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# Green's Function Method for the Analysis of Soil Heat Flux in the Mountain Group Gesäuse

**MASTER'S THESIS**

to achieve the university degree of
Diplom-Ingenieur

Master's degree programme:
Technical Physics

submitted to
**Graz University of Technology**

**Supervisor**

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Institute of Physics

in cooperation with the Nationalpark Gesäuse

Graz, July 2023

# Abstract

The systematic observation of the climate as well as of ecosystems is methodically based on statistical thermodynamics. The state of these systems is therefore determined by state variables. How much and which state variables are meaningful for the respective system is defined by knowledge consortia. There is a strong coupling between the climate system and ecosystems. Highly integrated numerical models, including Earth system models, take this coupling into account. Consequently, there are common state variables of the climate and of ecosystems. Specifically, these are the surface temperature of the Earth and the heat flux at the Earth's surface. Using the diffusion equation and Green's function method, these two state variables are generated from space-time temperature data. The resulting model is defined by only two parameters, the depth at which the temperature is measured and the diffusion constant of the soil. The validation of the Green's function method is carried out by a rigorous consideration of the distribution theory. The appropriate mathematical framework is provided by functional analysis. The physical problem and the fundamental solution of the diffusion equation are presented. Based on the fundamental solution, the Green's function of the problem is constructed. The method is implemented numerically and provides the ground heat flux and thus total heat flux and temperature profile of the soil, which is guaranteed by the Green's function method. The input data for this consists of the temperature time series of the Gesäuse National Park. The method presented here offers a clear advantage over the conventional method using gradient methods. Only by using maintenance-free and inexpensive temperature loggers, the entire soil heat flux profile and soil temperature profile can be generated with the Green's function method and thus essential state variables for the climate and for ecosystems can be measured in a simple way.

# Kurzfassung

Die ganzheitliche Betrachtung des Klimas als auch von Ökosystemen fußt methodisch in der statistischen Thermodynamik. Der Zustand dieser Systeme wird daher durch Zustandsgrößen festgelegt. Wieviel und welche Zustandsgrößen für das jeweilige System aussagekräftig sind, wird von Wissenskonsortien definiert. Es besteht eine starke Kopplung zwischen dem Klimasystem und den Ökosystemen. Hochintegrierte numerische Modelle, wozu Erdsystemmodelle gehören, berücksichtigen diese Kopplung. Folglich decken sich einige Zustandsgrößen des Klimasystems und von Ökosystemen. Konkret sind das die Oberflächentemperatur der Erde und der Wärmestrom an der Erdoberfläche. Mithilfe der Diffusionsgleichung und der Methode der Green's Funktion, werden diese beiden Zustandsgrößen aus Raumzeitpunkttemperaturdaten generiert. Das so entstandene Modell wird lediglich durch zwei Parameter festgelegt, die Tiefe, in welcher die Temperaturmessung stattfindet und die Diffusionskonstante des Erdbodens. Die Validierung der Green's Funktion Methode wird durch eine rigorose Betrachtung der Distributionentheorie untermauert. Den geeigneten mathematischen Rahmen bietet hierbei die Funktionalanalysis. Das physikalische Problem und die Fundamentallösung der Wärmeleitungsgleichung wird vorgestellt. Aus ihr wird die Green's Funktion des Problems konstruiert. Die Methode wird numerisch implementiert und liefert den Bodenwärmestrom und mit ihm das gesamte Wärmestrom- und Temperaturprofil des Erdbodens, was durch die Green's Funktion Methode gewährleistet wird. Die Eingangsdaten hierzu bestehen aus den Temperaturzeitreihen des Nationalparks Gesäuse. Die hier vorgestellte Methode bietet einen klaren Vorteil gegenüber der konventionellen Methode mittels Gradientenverfahren. Lediglich unter Einsatz wartungsfreier und günstiger Temperaturlogger, kann mit der Methode der Green's Funktionen das gesamte Bodenwärmestromprofil und Bodentemperaturprofil generiert werden und somit essentielle Zustandsgrößen für das Klima und für Ökosysteme, auf einfache Weise, gemessen werden.

# Danksagung

Seit mir der Fachbereichsleiter im Nationalpark Gesäuse für Naturschutz und Forschung, Mag. Alexander Maringer, von der Bodentemperaturmesskampagne im Park erzählt hatte, ist viel Wasser die Enns hinunter geflossen. Mit den großartigen Methoden, welche uns im Physikstudium gelehrt wurden, war sofort klar, dass sich aus den Daten viel Information herausholen ließe. Die Methode der Green's Funktion, angewandt auf die Wärmeleitungsgleichung, machte die Zustandsgrößen Bodenwärmestrom und Oberflächentemperatur zugänglich. Die Ausarbeitung war anspruchsvoll aber sehr lehrreich, vor allem in mathematischer und interdisziplinärer Hinsicht. Ich durfte einige mathematische Verfahren aus dem Studium festigen und konnte meinen Horizont bezüglich Ökosystemforschung erweitern. Für diese Möglichkeit bedanke ich mich vielmals beim Nationalpark Gesäuse und hier insbesondere bei Mag. Alexander Maringer für seine großartige Fachkenntnis und freundliche und wertschätzende Unterstützung.

Ganz herzlich möchte ich mich auch bei meinem Betreuer Herrn Prof. Ulrich Foelsche bedanken. Nicht nur aufgrund seiner ausgesprochen großen fachlichen Expertise, sondern auch wegen seiner unkomplizierten und immer freundlichen Art, bei der man gern ins Privatissimum geht, wo auch mal unbekannte Skitourenziele erörtert werden konnten. Ihre Vorlesungen über Klimaphysik und das Erdsystem während des Studiums waren inspirierend, ausgesprochen lehrreich und immer besonders unterhaltsam.

Ein großer Dank gilt auch meinen sehr guten Freunden. Ohne euch wäre die Studienzeit nur halb so lustig und das Leben nur halb so aufschlussreich geblieben. Speziell möchte ich mich bei Mag. Gerd Egner bedanken, unsere gemeinsamen Bergabenteuer und die obligatorischen Prüfungsbiere werde ich nie vergessen. Ich freue mich schon, wenn wir wieder gemeinsam in die Berge ziehen und ein paar Prüfungsbiere wird es bestimmt auch noch geben.

Ganz herzlich möchte ich mich auch bei Frau Dr. Victoria Reichel bedanken.

Sie ist eine große Inspiration und ich kenne niemanden der mit soviel wissenschaftlicher Integrität und Hingabe arbeitet. Ein Fels in der Brandung für ihre Mitmenschen und die Wissenschaft.

Ein ganz großer Dank gilt meiner Familie, meinen Eltern und insbesondere meinen Brüdern und meiner Schwester, die immer ein offenes Ohr für mich haben und hatten und auf die ich immer zählen konnte. Ich hoffe ihr wisst, dass dies auf Gegenseitigkeit beruht. Der allergrößte Dank gilt meiner Mutter. Ihre bedingungslose Unterstützung und ihr unerschütterlicher Glaube in mich war und ist die größte Stütze die man sich wünschen kann, ich hoffe ich kann dir zumindest eine leise Vorstellung davon geben wie viel mir das bedeutet.

Zuletzt möchte ich noch meiner liebsten Eisprinzessin Verena Danke sagen. Ich bin so froh, dass ich dich kennen- und schätzen lernen durfte. Wenn die geraden Wege nicht mehr weiterführen machst du sie für mich krumm. Du bist die beste Seil- und Lebensgefährtin die man sich nur wünschen kann und außerdem die beste Pharmazeutin aller Zeiten.

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# 1. Introduction

Inside the pedosphere, the atmosphere, biosphere, hydrosphere, cryosphere and lithosphere overlap. Across their boundary layers, processes occur that also change the state of the climate. To complement the climate system, only the external influences to the pedosphere are missing, namely the dynamical properties of the sun itself and the earth's orbit parameters in relation to the sun, other cosmic influences are neglected. If we know all the state variables and processes of the pedosphere and the cosmic variables, than the state of the climate is known. This state and the processes are mapped with the help of models. To correct systematic errors in the current global and regional Earth System Models (ESM) used in climate research, these processes are already directly integrated or parameterized within the models. The different components of the climate system are thereby considered in the form of modules in the ESM's. The Land Surface Model (LSM) is such a module, which contains system variables like vegetation, soil properties and groundwater. Furthermore, it should be mentioned that an increased integration of the models allows a better coverage of small-scale climate phenomena and regional variability. If you neglect the biosphere for example, the variability of the regional climate will reduce, because the coupling between biosphere and atmosphere is not mentioned. As with all other modules, data are also required for the LSM in order to specify initial and especially boundary conditions of the model equations or to carry out the parameterization of the system variables. Furthermore, the data are of particular importance to validate the climate models. The data products are versatile, e.g. in situ measurements, remote sensing and reanalysis data or a combination thereof.

