parabolic PDGL. This PDGL is called parabolic because the quadratic form Eq. (2.32) or (2.33) describes a parabola. (This is of course an analogy. You have to replace the differential operators with coordinates for this to work). Without restriction of generality, let $\lambda_2 = 0$. Then we get

$$\frac{\partial^2 u}{\partial x'^2} = 0. \quad (2.38)$$

This is the canonical form of a parabolic PDGL.

- The case $\det \underline{C} = \lambda_1 \lambda_2 = ac - b^2/4 > 0$ leads to an elliptic PDGL. This PDGL is called elliptic because the quadratic form Eq. (2.32) or (2.33) describes an ellipse for a constant right-hand side. (For $\lambda_1 = \lambda_2$ it is a circle). We now convert the equation for the elliptical case to a standardized form and introduce the scaled coordinates $x' = \sqrt{\lambda_1} x''$ and $y' = \sqrt{\lambda_2} y''$. Eq. (2.36) then becomes the canonical elliptic PDGL

$$\frac{\partial^2 u}{\partial x''^2} + \frac{\partial^2 u}{\partial y''^2} = 0. \quad (2.39)$$

The canonical elliptic PDGL is therefore the Laplace equation, Eq. (2.39) (here in two dimensions). Solutions of the Laplace equation are called *harmonic functions*.

- The case $\det \underline{C} = \lambda_1 \lambda_2 = ac - b^2/4 < 0$ results in the so-called hyperbolic PDGL. This PDGL is called hyperbolic because the quadratic form Eq. (2.32) or (2.33) for a constant right-hand side describes a hyperbola. Without restricting the generality, we now require $\lambda_1 > 0$ and $\lambda_2 < 0$. Then we can again introduce scaled coordinates $x' = \sqrt{\lambda_1} x''$ and $y' = \sqrt{-\lambda_2} y''$ so that

$$\frac{\partial^2 u}{\partial x''^2} - \frac{\partial^2 u}{\partial y''^2} = \begin{pmatrix} \partial u / \partial x'' \\ \partial u / \partial y'' \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} \partial u / \partial x'' \\ \partial u / \partial y'' \end{pmatrix} = 0. \quad (2.40)$$

We can now use a further coordinate transformation, namely a rotation by 45° , to bring the coefficient matrix in Eq. (2.40) to a form in which the diagonal elements are 0 and the secondary diagonal elements are 1. This results in the differential equation

$$\frac{\partial^2 u}{\partial x''' \partial y'''} = 0, \quad (2.41)$$

where x''' and y''' are the corresponding rotated coordinates. This equation is the canonical form of a hyperbolic PDGL and equivalent to Eq. (2.31) in the new variables x''' and y''' .

For higher dimensional problems, we need to look at the eigenvalues of the coefficient matrix \underline{C} . The PDGL is called *parabolic* if there is an eigenvalue that vanishes, but all other eigenvalues are either greater or less than zero. The PDGL is called *elliptic* if all eigenvalues are either greater than zero or less than zero. The PDGL is called *hyperbolic* if there is exactly one negative eigenvalue and all others are positive or if there is exactly one positive eigenvalue and all others are negative. It is clear that for PDGLs with more than two variables, these three classes of PDGLs are not exhaustive and there are coefficient matrices that fall outside this classification scheme. For problems with exactly two variables, this classification leads to the conditions for the determinants of the coefficient matrix mentioned above.

These three types of 2nd order linear PDEs can also be solved analytically for some problems can also be solved analytically. In the following we give an example of this.

Example: We solve the one-dimensional wave equation.

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = 0 \quad (2.42)$$

by separating the variables. To do this, we take the approach $u(x, t) = X(x)T(t)$, which leads to

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} = \frac{1}{c^2} \frac{1}{T} \frac{\partial^2 T}{\partial t^2} \quad (2.43)$$

leads. In Eq. (2.43), the left-hand side depends only on the variable x , while the right-hand side depends only on t . For any x and t , this equation can only be equation can only be fulfilled if both sides are equal to a constant and we thus obtain

$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} = -k^2 = \frac{1}{c^2} \frac{1}{T} \frac{\partial^2 T}{\partial t^2}. \quad (2.44)$$

This results in the following two equations

$$\frac{\partial^2 X}{\partial x^2} + k^2 X = 0$$

with the solution $X(x) = e^{\pm ikx}$ and

$$\frac{\partial^2 T}{\partial t^2} + \omega^2 T = 0$$

with the solution $T(t) = e^{\pm i\omega t}$, where we have set $\omega^2 = c^2 k^2$. have set. This example needs initial conditions to be completed so that we can find a solution.

Chapter 3

Transport theory

Context: This learning module introduces the basics of the model problem, which we will solve with numerical methods during the course. First of all, it deals with the basics of transport theory.

3.1 Diffusion and drift

Diffusive transport is easily accessible via the image of the “random walk”, a random stochastic movement of particles. Such random motion processes were first described by the botanist *Robert Brown* (1773-1858) and are called *Brownian motion* or *Brownian molecular motion*. However, Robert Brown did not know about molecules at the time and thought during his lifetime that this movement was due to active processes (the “life force” of the pollen). Today we know that this movement is caused by thermal fluctuations, i.e. molecules that randomly hit the pollen and push it in one direction. This explanation requires the existence of atoms and was only popularized in 1905 by Albert Einstein (?).

Brownian molecular motion leads to diffusive transport. Figure 3.1 shows a simple qualitative thought experiment. The configuration in Fig. 3.1a shows a localization of the “pollen” in the left half of the domain shown. Due to their random movement (shown as an example by the red line in Fig. 3.1a), some of the pollen will cross the dashed boundary line into the right half and also come back again. After a certain time, the initial state can no longer be identified and the pollen is distributed throughout the domain (Fig. 3.1b). The concentration is now constant. The pollen continues to move, but on average the same number of pollen moves to the left as to the right. In the case shown in Fig. 3.1a, this symmetry is broken.

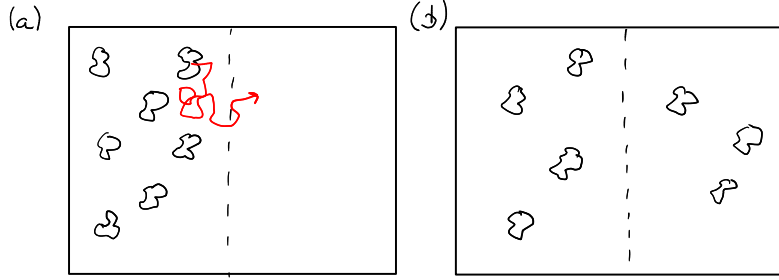


Figure 3.1: Illustration of a diffusion process. The “pollen” in (a) move randomly in the domain shown. After a certain time (b), the initial concentration difference between the left and right parts of the domain is equalized.

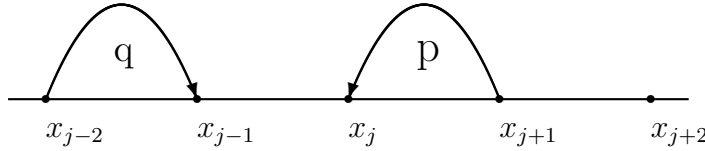


Figure 3.2: Random movement in one dimension is given by transition probabilities p (for a movement to the left) and q for a movement to the right.

This thought experiment can be easily formalized mathematically. We consider a particle that performs a random movement in one dimension is performed. We start with a particle that randomly jumps back and forth on a straight line. back and forth. The straight line lies along the x-direction. The particle can only move to predetermined positions on the x-axis, which we denote by x_j and which are equidistantly distributed, $x_j - x_{j-1} = \Delta x$ for $j \in \mathbb{Z}$ (see Fig. 3.2).

A particle jumps to the left with a probability p and to the right with a probability probability q to the right. In addition, we have the probability of finding a particle at all at time t at position x . This is given on the 1D grid by the function $P(x, t)$.

3.1.1 Diffusion

We first consider the case $p = q = 1/2$, i.e. that the probabilities for the jumps to the left and right are identical. We assume that the particle jumps from one place to the neighboring one in a discrete, finite and constant time step τ . Then the probability of finding a particle at time $t + \tau$ at location x is if at time t there is a probability $P(x - \Delta x, t)$ of finding a particle at position particle could be found at the position $x - \Delta x$ and with the probability

$P(x + \Delta x, t)$ of one at $x + \Delta x$, given by

$$P(x, t + \tau) = \frac{1}{2}P(x + \Delta x, t) + \frac{1}{2}P(x - \Delta x, t). \quad (3.1)$$

By subtracting $P(x, t)$ on both sides and dividing by τ , we obtain the following equivalent form:

$$\frac{P(x, t + \tau) - P(x, t)}{\tau} = \frac{\Delta x^2}{2\tau} \frac{P(x + \Delta x, t) - 2P(x, t) + P(x - \Delta x, t)}{\Delta x^2} \quad (3.2)$$

We can now make the limit transition to the “continuum”. For $\tau \rightarrow 0$ and at the same time $\Delta x \rightarrow 0$ under the condition that

$$\lim_{\Delta x \rightarrow 0, \tau \rightarrow 0} \frac{\Delta x^2}{2\tau} = D \quad (3.3)$$

you get

$$\frac{\partial P(x, t)}{\partial t} = D \frac{\partial^2 P(x, t)}{\partial x^2}. \quad (3.4)$$

This is the well-known diffusion equation. In several dimensions, the second derivative becomes the Laplace operator ∇^2 ,

$$\frac{\partial P(x, t)}{\partial t} = D \nabla^2 P(x, t). \quad (3.5)$$

This equation is only correct if the diffusion constant is actually constant and does not vary spatially.