The state of the climate is characterized by so called Essential Climate Variables (ECV) from the Global Climate Observing System (GCOS). It is an physical, chemical or biological variable, or a group of linked variables, that critically contributes to the characterization of earth's climate. As a result, there are ECV

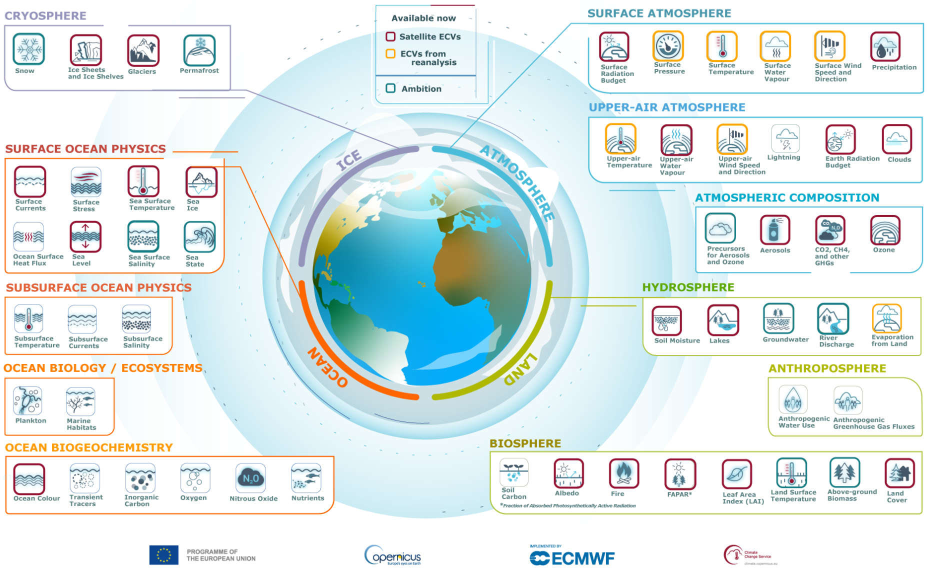


Figure 1.1.: Chart of the 22 Essential Climate Variables definesd by Global Climate Observing System (GCOS). Figure from Zemp et al. (2022b).

products which are defined as a measurable parameter needed to characterize the ECV according to Zemp et al. (2022a, Ch. 1). One can see the 22 ECV's in Fig. 1.1 where in particular the Land Surface Temperature (LST) is mentioned as an ambition.

The National Park Gesäuse, in turn, has now recorded soil temperature data in high spatial and temporal resolution over 10 years. The motivation for these time series is based on ecosystem monitoring. The research network european Long Term Ecosystem Monitoring (eLTER) defines and discusses so called Standard Observations (SO), which determine the state and system variables of an ecosystem according to Zacharias et al. (2021, Ch. 1.1).

Because climate research today is a highly interdisciplinary one, it has become apparent that there are common system variables which are both, SO and ECV. These quantities are listed in the table 1.1. The ECV's listed here are used to close the energy balance. Thereby the fluxes of the soil, especially the ground heat flux $B$, the latent heat $L$ and the sensible heat $H$ must be known H. Kraus (2008, Ch. 11). The energy balance directly at the earth's

Table 1.1.: Essential Climate Variables and Standard Observations.

| **Essential Climate Variable (ECV)** (Climate Modelling) | **Standard Observation (SO)** (Ecosystem Modelling) |
|---|---|
| 9.3 **Evaporation from Land** | SOATM_098 Ground Heat Flux |
| 9.3.1 Sensible Heat Flux | SOATM_099 Sensible Heat Flux |
| 9.3.2 Latent Feat Flux | SOATM_097 Latent Heat Flux |
| 9.7 **Land surface Temperature** | |
| 9.7.1 Land Surface Temperature | SOGEO_002 Soil Temperature |
| 9.7.2 Soil Temperature[1] | |

surface with the global radiation of $Q_0$, indicated by the index 0, is then

$$Q_0 - B_0 - H_0 - L_0 = 0\,. \tag{1.1}$$

The soil temperature loggers installed in the Gesäuse measure the temperatures within the soil in high spatial and temporal resolution, whereby the spatial resolution here relates to the geographical latitudes and longitudes, not the depth in the soil. The individual temperature data are integrated into a spatiotemporal grid $T_i = T(\boldsymbol{r}_i, t)$, with the $i$-th temperature logger (GIS-Metadata). Temperature measurements are known to be scalar quantities. The individual measured values of the temperature loggers are therefore scalars in space and time. Together with the heat equation

$$\frac{\partial}{\partial t} u(\boldsymbol{r}, t) = -a \Delta u(\boldsymbol{r}, t)$$

results in a combined initial and boundary value problem with these measured values $T_i$, where $a$ is the thermal diffusivity of the soil. With the help of the Green's Function to the problem, this can be used to generate the fluxes and a temperature profile, and to generate the system variables in Table 1.1. The necessary metadata and especially the soil parameters, which are included in $a$, are obtained by field study. Data from WegenerNet can be used to complement and validate the analysis. Furthermore, the data should be qualitatively put into a larger context (keyword ESM).

[1] „Soil Temperature is a new ECV product temporary included under the ECV Land-Surface Temperature. His positioning will be subjected to evaluation of TOPC Panel and GCOS Steering Committee" (Zemp et al. 2022a)

Figure 1.2.: View of the south-eastern side of the Buchstein group above the Hieflau weir. With kind permission of Mag. Verena Lewenhofer.

## 1.1. The Gesäuse Mountain Group

The Gesäuse Mountains are a wild natural landscape in the east of the Northern Limestone Alps. The Gesäuse gets its name from the Enns River, which pierces the walls of the Himbeerstein and Haindlmauer near Krumau. This natural monument is called the Gesäuse entrance. Afterwards, the Enns runs through a breakthrough valley, carved between the Reichenstein, Hochtor and Buchstein groups (Fig. 1.2).

Himbeerstein and Haindlmauer have held back the alpine glaciers of the last

Figure 1.3.: Megabunus Lesserti or the northern giant-eye harvestmen. Figure from Lemke (2016).

pleistocene glaciation, which has allowed the survival of many rare species of flora and fauna that today live endemically in the Gesäuse mountains. Among a lot of other things, this makes the Gesäuse very interesting for ecosystem research of rare species in extreme habitats. The northern giant-eye harvestmen, a species of weaver's foot endemic to the Northern Limestone Alps, is mentioned here as a representative example (Fig. 1.3).

### 1.1.1. Measurement Sites

As already mentioned, soil temperature measurement series are available from the Gesäuse National Park. The sites were selected according to various aspects. A large number of the measuring stations are located in avalanche gullies in order to observe the temperature developments there. Further measuring sites are located in the areas of the WegenerNet stations, whereby the soil temperature data are to supplement the measurements here.
The Gesäuse with its high relief energy is an exciting but challenging measuring region. There are very many natural processes with destructive power. Rockfall, avalanches and the rough weather are just a few examples. With all the theoretical considerations about the measurements, this component must not be neglected. All data must be critically questioned and verified for plausibility.

Figure 1.4.: The Gscheideggkogel measuring station of the WegenerNet. A soil temperature logger is buried in the very close neighbourhood. With kind permission of the Nationalpark Gesäuse.

The station at Gscheideggkogel is presented as a representative example of all measuring stations.

### Measurement Site Gscheideggkogel

The Gscheideggkogel[2] is a 1788 m high mountain at the south-east edge of the national parc. He is popular for ski touring and generally offers guaranteed snow. The mountain is sparsely tree-covered up to the summit area and extensively covered with blueberry bushes. The measurement site is located about hundred metres altitude below the summit on the north-west side of the mountain (see Fig. 1.4). The temperature logger (see Fig.1.5) are buried in some depth not far from the surface. The data is read out at regular intervals. The time interval between the measurements is constantly one hour.

[2]Coordinates: 475000E 5262000N. UTM (33T), WGS 84.

Figure 1.5.: The soil temperature logger on the Gscheideggkogel. With kind permission of the Nationalpark Gesäuse.

The next chapter presents the methodological framework of the thesis. It begins with an introduction to the climate system and the earth's energy budget. The physical problem of heat flow and temperature in the soil is presented. What follows is the mathematical representation of the problem and the solution of it using Green's function method.

# 2. Methods

To solve the task of analysing the temperature and flux profile, the necessary mathematical and physical theory will be presented. Already with respect to the conclusio and the outlook, special emphasis is put on generality, especially the mathematical concepts around the partial differential equations are treated more rigorously. This includes an introduction to the functional analysis, the distribution theory and the method of green's functions. With these tools, the problem of the heat equation can be countered and a solution can be found for the given framework.
However, it starts with an introduction to system dynamics theory in section 2.1.1, which is essential for dealing with the climate system as well as ecosystems. To make this abstract approach more concrete, an instructive zero dimensional radiation balance model for the earth is set up. Afterwards we focus into the subsystem pedosphere and there specifically into the uppermost soil layer of the lithosphere, where the consideration lies, more or less decoupled from the superior systems, on the problem of the temperature distribution and the temperature flux within the soil. Particularly, this problem is then solved with the Heat equation, respectively the Green's function of the problem will be found. Once the Green's function is found, the problem can be considered as solved, since the convolution theorem allows to construct particular solutions. This approach is physically equivalent to the superposition principle, as shown in chapter 2.2.5. By means of simple algebra, the ground heat flux $B_0$ in (1.1) can than be determined from the temperature, which is known from the measurements and the energy closure problem can be discussed. If $B_0$ is known, the whole temperature and heat flux profile of the soil can be reconstructed in turn.
Consequently, the remaining chapter 2.2 deals with the previously mentioned mathematical theory for the solution of partial differential equations.

## 2.1. The Climate System

The climate is a complex system. There are different formal approaches to this science. A special and appropriate formulation can be given with the help of system theory, which is therefore outlined below.

### 2.1.1. Review of Dynamical System Theory

In the following, the problem is outlined on the basis of the climate system. With a general systemic approach to such a problem, however, all other systems can be treated analogously. This includes ecosystems as well.