3.1.2 Drift

What happens if the probabilities for the jumps to the right or left are not equal right or left are not equal, $p \neq q$ (but of course $p + q = 1$)? We still assume discrete, uniform time steps and equidistant sampling points.

In this case, we have

$$P(x, t + \tau) = pP(x + \Delta x, t) + qP(x - \Delta x, t) \quad (3.6)$$

and therefore follows

$$\frac{P(x, t + \tau) - P(x, t)}{\tau} = \frac{\Delta x^2}{\tau} \frac{pP(x + \Delta x, t) - P(x, t) + qP(x - \Delta x, t)}{\Delta x^2}. \quad (3.7)$$

We write

$$p = \frac{1}{2} - \varepsilon \quad \text{and} \quad q = \frac{1}{2} + \varepsilon \quad \text{with} \quad 0 \leq |\varepsilon| \leq \frac{1}{2} \quad \text{or} \quad 2\varepsilon = q - p, \quad (3.8)$$

where ε now indicates how much more likely a jump to *right* is than to the left. A positive ε therefore means that the particles will move to the right on average – this is the drift movement. We can now express Eq. (3.7) using ε as

$$\frac{P(x, t + \tau) - P(x, t)}{\tau} = \frac{\Delta x^2}{2\tau} \frac{P(x + \Delta x, t) - 2P(x, t) + P(x - \Delta x, t)}{\Delta x^2} - \frac{2\varepsilon \Delta x}{\tau} \frac{P(x + \Delta x, t) - P(x - \Delta x, t)}{2\Delta x} \quad (3.9)$$

express. In the limiting cases $\tau \rightarrow 0$ and $\Delta x \rightarrow 0$ we require

$$\lim_{\Delta x \rightarrow 0, \tau \rightarrow 0} \frac{\Delta x^2}{2\tau} = D \quad \text{and} \quad \lim_{\Delta x \rightarrow 0, \tau \rightarrow 0} \frac{2\varepsilon \Delta x}{\tau} = v \quad (3.10)$$

and thus obtain the drift-diffusion equation

$$\frac{\partial P(x, t)}{\partial t} = \left(D \frac{\partial^2}{\partial x^2} - v \frac{\partial}{\partial x} \right) P(x, t). \quad (3.11)$$

Here, the first summand on the right-hand side again describes the diffusion process. The second summand is a drift process and v is a constant *drift* velocity. (From Eq. (3.10) and (3.11) it can be seen that the unit of v corresponds exactly to a velocity). It is the speed at which the particle moves (on average) along the x -axis. The solution to this equation has already been discussed in the previous chapter. From the solution of the previous chapter, it is also clear that the drift motion for positive v is in the direction of the positive x -axis. This is consistent with the above definition of ε .

Note: The motion of our particle was modeled using a residence *probability* P . In the thermodynamic limit, i.e. for many particles (usually of the order of Avogadro's number N_A), this probability becomes the density ρ or the concentration c . We can therefore simply replace the probability P in the above equations with a particle concentration c . The reason for this is that we can write the particle concentration as an *ensemble* mean,

$$c(x, t) = \langle 1 \rangle(x, t), \quad (3.12)$$

where the mean value

$$\langle f(x) \rangle(x, t) = f(x)P(x, t). \quad (3.13)$$

3.2 Continuity

The equations (3.5) and (3.11) mix two concepts that we want to treat separately here: The conservation of the number of particles (continuity) and the process that leads to a flow of particles (diffusion or drift). The number of particles is conserved simply because we cannot create atoms out of nothing or destroy them into nothing. So, if we have a certain number of particles N_{tot} in our overall system, we know that this number is

$$N_{\text{tot}} = \int d^3 r c(\vec{r}) \quad (3.14)$$

cannot change over time: $dN_{\text{tot}}/dt = 0$.

For a small section with volume V from this total volume, the number of particles can change because they can flow over the walls of the sample volume (see Fig. 3.3). The change in the number of particles is given by

$$\dot{N} = \frac{\partial}{\partial t} \int_V d^3 r c(\vec{r}, t) = \int_V d^3 r \frac{\partial c}{\partial t}. \quad (3.15)$$

However, the change \dot{N} must also be given by the number of particles flowing down the side walls. For a cube (Fig. 3.3) with six walls, the following applies

$$\begin{aligned} \dot{N} = & -j_{\text{right}} A_{\text{right}} - j_{\text{left}} A_{\text{left}} \\ & -j_{\text{above}} A_{\text{above}} - j_{\text{bottom}} A_{\text{bottom}} \\ & -j_{\text{front}} A_{\text{front}} - j_{\text{back}} A_{\text{back}} \end{aligned} \quad (3.16)$$

if the walls are small enough so that j is almost constant over A . (The current density j has the unit number of particles/time/area).

Here the scalar current j denotes the current flowing out of the surface. For a general vectorial current density \vec{j} , which indicates the strength and direction of the particle current, $j_i = \vec{j}_i \cdot \hat{n}_i$ where \hat{n}_i is the normal vector to the wall i . The current through the wall is therefore only the component of \vec{j} that is parallel to the surface normal. With this argument, we can generally express the change in the number of particles as

$$\dot{N} = - \int_{\partial V} d^2 r \vec{j}(\vec{r}) \cdot \hat{n}(\vec{r}) \quad (3.17)$$

where ∂V denotes the surface area of the volume V . This equation explicitly indicates that both the flux \vec{j} and the surface normal \hat{n} depend on the position \vec{r} on the surface.

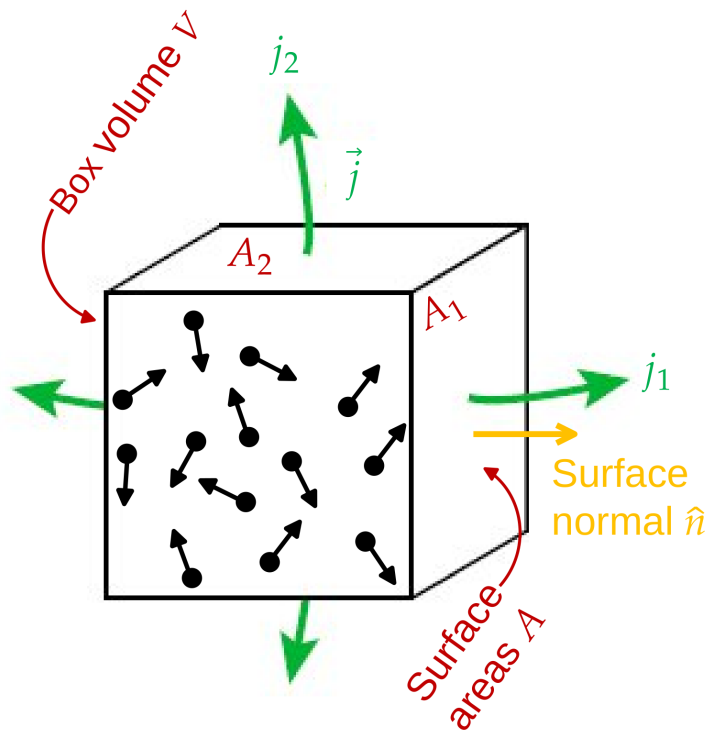


Figure 3.3: Particles can only leave the volume V through the side walls. The change in the number of particles N over a time interval τ is therefore given by the number of particles flowing through the walls. For this we need the particle flows j . The number of particles flowing through a surface is then given by $j A \tau$, where A is the area of the side wall

Alternatively, we can also group the change in the number of particles Eq. (3.16) as follows:

$$\begin{aligned}\dot{N} = & -(j_{\text{right}} + j_{\text{left}})A_{\text{right/left}} \\ & -(j_{\text{top}} + j_{\text{bottom}})A_{\text{top/bottom}} \\ & -(j_{\text{front}} + j_{\text{rear}})A_{\text{front/back}}\end{aligned}\quad (3.18)$$

Here we have used the fact that $A_{\text{right}} = A_{\text{left}} \equiv A_{\text{right/left}}$. But now

$$\begin{aligned}j_{\text{right}} &= \hat{x} \cdot \vec{j}(x + \Delta x/2, y, z) = j_x(x + \Delta x/2, y, z) \quad \text{and} \\ j_{\text{left}} &= -\hat{x} \cdot \vec{j}(x - \Delta x/2, y, z) = -j_x(x - \Delta x/2, y, z)\end{aligned}\quad (3.19)$$

since $\hat{n} = \hat{x}$ for the right wall but $\hat{n} = -\hat{x}$ for the left wall. Here, \hat{x} is the normal vector along the x -axis of the coordinate system. The sign of the surface normal is therefore reversed between the right and left surfaces. The same applies to the top/bottom and front/back walls. We can further rewrite this equation as

$$\begin{aligned}\dot{N} = & -\frac{j_x(x + \Delta x/2, y, z) - j_x(x - \Delta x/2, y, z)}{\Delta x}V \\ & -\frac{j_y(x, y + \Delta y/2, z) - j_y(x, y - \Delta y/2, z)}{\Delta y}V \\ & -\frac{j_z(x, y, z + \Delta z/2) - j_z(x, y, z - \Delta z/2)}{\Delta z}V,\end{aligned}\quad (3.20)$$

since $V = A_{\text{right/left}}\Delta x = A_{\text{top/bottom}}\Delta y = A_{\text{front/back}}\Delta z$. However, the factors in front of the volume V in Eq. (3.20) are now exactly the difference quotients of the flows j_i , in the x , y and z directions respectively. For small volumes (and small Δx , etc.) this becomes

$$\dot{N} = -\int_V d^3r \nabla \cdot \vec{j}(\vec{r}).\quad (3.21)$$

We have just heuristically derived Gauss's theorem ("divergence theorem" - see also Eq. (3.22)) to express Eq. (3.17) as a volume integral.

Note: Gauss's theorem is an important result of vector analysis. It converts an integral over a volume V into an integral over the surface ∂V of this volume. For a vector field $\vec{f}(\vec{r})$ applies:

$$\int_V d^3r \nabla \cdot \vec{f}(\vec{r}) = \int_{\partial V} d^2r \vec{f}(\vec{r}) \cdot \hat{n}(\vec{r})\quad (3.22)$$

Here $\hat{n}(\vec{r})$ is the normal vector which points outwards on the edge ∂V of the volume V .

Equation (3.15) and (3.21) together result in

$$\int_V d^3 r \left\{ \frac{\partial c}{\partial t} + \nabla \cdot \vec{j} \right\} = 0. \quad (3.23)$$

Since this applies to any volume V , the following must also be true

$$\frac{\partial c}{\partial t} + \nabla \cdot \vec{j} = 0 \quad (3.24)$$

must be fulfilled. This equation is called *continuity equation*. It describes the conservation of the number of particles or the mass of the system.

Note: In the derivation presented here, we have already implicitly used the *strong* formulation and a *weak* formulation (“weak formulation”) of a differential equation. Equation (3.24) is the strong formulation of the continuity equation. This requires that the differential equation is satisfied for every spatial point \vec{r} . The corresponding weak formulation is Eq. (3.23). Here it is only required that the equation is fulfilled in a kind of mean value, here as an integral over a sample volume V . Within the volume, the strong form need not be satisfied, but the integral over these deviations (which we will later call “residuum”) must vanish. The weak formulation is thus an approximation for finite sample volumes V . In the finite element method, a weak equation is solved exactly for a certain (approximate) initial function. The weak formulation will therefore become important during this course.

We can still require that “particles” are produced within our sample volume. In the current interpretation of the equation, this would be, for example, chemical reactions that convert one type of particle into another. An identical equation applies to heat transport. Here, a source term would be the production of heat, e.g. by a heating element. Given a source flow Q (with unit number of particles/time/volume), the continuity equation can be reduced to

$$\frac{\partial c}{\partial t} + \nabla \cdot \vec{j} = Q \quad (3.25)$$

can be extended. The continuity equation with source term is also sometimes referred to as *balance equation*.

Note: Equation (3.25) describes the change in concentration c over time. A related question is how to solve this equation after a very long time - when a dynamic equilibrium has been reached. This equilibrium is characterized by the fact that $\partial c / \partial t = 0$. The equation

$$\nabla \cdot \vec{j} = Q \quad (3.26)$$

is the *stationary* variant of the continuity equation.

3.2.1 Drift

Let's come back to transport processes, first to drift. If all particles in our sample volume move with the speed \vec{v} , this leads to a particle flow

$$\vec{j}_{\text{drift}} = c\vec{v}. \quad (3.27)$$

When inserted into the continuity equation (3.24), this results in the drift contribution to the drift-diffusion equation (3.11).

3.2.2 Diffusion

From our thought experiment above, it is clear that the diffusion current must always go in the direction of the low concentration, i.e. in the opposite direction to the gradient ∇c of the concentration. The corresponding current is given by

$$\vec{j}_{\text{Diffusion}} = -D\nabla c. \quad (3.28)$$

When inserted into the continuity equation (3.24), this results in the diffusion equation (3.5).

The entire drift-diffusion equation therefore has the form

$$\frac{\partial c}{\partial t} + \nabla \cdot \{-D\nabla c + c\vec{v}\} = 0. \quad (3.29)$$

In contrast to equations (3.5) and (3.11), this equation also applies if the diffusion constant D or drift velocity \vec{v} varies spatially.

Note: We have introduced transport theory here in terms of a particle concentration c . However, the continuity equation generally describes the *conservation* of a certain quantity, in our case the number of particles

(or equivalently the mass). Other physically conserved quantities are momentum and energy. The continuity equation for the momentum leads to the Navier-Stokes equation. The continuity equation for the energy leads to the heat conduction equation.

Chapter 4

Numerical solution

Context: We will now put the transportation problem aside for a while and devote ourselves to the *numerical* solution of differential equations. This chapter shows the basics of the numerical analysis of differential equations and introduces a few important concepts, in particular the series expansion and the residual. The presentation here follows chapter 1 from ?.

4.1 Series expansion

In abstract notation, we are looking for unknown functions $u(x, y, z, \dots)$ that solve a set of differential equations

$$\mathcal{L}u(x, y, z, \dots) = f(x, y, z, \dots) \quad (4.1)$$

must be fulfilled. Here, \mathcal{L} is a (not necessarily linear) operator that contains the differential (or integral) operations. We now introduce an important concept for the (numerical) solution of the differential equation: We approximate the function u by a *series expansion*. We write

$$u_N(x, y, z, \dots) = \sum_{n=0}^N a_n \varphi_n(x, y, z, \dots) \quad (4.2)$$

where the φ_n are called “base functions”. We will discuss the properties of these basis functions in more detail in the next chapter.

We can now write the differential equation as,

$$\mathcal{L}u_N(x, y, z, \dots) = f(x, y, z, \dots). \quad (4.3)$$

This representation means that we have now replaced the question of the unknown function u with the question of the unknown coefficients a_n . We only have to let the differential operator \mathcal{L} act on the (known) basis functions φ_n and we can calculate this analytically.

What remains is to determine the coefficients a_n . These coefficients are numbers, and these numbers can be calculated by a computer. Equation (4.2) is of course an approximation. For certain basis functions, it can be shown that these are “complete” and can therefore represent certain classes of functions exactly. However, this is only true under the condition that the series Eq. (4.2) is extended to $N \rightarrow \infty$. For all practical applications (such as implementations in computer code), however, this series expansion must be aborted. A “good” series expansion approximates the exact solution already at low N with a small error. With this statement, we would of course have to specify how we want to quantify errors. Numerically, we then search for the exact coefficients a_n that minimize the error.

The choice of a good basis function is non-trivial. We will mainly use “finite elements” as basis functions here and briefly touch on other types. Before we go deeper into this topic, we need some more concepts to understand numerical analysis.

4.2 Residual

An important concept is that of *residuum*. Our goal is to solve Eq. (4.1). The exact solution would be $\mathcal{L}u - f \equiv 0$. However, since we can only construct an approximate solution, this condition will not be fulfilled exactly. We define the residual as exactly this deviation from the exact solution, namely

$$R(x, y, z, \dots; a_0, a_1, \dots, a_N) = \mathcal{L}u_N(x, y, z, \dots) - f(x, y, z, \dots). \quad (4.4)$$

The residual is therefore a kind of measure for the error we make. The strategy for numerically solving the differential equation Eq. (4.1) is now to determine the coefficients a_n in such a way that the residual Eq. (4.4) is minimal. We have thus mapped the solution of the differential equation to an optimization problem. The different numerical methods, which we will discuss in the next chapters, are mainly determined by the specific optimization strategy.

Note: Numerical methods for *optimization* are a central core of the numerical solution of differential equations and thus of simulation techniques. There are countless optimization methods that work better or worse in different situations. We will first treat such optimizers as “black boxes”.

At the end of the course, we will return to the question of optimization and discuss some well-known optimization methods. The term *minimization method* is often used synonymously with optimization methods. A good overview of optimization methods can be found in the book by ?.

4.3 A first example

We now want to concretize these abstract ideas using an example and introduce a few important terms. Let's look at the one-dimensional boundary value problem,

$$\frac{d^2 u}{dx^2} - (x^6 + 3x^2)u = 0, \quad (4.5)$$

with the boundary conditions $u(-1) = u(1) = 1$. (I.e. $x \in [-1, 1]$ is the domain on which we are looking for the solution.) In this case, the abstract differential operator \mathcal{L} takes the concrete form

$$\mathcal{L} = \frac{d^2}{dx^2} - (x^6 + 3x^2) \quad (4.6)$$

is given. The exact solution to this problem is given by

$$u(x) = \exp [(x^4 - 1)/4]. \quad (4.7)$$

We now guess an approximate solution as a series expansion for this equation. This approximate solution should already fulfill the boundary conditions. The equation

$$u_2(x) = 1 + (1 - x^2)(a_0 + a_1x + a_2x^2) \quad (4.8)$$

is constructed in such a way that the boundary conditions are fulfilled. We can express these as

$$u_2(x) = 1 + a_0(1 - x^2) + a_1x(1 - x^2) + a_2x^2(1 - x^2) \quad (4.9)$$

to exponentiate the basis functions $\varphi_i(x)$. Here $\varphi_0(x) = 1 - x^2$, $\varphi_1(x) = x(1 - x^2)$ and $\varphi_2(x) = x^2(1 - x^2)$. Since these basis functions are non-zero on the entire domain $[-1, 1]$, this basis is called a *spectral* basis. (Mathematically: The carrier of the function corresponds to the domain.)