Considering the Earth's climate system as a statistical system with many degrees of freedom, a microstate of the climate is completely determined by a point

$$\boldsymbol{\pi} = (\pi_1, \pi_2, \ldots, \pi_{ns}) \equiv (\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n)$$

in phase space $\Gamma$, where $\boldsymbol{q}_i$ is a generalized coordinate with dimension $s$, which are gouverning the system. The dimension of the phase space are than the degrees of freedom $ns$. Depending on how we look at the system, the number of dimensions or degrees of freedom can change for expediency or convinience and has a range from zero dimensional, as in the Zero Dimensional Radiation Balance Model in Chapter 2.1.3, to a huge number of degrees of freedom, as in the Earth system model.
The phase trajectory, i.e. the evolution of the system, is the set of all phase space points $\boldsymbol{\pi}$ occupied by the system over time. With given initial conditions and the dynamic of the system, the phase trajectory is uniquely computable and thus future states can be predicted. The dynamic is given by the processes, which are controlled e.g. by physical laws. For a specific process we call the dynamic, the equation of motion of this process. Thus the processes prescribed by equation of motion connect the states. With the evolution parameter $t$, which is often the time but not always, the state of the system is $\boldsymbol{\pi}(t)$ and can be determined from an initial state $\boldsymbol{\pi}(\boldsymbol{t} = \boldsymbol{0})$ if the dynamics, i.e. the processes, are known. We name $\mathcal{H} = \mathcal{H}(\boldsymbol{\pi}, t)$ the generalized Hamilton-function which describes the

abstract energy of the entire system. If $\boldsymbol{\pi}$ is known, every measurable variable, i.e. every so called observable of the system, can be specified with

$$F = F(\boldsymbol{\pi}, t)\,. \tag{2.1}$$

Such observables are thus our measurable quantities that describe the macroscopic state of the climate, such as the globally averaged near surface temperature of the atmosphere. Many microstates now realize the same macrostate, the microstates all lie on the same hypersurface in phase space. So it can be said, that a macrostate, in turn to a microstate, describes the system by a few state variables, which are those previously mentioned observables. Especially for Climate System this observables are called Essential Climate Variables. For Ecosystems they are called Standard Observations.

Note that this observables follow a equation of motion in particular as well, e.g. for Hamiltonian Systems

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, \mathcal{H}\} + \frac{\partial F}{\partial t}\,,$$

where the bracket $\{\ldots,\ldots\}$ is the Poisson-bracket defined by

$$\{F, H\} = \sum_{j}^{s} \left( \frac{\partial F}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial H}{\partial q_j} \right)\,.$$

Here $H$ is the classical Hamiltonian and $p_j$ is the conjungate momentum to the generalized coordinate $g_j$. Notice that this evolution equation only applies to Hamiltonian systems. For the climate system and also for ecosystems it applies in general, that they are nonlinear and chaotic, so the search for full dynamics is often hopeless if you considering a lot of degrees of freedom. With the help of the theory of dynamic systems, however, statements can be made about the system behavior, such as equilibrium states, tipping points and attractors.
Because of the chaoticness of the climate system, it is not possible to consider it as an initial value problem over a long integration time and not necessary either. For this reason, the climate is a boundary value problem, which is driven by various influences, such as the magnitude of the Earth's orbit parameters or the concentration of greenhouse gases, to name a few popular representatives. For comparising, the numerical wheater forecast is an initial value Problem. It does not depend on slowly varying boundary conditions like trace gases in the atmosphere but depends e.g. on the current atmospheric pressure.

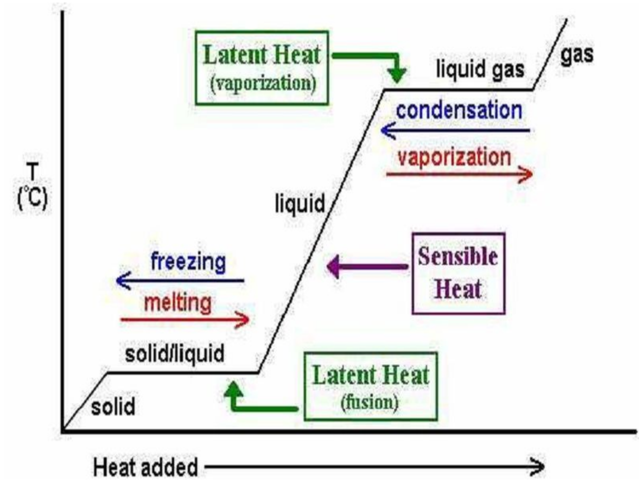


Figure 2.1.: To illustrate the difference between latent and sensible heat. Figure from SG (2007).

### 2.1.2. Latent and Sensible Heat

The quantities latent heat $L$ and sensible heat $H$ introduced in (1.1) are thermodynamically motivated. If you look at a body and supply it with heat from the environment, the change in heat can manifest itself as latent or sensible heat.

If it is a latent heat change, the measured temperature in °Celsius remains the same. The supplied energy is required for a phase transition and is then retained in this phase. If it is transformed back again, the stored energy is released back into the environment. Of course, this process can also be viewed vice versa.
Sensible heat, on the other hand, is a measure of how the measured temperature, also in °Celsius, increases when heat is added from the environment. So it is really the sensed heat that a body sends to human receptors. This is why sensible heat is also called tactile heat. The difference between latent and sensible heat is illustrated in Fig. 2.1.

Concerning climate, these two heat terms have already been motivated by (1.1). At the boundary layer between the ground and the atmosphere, energy is not only transferred in the sense that the absolute temperature changes in

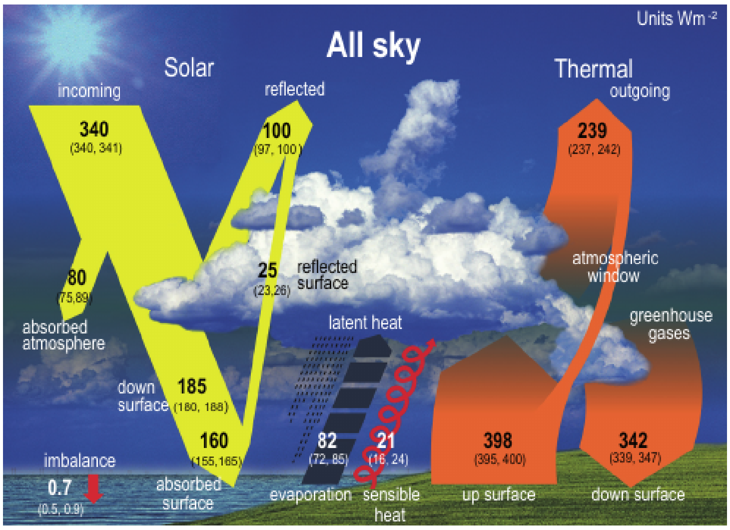


Figure 2.2.: Schematic scetch of the global mean energy budget of the earth. The values gives the estimates for the magnitudes of the globally averaged energy balance components in $Wm^{-2}$ together with their uncertainty ranges (5–95% confidence range), representing climate conditions at the beginning of the 21st century. Figure from Masson-Delmotte et al. (2021, ch. 7, p. 934).

both spheres, but phase transitions also take place continuously, which manifest themselves in latent heat.
An important quantity is the ratio between sensible and latent heat, the so called Bowen ratio:

$$\beta = \frac{H}{L} \,. \tag{2.2}$$

This parameter not only plays an outstanding role when talking about climate conditioning of cities, but also for micrometeorological questions. As shown in H. Kraus (2008, Ch. 11.5, p. 140ff), $\beta$ is used for the conventional measurement of energy balance terms and thus for the budget closure problem of (1.1).

Next, we take a closer look at the Earth's energy budget.

### 2.1.3. Earth's Energy Budget

This chapter is a brief summary of Foken (2016, Ch. 1.4) and of H. Kraus (2008, Ch. 11).

The energy input into the Earth's climate system can be attributed for the very most part to the sun. Other contributions, such as geothermal energy generated by radioactive decay or tidal friction will be neglected. In the following, there will therefore only be talk of the radiation budget. So the sun is the main driver of earth's climate and one can quantify her contribution by means of the solar constant. All processes which come after are conditioned by the influence of the sun. As far as the radiation balance of the earth is concerned, this fact is very well visible in Fig. 2.2.

The solar constant $S_0 = 1361\,\frac{\mathrm{W}}{\mathrm{m}^2}$ is the measured mean flux density of the solar electromagnetic radiation at a distance of one astronomical unit (AU), where the rays of the sun hit the earth's surface perpendicular to the beam direction without influence of the atmosphere. In Fig. 2.2, the incoming flux is given with $340\,\frac{\mathrm{W}}{\mathrm{m}^2}$. This corresponds to a quarter of the solar constant , wich is the daily average incoming radiant power at the TOA for half a spherical surface.