In the next step, we must find the residual

$$R(x; a_0, a_1, a_2) = \frac{d^2 u_2}{dx^2} - (x^6 + 3x^2)u_2 \quad (4.10)$$

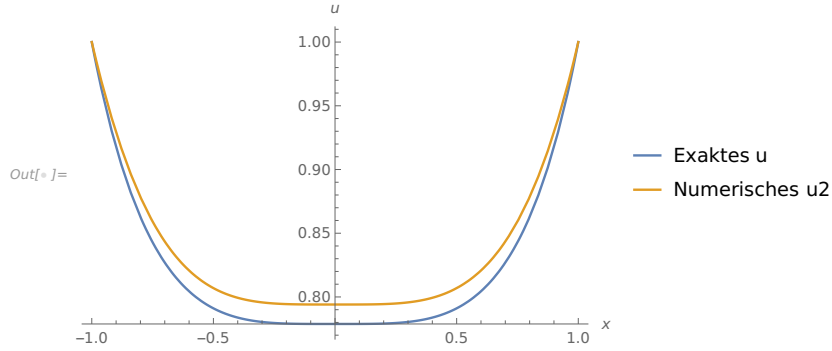


Figure 4.1: Analytical solution $u(x)$ and “numerical” approximate solution $u_2(x)$ of the GDGL (4.5).

minimize. For this we choose a strategy called *collocation*: We require that the residual vanishes exactly at three selected points:

$$R(x_i; a_0, a_1, a_2) = 0 \quad \text{for} \quad x_0 = -1/2, x_1 = 0 \text{ und } x_2 = 1/2. \quad (4.11)$$

Note: The disappearance of the residual at x_i does not mean that $u_2(x_i) \equiv u(x_i)$, i.e. that at x_i our approximate solution corresponds to the exact solution. We are still restricted to a limited set of functions, namely the functions covered by Eq. (4.8).

From the collocation condition we now get a linear system of equations with three unknowns:

$$R(x_0; a_0, a_1, a_2) \equiv -\frac{659}{256}a_0 + \frac{1683}{512}a_1 - \frac{1171}{1024}a_2 - \frac{49}{64} = 0 \quad (4.12)$$

$$R(x_1; a_0, a_1, a_2) \equiv -2(a_0 - a_2) = 0 \quad (4.13)$$

$$R(x_2; a_0, a_1, a_2) \equiv -\frac{659}{256}a_0 - \frac{1683}{512}a_1 - \frac{1171}{1024}a_2 - \frac{49}{64} = 0 \quad (4.14)$$

$$(4.15)$$

The solution of these equations results in

$$a_0 = -\frac{784}{3807}, \quad a_1 = 0 \quad \text{and} \quad a_2 = a_0. \quad (4.16)$$

Figure 4.1 shows the “numerical” solution $u_2(x)$ in comparison with the exact solution $u(x)$.

In the numerical example shown here, both the basis functions and the strategy for minimizing the residual can be varied. In the course of this

lecture, we will establish the finite elements as basis functions and use the Galerkin method as minimization strategy. To do this, we must first discuss properties of possible basis functions.

Note: The example shown here is a simple case of *discretization*. We have gone from a continuous function to the discrete coefficients a_0 , a_1 , a_2 .

Chapter 5

Function spaces

Context: Before we delve deeper into the numerical solution of partial differential equations, we need to introduce a slightly abstract concept here: The concept of *function spaces*, or more concretely *silver space*. Function spaces are useful because they formalize the series expansion and provide easy access to the coefficients of a series expansion through the concept of basis functions.

5.1 Vectors

As an introduction, let us recall the usual Cartesian vectors. We can represent a vector $\vec{a} = (a_0, a_1, a_2)$ as a linear combination of basis vectors \hat{e}_0 , \hat{e}_1 and \hat{e}_2 ,

$$\vec{a} = a_0\hat{e}_0 + a_1\hat{e}_1 + a_2\hat{e}_2, \quad (5.1)$$

can be written. The unit vectors \hat{e}_0 , \hat{e}_1 and \hat{e}_2 are of course the vectors that span the Cartesian coordinate system. (In previous chapters, the notation $\hat{x} \equiv \hat{e}_0$, $\hat{y} \equiv \hat{e}_1$ and $\hat{z} \equiv \hat{e}_2$ was also used). The numbers a_0 , a_1 and a_2 are the components or *coordinates* of the vector, but also the coefficients of the unit vectors. In this sense, they are identical to the evolution coefficients of the series expansion, with the difference that the \hat{e}_i are orthogonal, i.e.

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} \quad (5.2)$$

where δ_{ij} is the Kronecker- δ . Two Cartesian vectors \vec{a} and \vec{b} are orthogonal if the scalar product between them vanishes:

$$\vec{a} \cdot \vec{b} = \sum_i a_i b_i = 0 \quad (5.3)$$

Using the basis vectors and the scalar product, we can directly obtain the components: $a_i = \vec{a} \cdot \hat{e}_i$. This is a direct consequence of the orthogonality of the basis vectors \hat{e}_i .

5.2 Functions

In the previous section, we asserted that the basis functions from Chapter 5 are not orthogonal. For this we need an idea for orthogonality of functions. With a definition of a scalar product between two *functions*, we could then define orthogonality as the vanishing of this scalar product.

We now introduce scalar product on functions (spaces) that also fulfill these properties. Given two functions $g(x)$ and $f(x)$ on the interval $x \in [a, b]$, *define* the scalar product as

$$(f, g) = \int_a^b dx f^*(x)g(x), \quad (5.4)$$

where $f^*(x)$ is the complex conjugate of $f(x)$. This inner product or scalar product is a mapping with the properties

- Positive definite: $(f, f) \geq 0$ and $(f, f) = 0 \Leftrightarrow f = 0$
- Sesquilinear: $(\alpha f + \beta g, h) = \alpha^*(f, h) + \beta^*(g, h)$
- Hermitian: $(f, g) = (g, f)^*$

The scalar products Eq. (5.3) and (5.4) both fulfill these properties.

Note: The scalar product between two functions is often defined more generally with a weight function $w(x)$,

$$(f, g) = \int_a^b dx f^*(x)g(x)w(x). \quad (5.5)$$

The question of orthogonality between functions can thus only be answered with respect to a certain definition of the scalar product. For example, the Chebyshev polynomials or the weight function $w(x) = (1 - x^2)^{-1/2}$ are orthogonal. Within this course we will only need the case $w(x) = 1$.

5.3 Basis functions

Let us now return to the series expansion,

$$f_N(x) = \sum_{n=0}^N a_n \varphi_n(x). \quad (5.6)$$

The functions $\varphi_i(x)$ are called *base functions*. A necessary property of the basis functions is their linear independence. The functions are linearly independent if none of the basis functions themselves can be written as a linear combination, i.e. in the form of the series expansion Eq. (5.6), of the other basis functions. This means that it must be fulfilled that

$$\sum_{n=0}^N a_n \varphi_n(x) = 0 \quad (5.7)$$

if and only if all $a_n = 0$. Linearly independent elements form a basis.

This basis is called complete if all relevant functions (= elements of the underlying vector space) can be mapped by the series expansion (5.6). (Proofs of the completeness of basis functions are complex and outside the focus of this course). The coefficients a_n are called coordinates or coefficients. The number of basis functions or coordinates N is called the *dimension* of the vector space.

Note: A *vector space* is a set on which the operations of addition and scalar multiplication are defined with the usual properties, such as the existence of neutral and inverse elements and associative, commutative and distributive laws. If this space is defined on functions, it is also referred to as a *function space*. If there is also a scalar product such as Eq. (5.4), then we speak of a *inner product space*.

Particularly useful basis functions are orthogonal. Using the scalar product, we can now define orthogonality for these functions. Two functions f and g are orthogonal if the scalar product vanishes, $(f, g) = 0$. A set of mutually orthogonal basis functions satisfies

$$(\varphi_n, \varphi_m) = \nu_n \delta_{nm}, \quad (5.8)$$

where δ_{nm} is the Kronecker- δ . For $\nu_n \equiv (\varphi_n, \varphi_n) = 1$ the basis is called *orthonormal*.

Orthogonality is useful because it shows us a way to obtain the coefficients of the series expansion (5.6):

$$(\varphi_n, f_N) = \sum_{i=0}^N a_i (\varphi_n, \varphi_i) = \sum_{i=0}^N a_i \nu_i \delta_{ni} = a_n \nu_n \quad (5.9)$$

resp.

$$a_n = \frac{(\varphi_n, f_N)}{(\varphi_n, \varphi_n)}. \quad (5.10)$$

I.e. the coordinates are given by the projection (the scalar product) of the function onto the basis vectors. Remember that the following also applies to Cartesian vectors: $a_n = \vec{a} \cdot \hat{e}_n$. (The normalization factor is omitted here because $\hat{e}_n \cdot \hat{e}_n = 1$.) The coordinates given by Eq. (5.10) are to be seen in exactly the same context.