The sun as the driver of earth's climate is almost an perfect black body. According to Planck's radiation law, the spectral radiance is

$$B(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{k_B \lambda T}\right) - 1}\,, \tag{2.3}$$

where the spectrum of a black body depends only on the absolute temperature $T$ of the body, as can be seen in Fig. 2.4. By setting the first derivative of (2.3) to zero, Wien's displacement law can be derived

$$\lambda_{max}(T) = \frac{2898\,\mu\mathrm{mK}}{T}\,, \tag{2.4}$$

where $\lambda_{max}$ is the maximum wavelength at the temperature $T$. Inserting the approximated values of the surface temperature of the sun $T_\odot \cong 5800\,\mathrm{K}$ and the mean earth temperature $T_\oplus \cong 290\,\mathrm{K}$, we get a maximum wavelength for the sun of $\lambda_{max,\odot} = 0.5\,\mu\mathrm{m}$, which corresponds to visible light. For the earth

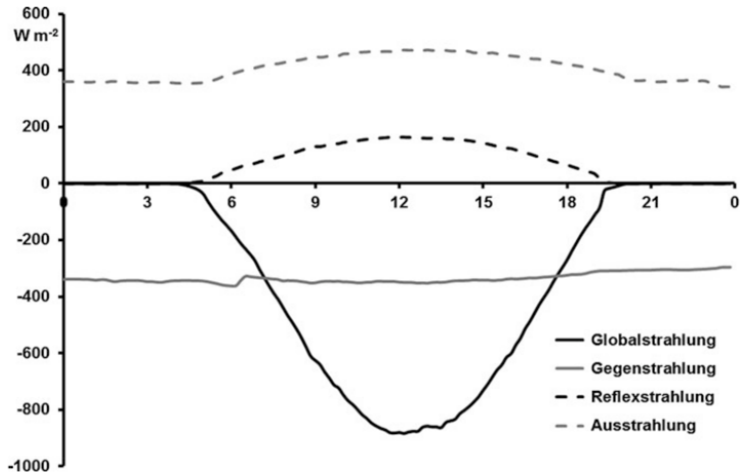


Figure 2.3.: Diurnal cycle of the components of the energy balance on 24.05.2012, Ecological-Botanical Garden of the University of Bayreuth. Figure from Foken (2016, p. 16).

the maximum wavelength $\lambda_{max,\oplus} = 10\,\mu$m lies in the thermal infrared.

The maximum intensity of the solar radiation is irradiated in the visible range which can pass the atmosphere almost unhindered. But the solar spectrum also contains other frequencies, which interact with the atmosphere. All in all, the incident shortwave radiation $Q_s$ must be divided into

$$Q_s = K \downarrow - K \uparrow = D + H - K \uparrow = (1 - A) K \downarrow \,. \tag{2.5}$$

Here $K \downarrow$ is global radiation, $K \uparrow$ is reflective radiation, $D$ is direct radiation, $H$ is diffusive radiation, and $A$ is albedo which is the ratio between the reflective radiation and the global radiation:

$$A = \frac{K \uparrow}{K \downarrow} \,. \tag{2.6}$$

In Fig. 2.3 you can see a representative of a diurnal cycle with the balance and the different flow components. The spectral intensity maximum of the Earth, on the other hand, lies in the long-wave IR, as has already been shown. Also this longwave radiation $Q_l$ can again be divided into terrestrial radiation of the earth's surface $I \uparrow$ and the back radiation (atmospheric gases, aerosols and

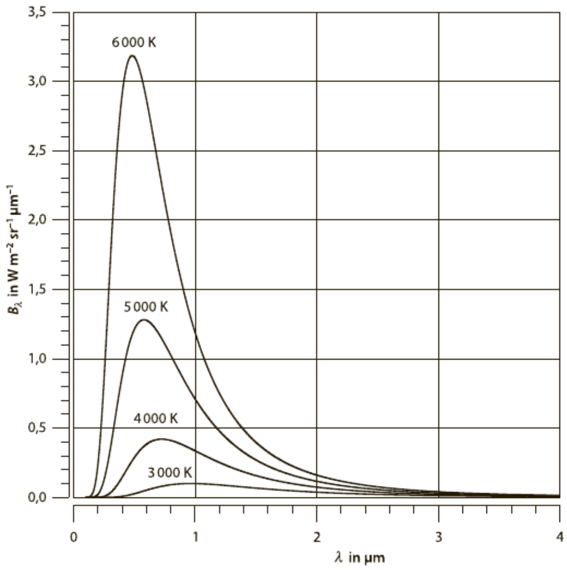


Figure 2.4.: Spectrum of the black body radiation as a function of wavelength for different temperatures. Figure from H. Kraus (2004, p. 100).

clouds) $I \downarrow$

$$Q_l = I \uparrow - I \downarrow \,. \tag{2.7}$$

The total radiation balance is therefore

$$Q = Q_s - Q_l = K \downarrow - K \uparrow - I \uparrow + I \downarrow \,. \tag{2.8}$$

At equilibrium, the sum of the radiative balance is 0, which is assumed in the zero dimensional model in the next section, with which the mean surface temperature of the earth is to be estimated. More details about the earth's energy budget are given in Foken (2016, Ch. 1.4).

## Zero Dimensional Radiation Balance Model

The zero dimensional radiation balance model allows an instructive access to the climate system considered as a boundary value problem. With it's help, it is possible to estimate a important state variable of the climate system, the mean surface temperature of the earth. Furthermore, it provides the definition of the greenhouse effect. More details about this topic can be found in H. Kraus (2004, ch. 9, p. 95) and Roedel (2017, ch. 1, p. 1).

By integrating the Planck spectrum (2.3) over the whole half-space into which the surface element radiates, as well as over all frequencies, you get the Stefan Boltzmann law

$$P(T) = \frac{2\pi^5}{15}\frac{k_B^4}{h^3c^2}T^4 := \sigma T^4 \,. \tag{2.9}$$

Here $\sigma$ is the Stefan-Boltzmann constant with the unit $\left[\frac{\mathrm{W}}{\mathrm{m^2K^4}}\right]$. This law indicates the radiation flux or the specific power per unit area of an ideal blackbody as a function of its absolute temperature. For non-ideal black bodies, the incident radiation is not completely absorbed. In any case, with $0 \leq \alpha \leq 1$ is the absorption coefficient and $0 \leq \varepsilon \leq 1$ is the emission coefficient, the Kirchhoff's radiation law states

$$\alpha = \varepsilon \,, \tag{2.10}$$

where $\varepsilon = 0$ would correspond to an ideal white body and $\varepsilon = 1$ to an ideal black body. This means that the absorption of a body is equal to its emission, but this is only true in thermodynamic equilibrium. The Stefan-Boltzmann law is only valid for ideal black bodies, as the sun is almost entirely one. In contrast the earth is not absorbing the whole incoming radiation. So (2.9) has to be modified for non black bodies by the emission coefficient:

$$P(T) = \varepsilon\sigma T^4 \,. \tag{2.11}$$

In the case of a wavelength independent emission coefficient $\varepsilon(\lambda) = \text{const.}$, one speaks of a gray body. For the earth as a whole in the infrared range, a emission coefficient of $\varepsilon = 0.95$ is valid, which means that the earth is such a gray body. With these ingredients, a first zero-dimensional model can already be constructed.

The radiation balance in equilibrium for the earth is simply given by

$$\text{incoming radiation} = \text{outgoing radiation} \,. \tag{2.12}$$

The incoming radiation is therefore the radition from the sun per square meter times the cross section of the earth:

$$\text{incoming radiation} = S_0(1-A)\pi R_\oplus^2 \,.$$

$A = 0.3$ denotes the mean albedo of the earth. The outgoing radiation from the earth is the earth's spherical area times the thermally radiated power $p$[1]:

$$\text{outgoing radiation} = \varepsilon\sigma T_{eff}^4 4\pi R_\oplus^2 \,.$$

Insert the outgoing and the incoming radiation in (2.12) gives than

$$S_0(1-A) = 4\varepsilon\sigma T_{eff}^4$$

and therefor an effective temperature of the earth of about $T_{eff,\oplus} = -14\,°\mathrm{C}$. But the measured mean surface temperature of the earth is nowadays about $+15\,°\mathrm{C}$[2]. This temperature difference is quite significant after all, the model is obviously incorrect. One essential system component of the earth has been ignored so far, which is the atmosphere and it's greenhouse gases in particular.

In this zero dimensional model, the contribution of the atmosphere and it's infrared active gases is easily added. Only a factor $\tau_{IR}$ must be multiplied on it, which is the transmissivity in the infrared and is about 0.65 for the earth's atmosphere. The global mean surface temperature is than calculated using

$$S_0(1-A) = 4\tau_{IR}\varepsilon\sigma T_{eff}^4$$

to $+15\,°\mathrm{C}$. So without an atmosphere and it's greenhouse gases, the mean earth's surface temperature would be about $30\,°\mathrm{C}$ lower in this model.

The measured temperatures at the top of the atmosphere (TOA), where they are measured by satelites, should really correspond approximately to the calculated value of $-14\,°\mathrm{C}$, because the radiation balance must be given. This value is therefore independent of the greenhouse gas concentration within the

[1]According to Spektrum (1998) the effective temperature $T_{eff}$ is the temperature of an object that a black body would have if it had the same luminosity as the object.

[2]If the state variable of global mean temperature is used in this thesis, it is only for a didactic purpose. In climate science, mainly temperature differences are the object of investigation, not absolute temperatures.