5.3.1 Fourier basis

A famous and important set of basis functions is the *fourier-basis*,

$$\varphi_n(x) = \exp(iq_n x), \quad (5.11)$$

on the interval $x \in [0, L]$ with $q_n = 2\pi n/L$ and $n \in \mathbb{Z}$. The Fourier basis is periodic on this interval and is shown in Fig. ?? . It can easily be shown that

$$(\varphi_n, \varphi_m) = L \delta_{nm}, \quad (5.12)$$

so that the Fourier basis is orthogonal. The coefficients a_n of the Fourier series,

$$f_N(x) = \sum_{n=-N}^N a_n \varphi_n(x), \quad (5.13)$$

can thus be used for a series $f_N(x)$ directly as

$$a_n = \frac{1}{L} (\varphi_n, f_N) = \frac{1}{L} \int_0^L dx f_N(x) \exp(-iq_n x) \quad (5.14)$$

can be determined. This is the well-known formula for the coefficients of the Fourier series. Note that the sum in Eq. (5.13) runs from $-N$ to N and you get $2N + 1$ coefficients.

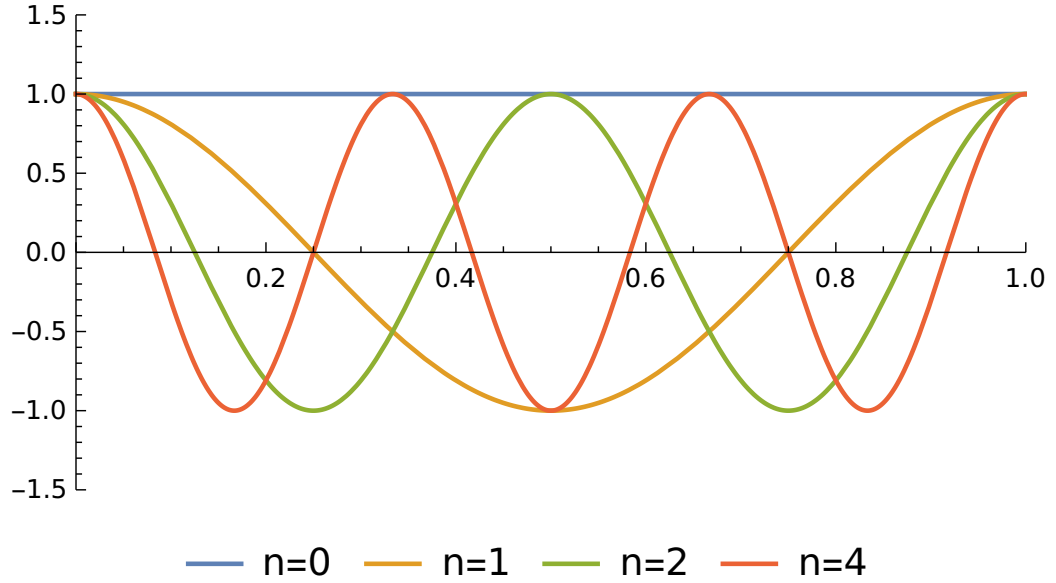


Figure 5.1: real part of the Fourier basis functions, Eq. (5.11), for $n = 1, 2, 3, 4$. The higher order basis functions oscillate with a smaller period and represent higher frequencies

Note: Conceptually, the Fourier basis describes different frequency components, while the basis of the finite elements described in the next section describes different spatial ranges.

5.3.2 Finite elements

We will mainly work with the finite element basis here. In contrast to the Fourier basis, which only becomes zero at isolated points in the entire domain, the finite element basis is localized in space and is zero for large areas of the domain. It thus divides the domain into spatial sections.

In its simplest form, the basis consists of localized section-wise linear functions, the “tent” function,

$$\varphi_n(x) = \begin{cases} \frac{x-x_{n-1}}{x_n-x_{n-1}} & \text{for } x \in [x_{n-1}, x_n] \\ \frac{x_{n+1}-x}{x_{n+1}-x_n} & \text{for } x \in [x_n, x_{n+1}] \\ 0 & \text{other} \end{cases} \quad (5.15)$$

Here, the x_n are the nodes (also known as grid points or nodes) between

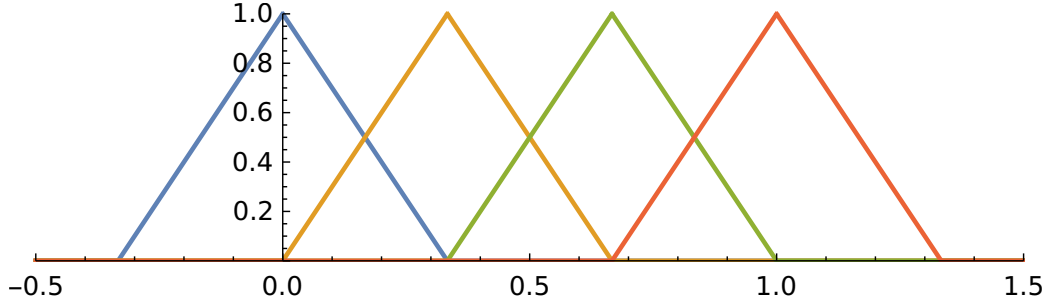


Figure 5.2: The base of the finite elements in its simplest, linear incarnation. Each basis function is a “marquee” that runs over a certain interval between 0 and 1 and back again, see also Eq. (5.15).

which the tents are spanned. The functions are constructed in such a way that $\int_0^L dx \varphi_n(x) = (x_{n+1} - x_{n-1})/2$. This basis is the simplest form of the finite element basis and is shown in Fig. 5.2. Higher order polynomials are also used for greater accuracy.

An important note at this point is that the base of the finite elements *not* is orthogonal. In our one-dimensional case, the scalar product does not vanish for the nearest neighbors. This is the case because two neighbors each have an overlapping rising and falling edge. One obtains

$$M_{nn} \equiv (\varphi_n, \varphi_n) = \frac{1}{3}(x_{n+1} - x_{n-1}) \quad (5.16)$$

$$M_{n,n+1} \equiv (\varphi_n, \varphi_{n+1}) = \frac{1}{6}(x_{n+1} - x_n) \quad (5.17)$$

$$M_{nm} \equiv (\varphi_n, \varphi_m) = 0 \quad \text{for } |n - m| > 1 \quad (5.18)$$

for the scalar products.

Nevertheless, we can use these relations to determine the coefficients of a series expansion,

$$f_N(x) = \sum_{n=0}^N a_n \varphi_n(x) \quad (5.19)$$

can be calculated. You get

$$\begin{aligned} (\varphi_n, f_N(x)) &= a_{n-1}(\varphi_n, \varphi_{n-1}) + a_n(\varphi_n, \varphi_n) + a_{n+1}(\varphi_n, \varphi_{n+1}) \\ &= M_{n,n-1}a_{n-1} + M_{nn}a_n + M_{n,n+1}a_{n+1}. \end{aligned} \quad (5.20)$$

We can express this as

$$(\varphi_n, f_N(x)) = [\underline{M} \cdot \vec{a}]_n \quad (5.21)$$

where $[\vec{v}]_n = v_n$ denotes the n th component of the vector enclosed by the two square brackets $[\cdot]_n$. The matrix \underline{M} is *sparse*. For an orthogonal basis, such as the Fourier basis in section 5.3.1, this matrix is diagonal. For a basis with identical distances $x_{n+1} - x_n = 1$ of the grid points x_n , the matrix has the following form

$$\underline{M} = \begin{pmatrix} 2/3 & 1/6 & 0 & 0 & 0 & 0 & 0 & \dots \\ 1/6 & 2/3 & 1/6 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1/6 & 2/3 & 1/6 & 0 & 0 & 0 & \dots \\ 0 & 0 & 1/6 & 2/3 & 1/6 & 0 & \dots & \\ 0 & 0 & 0 & 1/6 & 2/3 & 1/6 & \dots & \\ 0 & 0 & 0 & 0 & 1/6 & 2/3 & \dots & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (5.22)$$

To find the coefficients a_n , a (sparse) linear system of equations must be solved. We will meet \underline{M} again later under the name *mass matrix*.

Note: Basis sets that are different from zero only at individual points are called *spectral* basis sets. In particular, the Fourier basis is a spectral basis set for periodic functions. In principle, the *orthogonal polynomials* are important spectral basis theorems that are also used in numerics. For example, the Chebyshev polynomials are good basis theorems for non-periodic functions defined on closed intervals. The finite element basis is not a spectral basis.

Chapter 6

Approximation and interpolation

Context: We now apply the idea of basis functions to approximate functions. To do this, we return to the concept of the residual. The goal of function approximation is that the approximated function minimizes the residual. Building on these ideas, we will then discuss the approximation of differential equations in the next chapter.

6.1 Residual

In the previous section, we described how a series expansion can be constructed using basis functions. A typical series expansion contains a finite number of elements $N + 1$ and has the form

$$f_N(x) = \sum_{n=0}^N a_n \varphi_n(x), \quad (6.1)$$

where $\varphi_n(x)$ are the basis functions introduced in the previous chapter.

We now want to approach the question of how we can approximate an arbitrary function $f(x)$ via such a basis function development. To do this, we define the residual

$$R(x) = f_N(x) - f(x), \quad (6.2)$$

which vanishes at every point x if $f_N(x) \equiv f(x)$. For an approximation we want to “minimize” this residual. (By minimize here we mean to bring it as close to zero as possible.) So we are looking for the coefficients a_n of the series expansion, which approximates the function $f(x)$ in the sense of minimizing the residual.

At this point, it should be noted that the basis functions must be defined in the same space for the target function $f(x)$. For the approximation of a periodic function $f(x)$, a periodic basis set should also be used.

6.2 Collocation

The first minimization strategy introduced here is *collocation*. This method requires that the residual disappears at selected collocation points y_n ,

$$R(y_n) = 0 \quad \text{or} \quad f_N(y_n) = f(y_n). \quad (6.3)$$

The number of collocation points must correspond to the number of coefficients in the series expansion. The choice of ideal collocation points y_n itself is non-trivial, and we will only discuss specific cases here.

As a first example, we discuss here an evolution with N finite elements. As collocation points we choose the interpolation points of the base, $y_n = x_n$. At these sampling points, only one of the basis functions is non-zero, $\varphi_n(y_n) = 1$ and $\varphi_n(y_k) = 0$ if $n \neq k$. This means that the condition

$$R(y_n) = 0 \quad (6.4)$$

trivially leads to

$$a_n = f(y_n). \quad (6.5)$$

The coefficients a_n are therefore given by the function value of the function to be approximated at the collocation point. The approximation is therefore a piecewise linear function between the function values of $f(x)$.

As a second example, we discuss a Fourier series with corresponding $2N + 1$ Fourier basis functions,

$$\varphi_n(x) = \exp(iq_n x). \quad (6.6)$$

In the context of a collocation method, we require that the residual vanishes on $2N + 1$ equidistant points, $R(y_n) = 0$ with

$$y_n = nL/(2N + 1). \quad (6.7)$$

The condition for this is then

$$\sum_{k=-N}^N a_k \exp(iq_k y_n) = \sum_{k=-N}^N a_k \exp\left(i2\pi \frac{kn}{2N + 1}\right) = f(y_n). \quad (6.8)$$

Equations (6.8) can now be solved for a_k . We use the fact that for equidistant collocation points the Fourier matrix $W_{kn} = \exp(i2\pi kn/(2N + 1))$ is unitary

(except for one factor), i.e. its inverse is given by the adjoint: $\sum_n W_{kn} W_{nl}^* = (2N+1)\delta_{kl}$. We can therefore multiply Eq. (6.8) by W_{nl}^* and sum over n . This results in

$$\sum_{n=-N}^N \sum_{k=-N}^N a_k \exp \left[i2\pi \frac{(k-l)n}{2N+1} \right] = \sum_{k=-N}^N N a_k \delta_{kl} = N a_l \quad (6.9)$$

where

$$\sum_{n=-N}^N \exp \left[i2\pi \frac{(k-l)n}{2N+1} \right] = (2N+1)\delta_{kl} \quad (6.10)$$

was used. This means that the coefficients can be expressed as

$$a_l = \frac{1}{2N+1} \sum_{n=-N}^N f \left(\frac{nL}{2N+1} \right) \exp \left(-i2\pi \frac{ln}{2N+1} \right), \quad (6.11)$$

can be determined. This is the *discrete Fourier transform* of the function $f(y_n)$ discretized on the collocation points.

As a simple example, we show the approximation of the example function $f(x) = \sin(2\pi x)^3 + \cos(6\pi(x^2 - 1/2))$ using the Fourier basis and finite elements. Figure 6.2 shows this approximation for $2N+1 = 5$ and $2N+1 = 11$ basis functions with equidistant collocation points.

The figure shows that all approximations run exactly through the collocation points, as required by the collocation condition. The two approaches interpolate differently between the collocation points *interpolate*. The finite elements lead to a linear interpolation between the points. The Fourier basis is more complicated. The curve between the collocation points is called *Fourier interpolation*.

6.3 Weighted residuals

We would now like to generalize the collocation method. To do this, we introduce the concept of *test function*. Instead of requiring that the residual vanishes at individual points, we require that the scalar product

$$(v, R) = 0 \quad (6.12)$$

with a function $v(x)$ disappears. If Eq. (6.12) vanishes for any test function $v(x)$, then the “weak” formulation Eq. (6.12) is identical to the strong formulation $R(x) = 0$. Equation (6.12) is called a “weak” formulation because the condition is only fulfilled in the integral sense. In particular, it is shown in

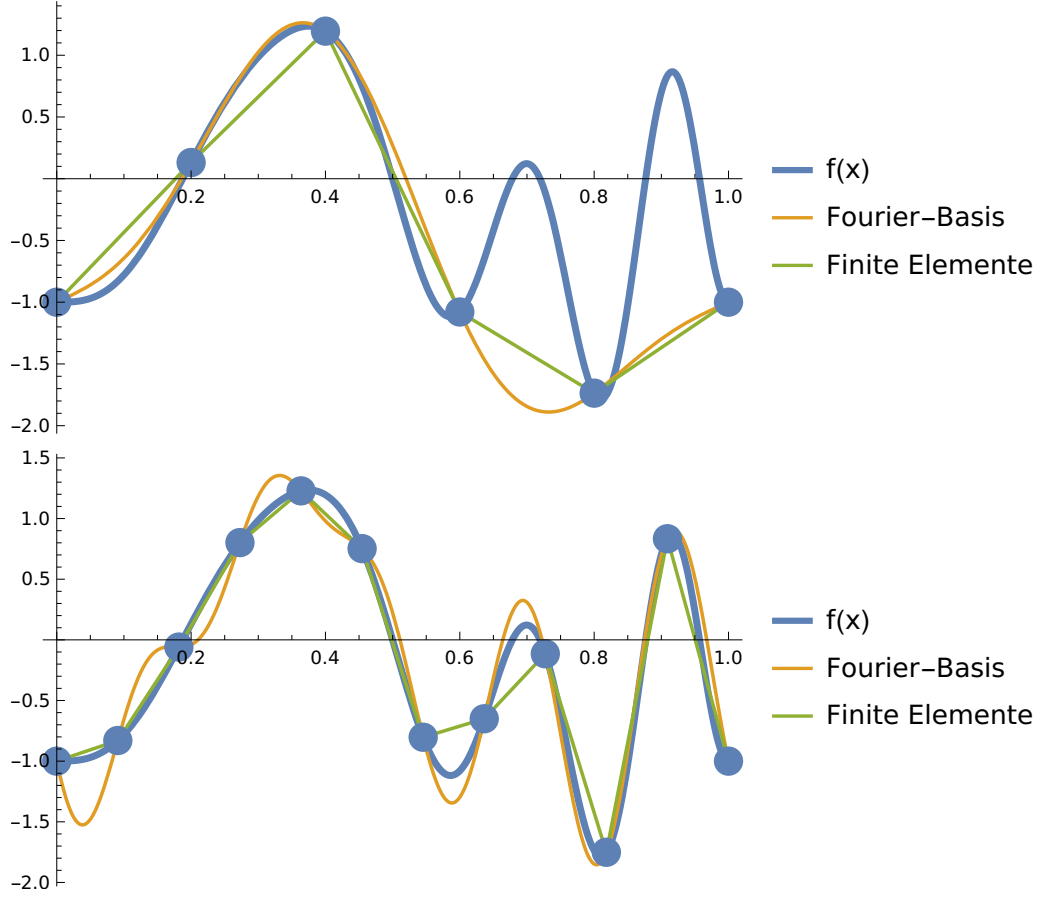


Figure 6.1: Approximation of the periodic function $f(x) = \sin(2\pi x)^3 + \cos(6\pi(x^2 - 1/2))$ on the interval $[0, 1]$ with a Fourier basis and finite elements. In each case 5 (top) and 11 (bottom) basis functions were used. The coefficients were determined using the collocation method. The round dots show the collocation points. Both approximations run exactly through these collocation points. (The right collocation point is identical to the left one due to the periodicity). The approximation with $N = 5$ basis functions cannot map the two right oscillations of the target function $f(x)$ in both cases

Chapter 9 that this weak formulation leads to a weak *solution*, which cannot satisfy the original (strong) PDGL at every point. The condition (6.12) is often subsumed under the term *weighted residuals*.

A special set of test functions leads directly to the collocation method. We choose the set of N test functions

$$v_n(x) = \delta(x - y_n) \quad (6.13)$$

where $\delta(x)$ is the Dirac δ function and y_n the collocation points. The condition $(v_n, R) = 0$ for all $n \in [0, N - 1]$ leads directly to the collocation condition $R(y_n) = 0$.

Note: The Dirac δ function should be familiar from lectures on signal processing. The most important property of this function is the filter property,

$$\int_{-\infty}^{\infty} dx f(x) \delta(x - x_0) = f(x_0), \quad (6.14)$$

i.e. the integral over the product of the δ function gives the function value at which the argument of the δ function disappears. All other properties follow from this, e.g.

$$\int dx \delta(x) = \Theta(x), \quad (6.15)$$

where $\theta(x)$ is the (Heaviside) step function.

6.4 Galerkin method

The Galerkin method is based on the idea of using the basis functions φ_n of the series expansion as test functions. This leads to the N conditions

$$(\varphi_n, R) = 0, \quad (6.16)$$

resp.

$$(\varphi_n, f_N) = (\varphi_n, f). \quad (6.17)$$

For an orthogonal set of basis functions, you directly obtain

$$a_n = \frac{(\varphi_n, f)}{(\varphi_n, \varphi_n)}. \quad (6.18)$$

This approach has already been discussed in section 5.3.