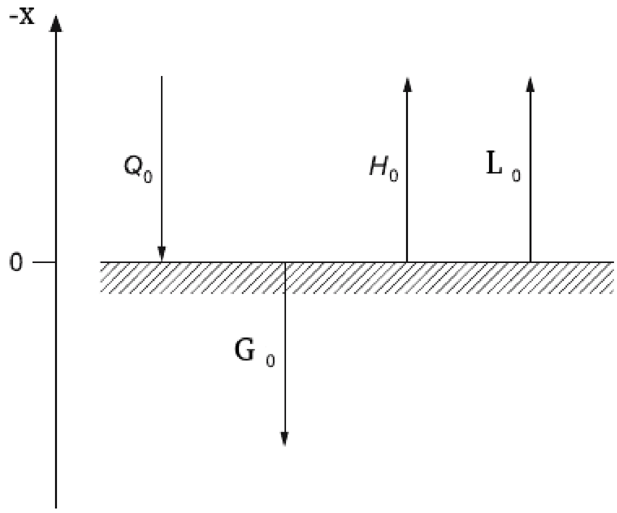


Figure 2.5.: Energy fluxes at the surface. Adapted from H. Kraus (2008, p. 33).

atmosphere but only dependent on the solar constant, if the albedo of the earth and the emissivity $\varepsilon$ remains the same. This immediately provides an indication of the discrimination between natural and anthropogenic climate change. If greenhouse gases increase, resulting in a temperature rise at the earth's surface, but the solar constant remains the same, the satellites do not measure any temperature change. Thus, a near-surface temperature change cannot be attributed to changes in e.g. solar activity.

### Energy Budget at the Earth's Surface

Let's concentrate on the subsystem pedosphere. As already mentioned, it is the interface between the Atmosphere, Biosphere, Hydrosphere, Cryosphere and Lithosphere and therfore the place where the diverse spheres and their numerous processes come together. A high degree of interdisciplinary expertise is required to understand and describe all processes and states at this interface. In the climate models, as mentioned at the beginning, the coupling was implemented and the ESM were created. These models have to be supplied with data, which requires a network of field measurements.
Anyway, the energy budget directly at the earth's surface has a great influence

on the processes in the pedosphere, especially for the microclimate. If one considers only the atmosphere and the soil and leaves all other spheres out, the energy budget at this interface is already given in Eq. (1.1) as

$$Q_0 - B_0 - H_0 - L_0 = 0\,.$$

and is vividly presented in Fig. 2.5. In Fig. 2.6 you can see a representative of a diurnal cycle with the balance and the different flow components.
The fact that the various energy flows add up to zero takes conservation of energy into account. Only vertical components need to be considered, as the horizontal ones average out. Above and below this boundary layer there are different profiles of the state variables, because the interaction processes in the atmosphere are different from those in the soil. Directly at the interface, however, the state variables must coincide, since continuity must be assumed. Let's talk about quantifying the variables in (1.1).

The radiation balance $Q_0$ is a standard meteorological measurement and the data are available, e.g. through the WegenerNet.
There exist a connection between the sensible heat and the ground heat flux as shown in Sadeghi et al. (2021), this will be discussed in more detail in the conclusion in Chapter 5. The sensible and the latent heat are connected through the bowen ratio (2.2), so the only value left to close the energy balance (1.1) is the ground heat flux $B_0$.

### Ground Heat Flux

The term soil must first be targeted. In the introductory view, the term soil is ambiguous. It was called the boundary layer between atmosphere and solid earth. However, this includes both the soil from loamy earth and the leaf of a tree. Further also stones, snow, sand and generally vegetation are included. For the following executions, however, we will speak of the loamy earth as soil, only with respect to this point of view, the heat equation can contribute meaningfully to the consideration. The fact that even the loamy soil represents a porous medium is not considered in the following and is discussed only in the summary in chapter 5 again. Thus, there is no convection in the soil considered here, which simplifies the problem immensely. So heat transfer in the floor really only takes place via conduction, as opposed to radiation and convection. According

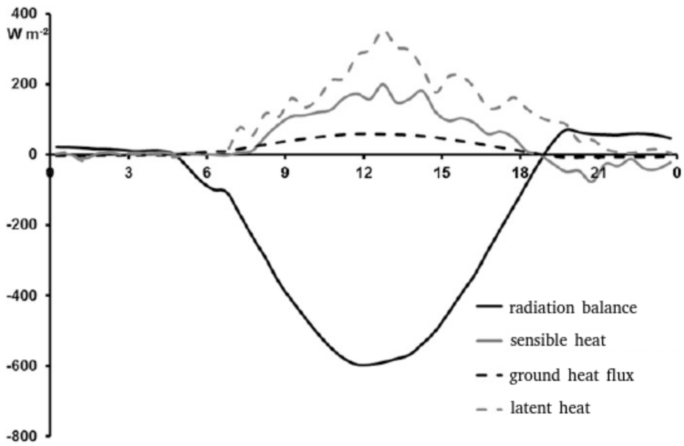


Figure 2.6.: Diurnal cycle of the components of the energy balance at the ground on 24.05.2012, Ecological-Botanical Garden of the University of Bayreuth. Adapted from Foken (2016, p. 14).

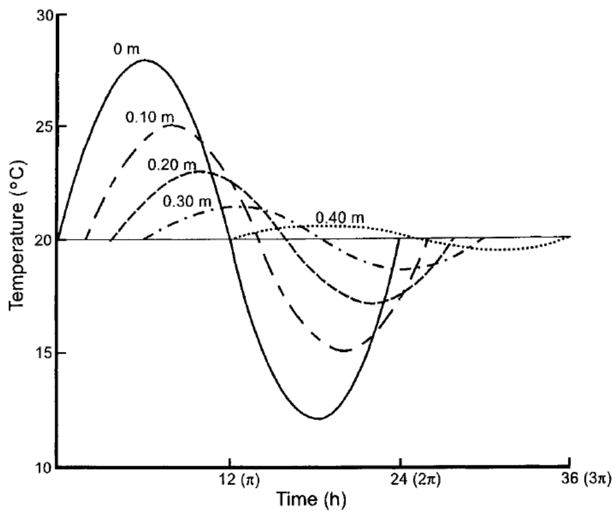


Figure 2.7.: Graph of the phenomenological solution to the heat conduction problem for different depths. The increasing phase shift with greater depth is clearly visible. Figure from Hillel (2003, p. 325).

to the second law of thermodynamics, heat always flows in the direction of lower temperature. The Further treatment to the ground heat flux are adapted from H. Kraus (2008, ch. 11.2, p. 129).

For solid soil with the above properties, Fourier's heat equation applies. Thereby the ground heat flux is a function of depth and time and is proportional to the temperature gradient

$$B(x,t) = -\lambda \frac{\partial T}{\partial x}\,, \tag{2.13}$$

where $\lambda$ is the thermal conductivity coefficient with the unit $\left[\frac{\mathrm{W}}{\mathrm{mK}}\right]$. The source of the soil heat flux is the change in temperature over time within the soil. If the temperature is stationary, the soil heat flux is sourceless. Therefore the dynamic relation

$$\rho c \frac{\partial T}{\partial t} = -\frac{\partial B}{\partial x} \tag{2.14}$$

is valid. Here $\rho$ is the density of the soil and $c$ the specific heat capacity which is related via the thermal diffusion constant $a$ to

$$a = \frac{\lambda}{\rho c}\,.$$

With (2.13), (2.14) and the diffusion coefficient $D$, the heat equation results

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial T^2}\,.$$

This equation is defined again in a more generally formulation in chapter 2.2.1 about the diffusion equation. The solution of the heat conduction problem will be given a lot of attention in chapter 3 where the Green's function to the problem is determined. First, however, a phenomenologically solution to the problem is to be found. With its help, the thermal profiles calculated later from the temperature data can be compared and the methodology verified. So, first of all, a usual daily temperature profile in the ground shall be created.

If one considers a radiative diurnal cycle, one can roughly assume a periodic

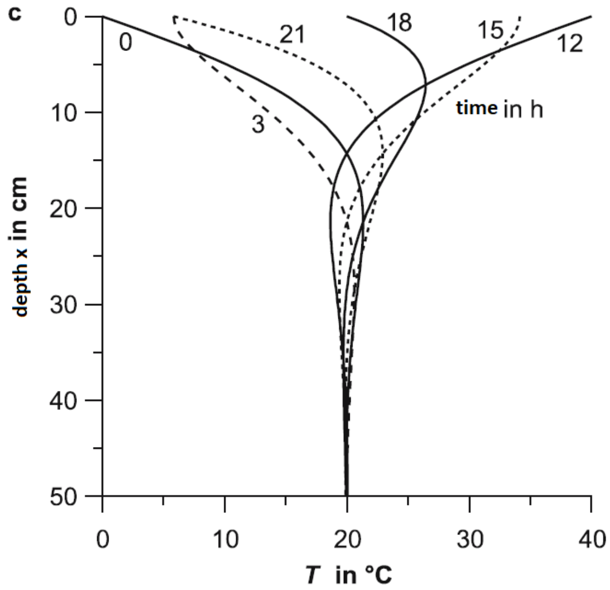


Figure 2.8.: Depth profiles of temperature (tautochrons) at six different times of a day calculated with (2.18). Adapted from H. Kraus (2008, p. 133).

insolation as upper boundary condition

$$T(0,t) = \overline{T} + A_0 \sin \omega t \,. \tag{2.15}$$

$A_0$ is the amplitude of the surface temperature fluctuation and $\omega = \frac{2\pi}{T}$ where $T = 24\,\mathrm{h}$. The other boundary condition is

$$T(x \to \infty, t) = \overline{T} \,. \tag{2.16}$$

The initial value is not really decisive, because after a long integration time an equilibrium is reached anyway, no matter from where you start. For simplicity we set $T(x,0) = 0$. The temperature at any depth $x$ is also a periodic function of time with a depth dependent amplitude and phase angle, as shown in Van Wijk and De Vries (1963):

$$T(x,t) = \overline{T} + A(x) \sin\left(\omega t + \phi(x)\right) . \tag{2.17}$$

Inserting this approach into the heat equation gives the solution by Hillel (2003) of

$$T(x,t) = \overline{T} + A_0 \exp\Big(-\frac{x}{d}\Big) \sin\Big(\omega t - \frac{x}{d}\Big) \,, \tag{2.18}$$

where $d$ is a called the damping depth at which $T(d,t) = A_0/e$ applies and is related to the thermal properties of the soil and the frequency of the temperature fluctuation:

$$d = \sqrt{\frac{2a}{\omega}} \, . \tag{2.19}$$

As can be seen in the sin factor of the solution (2.18) respectively vividly also in Fig. 2.7, there is a phase lag of the temperature peak what is typical for a temperature wave penetrating the ground.The depth profiles of temperature at six different times of day is shown in Fig. 2.9, this graphs are Tautochrones of the temperature profil within the soil.