For a non-orthogonal basis set, e.g. the basis of the finite elements, a linear system of equations is obtained,

$$\sum_{m=0}^N (\varphi_n, \varphi_m) a_m = (\varphi_n, f), \quad (6.19)$$

where the matrix $A_{nm} = (\varphi_n, \varphi_m)$ is sparse for the finite elements.

Let us now return to our example function $f(x) = \sin(2\pi x)^3 + \cos(6\pi(x^2 - 1/2))$. Figure 6.2 shows the approximation of this function with Fourier and finite element basis sets and the Galerkin method. There are no collocation points and the approximation using finite elements does not exactly match the function to be approximated at the interpolation points. The function is only approximated in the integral sense.

Note: The Galerkin condition (see also Eq. (6.16))

$$(\varphi_n, R) = 0, \quad (6.20)$$

means that the residual is *orthogonal* to all basis functions. In other words, the residual can only contain contributions to the function that cannot be mapped with the given basis set. However, this also means that we can systematically improve our solution by extending the basis set.

6.5 Least squares

An alternative approach to approximation is to minimize the square of the residual, (R, R) , also known as a *least squares* approach. For a general series expansion with N basis functions, we obtain

$$\begin{aligned} (R, R) &= (f, f) + (f_N, f_N) - (f_N, f) - (f, f_N) \\ &= (f, f) + \sum_{n=0}^N \sum_{m=0}^N a_n^* a_m (\varphi_n, \varphi_m) - \sum_{n=0}^N a_n^* (\varphi_n, f) - \sum_{n=0}^N a_n (f, \varphi_n). \end{aligned} \quad (6.21)$$

This error square is minimized if

$$\frac{\partial(R, R)}{\partial a_k} = \sum_{n=0}^N a_n^* (\varphi_n, \varphi_k) - (f, \varphi_k) = 0 \quad (6.22)$$

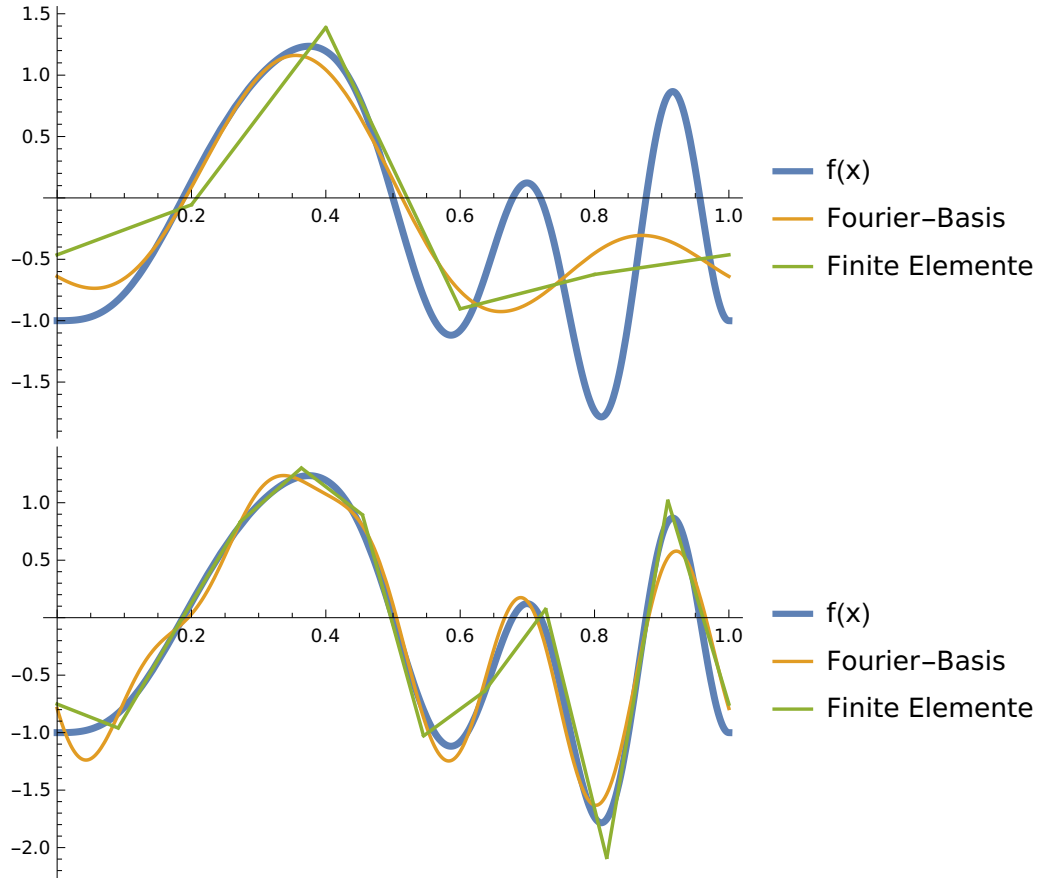


Figure 6.2: Approximation of the periodic function $f(x) = \sin(2\pi x)^3 + \cos(6\pi(x^2 - 1/2))$ on the interval $[0, 1]$ with a Fourier basis and finite elements. In each case 5 (top) and 11 (bottom) basis functions were used. The coefficients were determined using the Galerkin method. The approximation with 5 basis functions cannot map the two right oscillations of the target function $f(x)$ in both cases.

and

$$\frac{\partial(R, R)}{\partial a_k^*} = \sum_{n=0}^N a_n(\varphi_k, \varphi_n) - (\varphi_k, f) = 0. \quad (6.23)$$

This expression is identical to Eq. (6.19) of the Galerkin method.

Chapter 7

Spectral methods

Context: We now develop the ideas for solving partial differential equations outlined in the previous chapters. In this chapter, we deal with the Fourier basis. This leads to a solution method that is usually subsumed under the name *integral transform*. Although spectral methods can also be used for numerical solutions, here we only discuss the Fourier transform as an analytical solution method. In addition to the application of these methods, we also extend the solution approaches to multidimensional spaces.

7.1 Differential operators

To solve differential equations, we now use exactly the same methods that we developed in the previous chapter: Minimizing the residual using the Galerkin method. Our residual now has the general form

$$R(x, y, z, \dots; a_0, a_1, \dots, a_N) = \mathcal{L}u_N(x, y, z, \dots) - f(x, y, z, \dots), \quad (7.1)$$

where the unknown function u_N is represented here as a series expansion into a certain basis $\varphi_n(x, y, z)$. The Galerkin method requires

$$(\varphi_n, R) = 0 \quad (7.2)$$

for each n .

We first discuss the Fourier basis for periodic functions on $x \in [0, L]$ in one dimension,

$$\varphi_n(x) = \exp(iq_n x) \quad (7.3)$$

with $q_n = 2\pi n/L$. The operator \mathcal{L} can contain any differential operations that act on the basis functions, for example

$$\frac{d}{dx}\varphi_n(x) = iq_n\varphi_n(x) \quad (7.4)$$

$$\frac{d^2}{dx^2}\varphi_n(x) = -q_n^2\varphi_n(x). \quad (7.5)$$

I.e. the derivatives of the (Fourier) basis functions result in the *equal* basis function and an algebraic factor. It is also said that the basis functions *diagonalize* the differential operator. (This will be different for the finite elements discussed in the next chapter).

This property is particularly useful because, at least for linear differential equations, the residual becomes a trivial series expansion again and we can easily determine the coefficients due to the orthogonality of the basis.

7.2 Poisson equation in one dimension

We use the (one-dimensional) Poisson equation as a demonstrator for this behavior,

$$\nabla^2\Phi \equiv \frac{d^2\Phi}{dx^2} = -\frac{\rho}{\varepsilon}. \quad (7.6)$$

Here ρ is a charge density and Φ is the electrostatic potential. The residual is therefore

$$R(x) = \frac{d^2\Phi}{dx^2} + \frac{\rho}{\varepsilon}, \quad (7.7)$$

and the solution of Eq. (7.6) is given by $R(x) = 0$.

Formally, we now write the potential as the series expansion

$$\Phi(x) \approx \Phi_N(x) = \sum_{n=-N}^N a_n\varphi_n(x), \quad (7.8)$$

whereby we will not explicitly specify the summation limits in the following. We also develop the right-hand side of Eq. (7.6) into a series with the same basis functions,

$$\rho_N(x) = \sum_{n=-N}^N b_n\varphi_n(x). \quad (7.9)$$

Substituting this into Eq. (7.7) we obtain

$$R_N(x) = -\sum_n a_n q_n^2 \varphi_n(x) + \frac{1}{\varepsilon} \sum_n b_n \varphi_n(x). \quad (7.10)$$

We now multiply this from the left by the basis functions, (φ_k, R_N) (Galerkin method) and, due to the orthogonality of the basis functions, we obtain the equations

$$(\varphi_k, R_N) = -Lq_k^2 a_k + Lb_k/\varepsilon. \quad (7.11)$$

(The factor L appears because the basis functions are not normalized.) The condition $(\varphi_k, R_N) = 0$ leads to $a_k = b_k/(q_k^2 \varepsilon)$. The approximate solution of the Poisson equation is thus given by

$$\Phi_N(x) = \sum_n \frac{b_n}{q_n^2 \varepsilon} \varphi_n(x). \quad (7.12)$$

This is the Fourier series of the solution.

7.3 Transition to the Fourier transform

The Fourier basis Eq. (7.3) is periodic on a finite domain of length L . If we let the length L go to infinity, we get a formulation for non-periodic functions. This leads directly to the *Fourier transform*.

We write the series expansion as

$$\Phi_N(x) = \sum_{n=-N}^N a_n \varphi_n(x) = \sum_{n=-N}^N a_n \exp(iq_n x) = \sum_{n=-N}^N \frac{\Delta q}{2\pi} \tilde{\Phi}(q_n) \exp(iq_n x) \quad (7.13)$$

with $\Delta q = q_{n+1} - q_n = 2\pi/L$ and rescaled coefficients $\tilde{\Phi}(q_n) = La_n$. Here, only the factor $1 = L\Delta q/2\pi$ was inserted on the right-hand side of Eq. (7.13). This now helps to form the limits $L \rightarrow \infty$ and $N \rightarrow \infty$. In this case, $\Delta q \rightarrow dq$ and the sum becomes the integral. You get

$$\Phi(x) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{\Phi}(q) \exp(iqx), \quad (7.14)$$

the Fourier *backtransformation*.

The (outward) transformation is obtained via a similar argument. We now know that

$$\tilde{\Phi}(q_n) = La_n = L \frac{(\varphi_n, \Phi_N)}{(\varphi_n, \varphi_n)} = (\varphi_n, \Phi_N) = \int_0^L dx \Phi_N(x) \exp(-iq_n x). \quad (7.15)$$

In the limiting case $L \rightarrow \infty$ and $N \rightarrow \infty$ this becomes

$$\tilde{\Phi}(q) = \int_{-\infty}^{\infty} dx \Phi(x) \exp(-iqx), \quad (7.16)$$

of the Fourier transform. The Fourier transform is useful to obtain analytical solutions for partial differential equations on infinite domains.

Note: A tilde $\tilde{f}(q)$ denotes the Fourier transform of a function $f(x)$. The Fourier transform is a function of the wave vector q . In contrast, with the Fourier series we obtain countable coefficients a_n . The reason for this is the periodicity of the area under consideration.

7.4 Poisson equation in several dimensions

Similar to how we constructed an approximated solution for a differential equation using a series expansion, we can now use the approach Eq. (7.14) to obtain analytical solutions. In this section, this is demonstrated using the Poisson equation in three dimensions.

In three dimensions, the Poisson equation is

$$\nabla^2 \Phi \equiv \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} = -\frac{\rho}{\varepsilon}. \quad (7.17)$$

In contrast to Eq. (7.6), the partial derivative ∂ now appears here because $\Phi(x, y, z)$ now depends on three variables (the Cartesian coordinates).

The generalization of the Fourier basis and thus also of the Fourier transform to three dimensions is trivial. A basis is obtained by multiplying basis functions in the Cartesian directions (x , y and z). Usually, you now need three indices for the coefficients, which denote the basis in x , y and z respectively. The result is a series expansion

$$\begin{aligned} \Phi_{NMO}(x, y, z) &= \sum_{n=-N}^N \sum_{m=-M}^M \sum_{o=-O}^O a_{nmo} \varphi_n(x) \varphi_m(y) \varphi_o(z) \\ &\equiv \sum_{n=-N}^N \sum_{m=-M}^M \sum_{o=-O}^O a_{nmo} \varphi_{nmo}(x, y, z) \end{aligned} \quad (7.18)$$

with (possibly different) development order N , M and O . The basis theorem is given here by the set of functions $\varphi_{nmo}(x, y, z) = \varphi_n(x) \varphi_m(y) \varphi_o(z)$. Orthogonality of this basis theorem is trivially derived from the orthogonality of the one-dimensional basis functions $\varphi_n(x)$. The generalization of the Fourier transform follows directly from this. The Fourier inverse transform is written as

$$\Phi(x, y, z) = \int_{-\infty}^{\infty} \frac{d^3 q}{(2\pi)^3} \tilde{\Phi}(q_x, q_y, q_z) \exp(iq_x x + iq_y y + iq_z z), \quad (7.19)$$

where the Fourier transform $\tilde{\Phi}$ now naturally depends on three wave vectors q_x , q_y and q_z . The differential operator $\mathrm{d}^3 q = \mathrm{d}q_x \mathrm{d}q_y \mathrm{d}q_z$ is a shorthand notation for three-dimensional integration.

We can now insert Eq. (7.19) into the PDGL Eq. (7.17) and obtain

$$R(\vec{r}) = \int_{-\infty}^{\infty} \frac{\mathrm{d}^3 q}{(2\pi)^3} \left[\left(-q_x^2 - q_y^2 - q_z^2 \right) \tilde{\Phi}(\vec{q}) + \frac{\tilde{\rho}(\vec{q})}{\varepsilon} \right] \exp(i\vec{q} \cdot \vec{r}) = 0 \quad (7.20)$$

with $\vec{r} = (x, y, z)$ and $\vec{q} = (q_x, q_y, q_z)$. This equation must be fulfilled for every x, y, z and therefore the argument of the integration must disappear, i.e.

$$-q^2 \tilde{\Phi}(\vec{q}) + \frac{\tilde{\rho}(\vec{q})}{\varepsilon} = 0. \quad (7.21)$$

Note: An alternative argument is obtained by writing the Fourier transform of $R(x, y, z)$:

$$R(q'_x, q'_y, q'_z) = \int \mathrm{d}^3 r R(\vec{r}) \exp(-iq'_x x - iq'_y y - iq'_z z). \quad (7.22)$$

This contains terms of the form

$$\int_{-\infty}^{\infty} \mathrm{d}x \exp(i(q_x - q'_x)x) = 2\pi \delta(q_x - q'_x), \quad (7.23)$$

which are expressions of the orthogonality of the basis functions. Since the basis functions are now “parameterized” with a continuous q_x (instead of a discrete n), a Dirac δ function is obtained instead of the Kronecker δ in the orthogonality relation.

Equation (7.21) can easily be solved analytically. One obtains

$$\tilde{\Phi}(\vec{q}) = \frac{\tilde{\rho}(\vec{q})}{\varepsilon q^2} \quad (7.24)$$

with $q = |\vec{q}|$. This is equivalent to solving Eq. (7.12) for the Poisson equation on a periodic domain. The difficulty now lies in evaluating the back and forth transformation for a given $\rho(x, y, z)$.

Example: As an example, we now consider the solution for a point charge Q at the origin,

$$\rho(x, y, z) = Q \delta(x) \delta(y) \delta(z). \quad (7.25)$$

The Fourier transform of the charge density ρ is obtained from Eq. (7.16),

$$\tilde{\rho}(q_x, q_y, q_z) = Q. \quad (7.26)$$

I.e. the Fourier transform of the electrostatic potential is given by (see Eq. (7.24))

$$\tilde{\Phi}(\vec{q}) = \frac{Q}{\varepsilon q^2}, \quad (7.27)$$

and thus the representation in real space is

$$\begin{aligned} \Phi(\vec{r}) &= \int_{-\infty}^{\infty} \frac{d^3 q}{(2\pi)^3} \frac{Q}{\varepsilon q^2} \exp(i\vec{q} \cdot \vec{r}) \\ &= \frac{Q}{(2\pi)^3 \varepsilon} \int_0^{\infty} dq \int_0^{2\pi} d\phi \int_{-1}^1 d(\cos \theta) \exp(iqr \cos \theta) \end{aligned} \quad (7.28)$$

where $d^3 q = q^2 dq d\phi d(\cos \theta)$ with azimuth angle ϕ and elevation angle θ , was used (see also Fig. 7.1). We require here (without limiting the generality) that \vec{r} points in the direction of the zenith.

One obtains

$$\begin{aligned} \Phi(\vec{r}) &= \frac{Q}{(2\pi)^2 \varepsilon} \int_0^{\infty} dq \int_{-1}^1 d(\cos \theta) \exp(iqr \cos \theta) \\ &= \frac{Q}{(2\pi)^2 \varepsilon} \int_0^{\infty} dq \frac{\exp(iqr) - \exp(-iqr)}{iqr} \\ &= \frac{Q}{(2\pi)^2 \varepsilon} \int_{-\infty}^{\infty} dq \frac{\sin qr}{qr} \\ &= \frac{Q}{4\pi \varepsilon r}, \end{aligned} \quad (7.29)$$

where $\int dx \sin x/x = \pi$ was used. This is the known solution for the electrostatic potential of a point charge. It is also called the fundamental solution or *Green's function* of the (three-dimensional) Poisson equation.

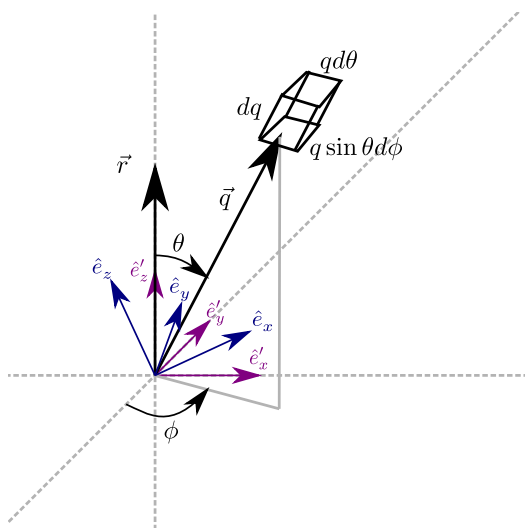


Figure 7.1: Volume element for integration in sphere coordination

Bibliography