Substituting the solution (2.18) into (2.13), gives the phenomenological soil heat flux

$$B(x,t) = \frac{\lambda}{d} A_0 \exp\Big(-\frac{x}{d}\Big)\sqrt{2}\sin\Big(\frac{\pi}{4} - \frac{x}{d} + \omega t\Big) \tag{2.20}$$

and the surface ground heat flux

$$B_0 = B(0,t) = \frac{\lambda}{d} A_0 \sqrt{2}\sin\Big(\frac{\pi}{4} + \omega t\Big) \, , \tag{2.21}$$

whose graph is shown in Fig. 2.9. The phase shift, with which the maxima or minima of the temperature wave occur at two different depths, provides a second good method to determine $a$ after the relation with the damping constant $d$. From

$$t_{max}(x_2) - t_{max}(x_1) = \frac{x_2 - x_1}{\sqrt{2a\omega}} \tag{2.22}$$

the thermal diffusion constant $a$ can be determined. For short integration times, $\overline{T}$ is not necessarily constant for not too large depths and the term $-\lambda\frac{\partial \overline{T}}{\partial x}$ is nonzero. This additional term in the bottom heat flux takes into account the e.g. seasons. After the end of winter, a time-independent heat flux is established until equilibrium is reached again. After that, this additional term goes back to zero and the soil heat flux follows again mainly the insolation and the nocturnal radiation.

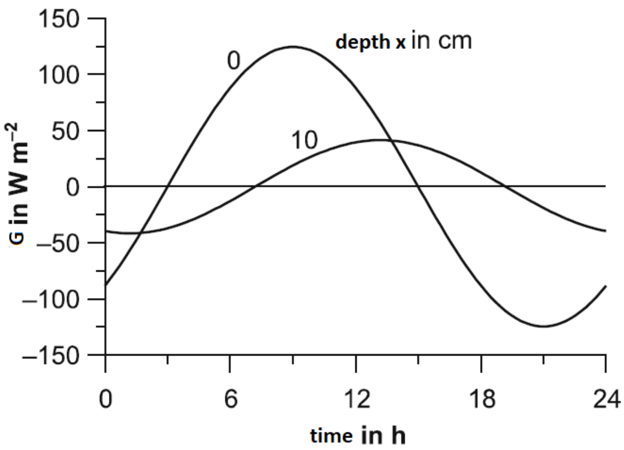


Figure 2.9.: Soil heat flux for two different depths, one for the surface and one for 10 cm depth, over the period of 24 hours, calculated with (2.20). The time lag in the depth can be seen well. Adapted from H. Kraus (2008, p. 133).

The periodic assumption is an idealizing and rough simplification because the real diurnal variation in surface temperature does not follow a periodic function. Equinox alone occurs on only two days of the year. This circumstance can be solved by using a Fourier series to accurately describe the diurnal variation in surface soil temperature as shown in Van Wijk and De Vries (1963), but the periodic approach is considered sufficient here.

In the previous modelling, the boundary layer between soil and atmosphere was assumed to be a homogeneous surface. Of course, this does not correspond to reality, where vegetation or snow is present above the ground. The ground alone is often a porous medium within which convection prevails; a more adequate model would result from the convection-advection equation or the porous medium equation. However, this work does not go that far, it is limited here only to the diffusion equation.

Before dealing with partial differential equations, a few words about the vegetation and snow above the ground.

### 2.1.4. Stock Climate

The following in this chapter is a brief summary of H. Kraus (2008, Ch.13) on stock climate. The stock is defined here as the sum of vegetation elements (leaves, branches, trunks, roots, etc.).

Plant cover naturally has an influence on the energy balance (1.1). The interface between soil and atmosphere can also no longer be clearly defined in this approach. In trees, for example, the surface of each leaf is the interface with the atmosphere. In this case, the problem of the soil heat flux must be defined differently, simply because of the transpiration, respiration and the albedo of the stock, just to name a few representatives.
The stock climate, i.e. the microclimate over plant cover, is difficult to model as a whole, there is no getting around numerical approaches. Nevertheless, one must or wants to understand the complex interactions that take place between the spheres. This is also necessary to integrate numerical Earth system models. The chapter on surface-vegetation-atmosphere transport in H. Kraus (ibid., Ch. 13.3) provides some incentives for this.
In the context of this work, these considerations are important because the quantities in (1.1) depend on the stock climate, respectively because the stock climate is a perturbation of the physical problem of the energy balance at the surface.

### 2.1.5. Microclimate above Snow

The following is a brief summary of H. Kraus (ibid., Ch. 14) on the microclimate above snow.

The balance equation (1.1) must be reevaluated in the presence of snow. The ground heat flux $B_0$ is thereby divided into two parts. The first part describes the heating of the ice and the second part the heat of melting, i.e. the melting enthalpy. The incident solar energy is therefore also used for phase transition and is converted into melting energy. The surface temperature remains constant at 0 °C, this influences the evaporation and the sensible heat considerably. A stable stratification is achieved above the ice and the heat flow is limited towards the top. If the radiation balance is positive, the excess energy is mainly used for melting. The remaining energy terms are then negligible. Overall, H. Kraus (ibid.) comes to the conclusion that the high albedo and melting processes with a positive energy balance prevent a warming of the air from the ground. This means that the sensible heat flow from the ground is prevented in the presence of snow.

For the soil itself and the temperature loggers in the ground, a snow cover means a very good insulation layer. The temperature dynamics will come to a standstill in the presence of snow, this will be noticeable by a ground heat flux identical to zero as will be shown in Ch. 4.

In the next section, there will be an overview of the theory of partial differential equation's. The diffusion equation will be derived. This is followed by an introduction to functional analysis and distribution theory, which can be used to define Green's function.

## 2.2. Partial Differential Equations

The most important definitions and theorems are given in this chapter in order to then give an overview to a solution theory of partial differential equation's (PDE)[3]. This includes elements of functional analysis, distributions and their application to linear PDE which leads to an solution calculus which is called Fundamental solution. If boundary value problems are considered, as it is the case here, the fundamental solution is concretized to the so called Greens's function. In chapter 3 this calculus is then used to determine the ground heat flux from the space-time-point temperature data and thus the temperature and flux field. All introduced elements are either described directly or referred to a description in the appendix.

The discussion in this chapter is largely based on Evans (2010), Kerner and Wahl (2013, Ch. 12) and Goldhorn, Heinz, and M. Kraus (2009) and therein in

[3]In this thesis the abbreviation PDE is ambiguous, it is used for the plural (partial differential equation's) as well as for the singular (partial differential equation) and can be understood from the context.

particular the chapters 7 on Banach- and Hilbert spaces, 11 on Distribution's and 13.D on Applications to linear differential equations.

### Well-poseness of a Problem

Partial differential equations are used to represent natural processes mathematically and thus to analyze them. In these equations, the solution function and its derivatives occur simultaneously. The PDE thus mathematically specify the dynamics for processes of various kinds, it remains only to find the solution, which turns out to be not always easy. First it must be clarified whether such a solution exists at all and whether it is unique, before one gives oneself on the search for it or to calculate the solution with numerical methods. Second, it is not said, that the solution is of the usual kind, what this means will become clear later.

Anyway it starts with the first issue, which leads to the informal definition of a well-posed problem which in Evans (2010, ch. 1.3.1) reads as follows:

(i) the solution indeed exist,

(ii) this solution is unique,

(iii) the solution depends continously on the data given in the problem.

The last condition means in summary, that the solution would not have a chaotic behaviour. But what conditions must a solution satisfy?

Is it necessary that the solution is classic[4]? Or does this ask too much and limit the solution set too much?

Just think of snow falling on the ground. The temperature of the snow has, directly at the impact on the earth, in general, another temperature than the earth surface. As will be shown later, the heat equation has a smoothing property, which means that, when two bodies with different temperatures are

[4] A classic solution informally means that the solution is out from $C^k$, where $k$ corresponds to the order of the PDE. With this claim, the derivatives appearing in the PDE at least exist and are continuous, even if derivatives higher than order $k$ exist.

joined together, the average temperature at the interface will be instantaneous. This means that the temperature gradient at the interface becomes infinite. This is unphysical, but this is how the heat equation is modeled and we have already identified it as an adequate equation for the problem presented here. The unphysicality can be defused, if one considers that the instantaneous temperature adjustment at the boundary surface is concentrated only on an infinite narrow surface, it then propagates instantaneously into the neighboring infinite narrow surfaces. Thus, we are dealing with singularities in time and space. How to model them mathematically is already shown to us by electrodynamics. If there e.g. a point charge is mentioned, then the mathematical calculation of the distribution becomes important which will be outlined in chapter 2.2.5. Especially the Delta Distribution will be used to describe such a process. But before that, some definitions are given and the concept of weak solution is briefly introduced, which is reasonably instructiv and trains the handling of so called test functions, which are essential for the theory. With these generalized solutions, the conditions (i)-(iii) of well-posed problems can then be shown much more easily than if we had to construct them laboriously with the help of classical solutions.

### Definition of a Partial Differential Equation

However, the heat equation, which will be derived in 2.2.1, is a PDE of second order. So this means that the differential operator of the heat equation will be of second order. It has the condition that it is linear and only linear operators are considered in this thesis. Operators in general will be discussed in more detail later. For now, with the definition of a linear operator, the topic of linear PDE is opened:

**Definition 1** *An operator $T : U \to V$ with real or complex vector spaces $U$ and $V$ over $\mathbb{K}$, is linear, if*

1. $T(x + y) = Tx + Ty$ ,
2. $T(\lambda x) = \lambda Tx$,

*for all $x, y \in U$ and for all $\lambda \in \mathbb{K}$, where $\mathbb{K}$ is $\mathbb{R}$ or $\mathbb{C}$.*

A differential operator is of this sort and is defined in general as follows:

**Definition 2** *Be $\Omega \subseteq \mathbb{R}^n$ an area. For multiindices*[5] $|\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n)| \leq k$, $a_\alpha(x) \in \mathcal{C}^\infty(\Omega)$ *are given functions. Than one define a* ***linear differential operator*** *of the order $k$ by*

$$L(x, D) := \sum_{|\boldsymbol{\alpha}| \leq k} a_\alpha(x) D^\alpha\,, \quad D = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right)\,. \tag{2.23}$$

*If the hieghest coefficient $a_\alpha$, with $\alpha = k$ enters nonlinearly, so $g(a)$, than the differential operator $L$ is not linear anymore.*

A PDE is an equation, which includes the seeked function and partial derivates of it:

**Definition 3** *A equation of the form*

$$F\left(x,\, u(x),\, \frac{\partial u(x)}{\partial x_1}, \ldots, \frac{\partial u(x)}{\partial x_n}, \frac{\partial^2 u(x)}{\partial x_1^2}, \frac{\partial^2 u(x)}{\partial x_1 \partial x_2}, \ldots, \frac{\partial^{k-1} u(x)}{\partial x_n^{k-1}}, \frac{\partial^k u(x)}{\partial x_n^k}\right) = F\left(x,\, u(x),\, Du(x), \ldots, D^{k-1}u(x),\, D^k u(x)\right) = 0 \tag{2.24}$$

*is called a partial differential equation of $k$-th order, where*

$$F : U \times \mathbb{R} \times \mathbb{R}^n \times \cdots \times \mathbb{R}^{n^{k-1}} \times \mathbb{R}^{n^k} \to \mathbf{R}^m$$

*and*

$$u : U \to \mathbb{R}$$

*is the solution of the equation.*

In this thesis the heat equation is considered, which is an linear PDE, where this property is defined as follows:

**Definition 4** *The PDE (2.24) is linear if it has the form*

$$\sum_{|\alpha| \leq k} a_\alpha(x) D^\alpha u =: L(x, D)u = f(x)$$

*for given function $a_\alpha$ ($|\alpha| \leq k$), $f$, and is homogeneous if $f \equiv 0$.*

[5]The multi index notation allows a more compact notation for linear differential operators and is presented in the appendix in chapter B.

The linear PDE is given again in a very compact form as

$$Lu = f\,, \tag{2.25}$$

with the inhomogenity $f$ on the right hand side. In contrast to ordinary differential equations (ODE), no closed solution theory exists for PDE. For ODE, the Picard-Lindelöf theorem guarantees the existence and uniqueness of initial value problems. Unfortunately, a corresponding counterpart for general PDE does not exist. Luckily something analogous exists for linear PDE, what leads to the lemma of Lax-Milgram. This lemma guarantees existence and uniqueness for at least weak solutions of linear PDE. Because of this we do not only speak of the above mentioned classical solution but extend the solution set by alternative solution terms instead. These solution functions are also able to model circumstances for which smooth properties are not sufficient, i.e. for which no classical solutions exist.

For motivation, it start's with the derivation of the Diffusion equation in Ch. 2.2.1. Afterwards the weak derivative is introduced to get used to the methodology of generalized solutions for PDE. Before that, function spaces are introduced in Ch. 2.2.2 where the so-called test functions play an outstanding role for the weak derivation and for distributions.

### 2.2.1. Diffusion Equation

If considering a conserved quantity, the continuity equation

$$u_t + \nabla \cdot \boldsymbol{j} = 0 \tag{2.26}$$

is valid. Here the first term is the change of the density $u(\boldsymbol{r}, t)$ of the observed quantity and the second term is the source term with the flux $\boldsymbol{j}$ of the diffusive quantity. On the other hand Fick's first law says, that the flux of a diffusive quantity is proportional to its gradient

$$j = -D(u,t)\,\nabla u(\boldsymbol{r}, t)\,. \tag{2.27}$$

Here $D(u,t)$ is the diffusion coefficient, which is in general dependent on $u$ and $t$ and therefore leads to a nonlinear PDE. These dependencies can be neglected for this problem posed here. However, the coefficient is set to a constant $D(u,t) \equiv D$. If diffusion is overlaid by convective flux $\boldsymbol{j} = \boldsymbol{v}u$, this convective component is added to the total flux

$$\boldsymbol{j} = \boldsymbol{j}_{\text{diff}} + \boldsymbol{j}_{\text{conv}} = -D\nabla u + \boldsymbol{v}u\,.$$

Substituting into the continuity equation leads to the convection-diffusion equation

$$u_t - D\Delta u + v \cdot \nabla u = 0\,. \tag{2.28}$$

The magnitude of the diffusion constant $D$ is irrelevant for the mathematical consideration in this chapter and is thus set to one. If there is no convection, a special case of the convection-diffusion equation is the diffusion equation or heat equation

$$u_t - \Delta u = 0\,,$$

which is used to find the temperature profile $u(\boldsymbol{r}, t)$ and is thus the object of investigation in this thesis.
Since the problem considered in this thesis is a one-dimensional one, the following applies to the general spatial coordinate $\boldsymbol{r} \equiv x$ and the problem of heat conduction can be written as

$$u_t - u_{xx} = 0\,. \tag{2.29}$$

### 2.2.2. Function Spaces

To work with PDE, the appropriate setting must first be defined. This leads to the so-called $L^p$ functions. Further function spaces, who lay dense in $L^p$, will be introduced successively within the next chapters.

**Definition 5** *Let* $1 \leq p < \infty$. *Let* $\Omega \subseteq \mathbb{R}^n$ *an open set. Than*

$$L^p(\Omega) := \left\{ f : \Omega \longrightarrow \mathbb{R}^n \;\middle|\; \int_\Omega |f(x)|^p \,\mathrm{d}x < \infty \right\}$$

*is the* ***space of p-fold integrable functions*** $L^p$.

The integration here is to be understood in the Lebesgue sense. This space is equipped with a norm, the so called $L^p$-**norm**:

**Definition 6** *The $L^p$-norm is defined as*

$$||f||_{L^p(\Omega)} := \left( \int_\Omega |f(x)|^p \, \mathrm{d}x \right)^{\frac{1}{p}} .$$

The $L^p$ space is complete with respect to the norm $||\cdot||_{L^p(\Omega)}$ and thus a Banach space.

Examples of $L^p$ functions are e.g. the probability density function of the normal distribution or bounded polynomial functions. So with boundedness one gets also functions in the $L^p$ space which would not be $p$-fold integrable on the whole space.

### Schwartz Functions

Schwartz functions are functions which are falling fast. This means that this functions fall faster than every polynomial function. One define the space of all Schwartz functions as the Schwartz space.

**Definition 7** *The set*

$$\mathcal{S}(\mathbb{R}^n) := \{f \in C^\infty(\mathbb{R}^n) \mid f \text{ falls faster than every polynomial function}\}$$

*is the* ***Schwartz space*** *or the* ***space of fast falling functions****.*

One important representative is the Gauss bell function. Because the Schwartz functions out of $C^\infty$ they are smooth.

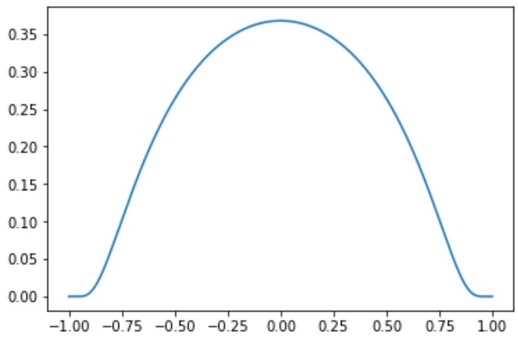


Figure 2.10.: Graph of the test function (2.30).

### Test Functions

Test functions are special $L^p$ functions, which are much more rigorous. They are zero outside a compact carrier and inside the compact carrier they are smooth, i.e. infinitely often differentiable. What's the use?

Transferred to the real world, one can imagine the test functions as a measurement. If, for example, one measures a length with the help of an ordinary tape measure, one can never specify the length exactly. One integrates so to say with the eyes over the approximate milimeter indication. If one reads off approximately 7mm for the length of a workpiece, then one can only say with certainty that 6mm is too short and 8mm too long. At these points, the solution function for the length of the workpiece must therefore have dropped to zero in any case. This would be an illustrative analog of a compact support. The smoothing property then becomes important for differential equations, because they involve derivatives of the solution function. Test functions can be collected in a vector space.

**Definition 8** *Let $\Omega \subseteq \mathbb{R}$ open. The vector **space of test functions** are the set*

$$\mathcal{D} := C_C^\infty(\Omega;\mathbb{R}) := \{\varphi \in C^\infty(\mathbb{R}) \mid \overline{\operatorname{supp}\varphi} \text{ is compact}\} .$$

*Here the support of a test function $\varphi$ is defined as*

$$\operatorname{supp}\varphi := \{x \in \Omega \mid \varphi(x) \neq 0\} .$$

*For compactness it must be valid that the support is closed and limited.*

An example of a test function is

$$\varphi(x) = \begin{cases} \exp\{\frac{-1}{1-x^2}\} & , \quad x \in (-1,1)\,, \\ 0 & , \quad \text{else}\,. \end{cases} \tag{2.30}$$

The graph of this function is shown in Fig. 2.10 where you can see the properties very well which are required for a test function. A very useful Lemma is given here about the inclusion of the different spaces.

**Lemma 1** *The space of the Test functions $\mathcal{D}(\mathbb{R}^n)$ lay dense in the Schwartz space $\mathcal{S}(\mathbb{R}^n)$.*
*The space of the Schwartz functions $\mathcal{S}(\mathbb{R}^n)$ lay dense in the space $L^p(\mathbb{R}^n)$ for all $1 \leq p < \infty$.*
*Because the denseness is transitive, the following is also true: The space $C_C^\infty(\Omega)$ lay dense in $L^p(\Omega)$ for all $1 \leq p < \infty$. Analogously one can write for instance*

$$\overline{C_C^\infty(\Omega)}^{||\cdot||_{L^p}} = L^p(\Omega)\,.$$

*It applies in total the inclusion chain*

$$\mathcal{D}(\mathbb{R}^n) \overset{\text{dense}}{\subseteq} \mathcal{S}(\mathbb{R}^n) \overset{\text{dense}}{\subseteq} L^p(\mathbb{R}^n)\,.$$

Lemma 1 means that any $L^p$-function can be approximated by Schwartz functions and any Schwartz function can approximated by test functions. Because denseness is transitive, also every $L^p$-function can approximated by test functions. This is advantageous, if we want to show a property for a $L^p$-function, it is sufficient to show the property for the test functions $C_C^\infty$, which are very well behaved because they are smooth.

With the help of the test functions, the weak derivation can now be defined.

### 2.2.3. Weak Derivation

In the case of weak solution, the limit value of the difference quotient is not used for the definition of the derivative, because this may not exist at all. Instead, the validity of the integration by parts is assumed and with its help the derivative of a function $f$ is rolled over to the differentiation of a test function.

Integration by parts is given by

$$\int_a^b f'(x)\varphi(x)\,\mathrm{d}x = [f(x)\varphi(x)]_a^b - \int_a^b f(x)\varphi'(x)\,\mathrm{d}x\,.$$

It is now necessary to guarantee that the boundary term $[f(x)\varphi(x)]_a^b$ is always zero. Test functions $\varphi \in C_C^\infty(\mathbb{R})$ have just this property that they are zero at the boundary and therefore the boundary terms are always omitted during integration. This results in

$$\int_a^b f'(x)\varphi(x)\,\mathrm{d}x = -\int_a^b f(x)\varphi'(x)\,\mathrm{d}x\,. \tag{2.31}$$

This representation now allows to define derivatives for functions that are classically non-differentiable.

**Definition 9** *Be $f \in L^p(\Omega)$. If for all test functions $\varphi \in C_C^\infty$ the equation*

$$\int_\Omega g(x)\varphi(x)\,\mathrm{d}x = -\int_\Omega f(x)\varphi'(x)\,\mathrm{d}x\,.$$

*is fullfiled, than is $g \in L^p(\Omega)$ the **weak derivation** of $f$. Symbolically, one writes $f' := g$ in short.*

The advantage is now that the derivative was rolled over to the test function. Thus you only need to search for the derivative of the test function, which has no pitfalls, because test functions are smooth. Of course, there must be correspondence between the two derivation terms. If a function is classically differentiable, it must also be weakly differentiable. This is always fulfilled with the above definition of the weak derivative.

Let us give an example. The absolute value function

$$f : \mathbb{R} \longrightarrow \mathbb{R}\,, \quad f(x) = |x| \tag{2.32}$$

is classically differentiable at the branches, but has a kink at $x = 0$, is therefore not classically differentiable at $x = 0$. Inserting the signum function

$$f : \mathbb{R} \longrightarrow \mathbb{R}\,, \quad \mathrm{sgn}(x) = \begin{cases} 1 & , \quad x > 0\,, \\ 0 & , \quad x = 0\,, \\ -1 & , \quad x < 0 \end{cases} \tag{2.33}$$

and a arbitrary test function $\varphi : (a, b) \longrightarrow \mathbb{R}$ into the definition for the weak derivation gives:

$$\begin{aligned} \int_a^b \varphi'(x) f(x)\,\mathrm{d}x &= -\int_a^0 \varphi'(x) x\,\mathrm{d}x + \int_0^0 \varphi'(x) f(x)\,\mathrm{d}x + \int_0^b \varphi'(x) x\,\mathrm{d}x \\ &= -\left(\int_a^0 \varphi(x)(-1)\,\mathrm{d}x + \int_0^b \varphi(x) 1\,\mathrm{d}x\right) \\ &= -\int_a^b \varphi(x)\mathrm{sgn}(x)\,\mathrm{d}x\,. \end{aligned}$$

So the sgn-function is the weak derivative of the absolute value function $f(x) = |x|$. In the first line we see that the second integral term disappears, because we integrate over a zero set $\{0\}$. This zero set is insignificant for the integration, therefore the value of the sign function at $x = 0$ can be set arbitrarily. The sign function itself is no longer weakly differentiable, but it can be differentiated in a distributional sense as will be shown in chapter 2.2.5.

The function space of weakly differentiable functions is called the Sobolev space which is also a Banach space. The Sobolev space links k-fold differentiability (in the weak sense) with p-fold integrability (in the Lebesgue sense). With the formulations worked out so far, we give the definition of Sobolev spaces.

**Definition 10** *Let $1 \leq p \leq \infty$. Let $\Omega \subseteq \mathbb{R}^n$ open, then the space*

$$W^{k,p}(\Omega) := \{f \in L^p(\Omega) \mid \text{for all } \alpha \text{ with } |\alpha| \leq k \text{ applies} : D^\alpha f \in L^p(\Omega)\}$$

*is called the **Sobolew space** of the order $k$ with exponent $p$. Here $D^\alpha f$ stands for the weak derivation.*

A helpful analogy is the following:

$$C^0(\Omega) \longleftrightarrow L^p(\Omega)\,,$$
$$C^k(\Omega) \longleftrightarrow W^{k,p}(\Omega)\,.$$

On the left is the classical setting, that is, the classical differentiability term. And on the right is the new setting, i.e. for the concept of weak differentiability.

An important remark about sobolev embedding theorem's also provides the motivation regarding PDE, why we introduce these spaces. These theorems indicate under which combination of the parameters $n$, $k$ and $p$ which space is hit. Thus, with the theorems one knows how to regulate the boundary and initial values so that the solution of the PDE lie in the desired space.

Finally, the **Theorem of Lax-Milgram** should be stated. This theorem ensures the existence and uniqueness of weak solutions of PDE problems.

**Theorem 1** *Let $U$ a Hilbert space and $a : U \times U \longrightarrow \mathbb{R}$ a bilinear mapping who fullfills the following two conditions:*

- *Continuity: There is a $k > 0$ such that $|a(u, v)| \leq k||u||_U||v|_U$,*
- *Coercivity: There is a $K > 0$ such that $|a(u, u)| \geq K||u||_U^2$.*

*Then for every $b \in U'$ there is a unique $u \in U$ such that for all $\varphi \in U$ holds:*

$$a(u, \varphi) = b(\varphi)\,.$$

The existence and uniqueness of weak solutions of such posed problems are thus assured. The theorem 1 looks very abstract. But this version is the most descriptive one for PDE. You can transform any PDE into the form $(u, \varphi) = b(\varphi)$. The functions $\varphi$ are the test functions which, as can be seen here again, are essential for the theory of PDE.

In the next section the most important definitions and spaces are introduced, which are needed for the distribution theory.

### 2.2.4. Operators and Functionals

A few important definitions and theorems of functional analysis are briefly given, which then lead in a natural way to the workhorse of this thesis, the distribution.

#### Operators

In functional analysis and especially for linear PDE, only linear operators are important and are considered. The definition of a linear operator has already been given in Def. 1. An important property of linear operators is that of limitedness:

**Definition 11** *Let $U$ and $V$ are normed vector spaces, than a linear operator $T : U \longrightarrow V$ is called limited, if there exists a $C > 0$ such that*

$$||Tx||_V \leq C||x||_U$$

*applies for all $x \in U$.*

The following theorem shows the equivalency of limitedness and continuity:

**Theorem 2** *A linear operator $T$ is limited exactly then when this operator is continuous.*

This is very helpful, because limitedness is a much more easier task to show than continuity. With these terms the space of continuous linear operators can be defined:

**Definition 12** *The* ***space of the continuous linear operators*** *are*

$$\mathcal{L}(U;V) := \{T : U \longrightarrow V \mid T \text{ is linear and continuous}\}.$$

This space is equipped with a norm, the so-called operator norm:

**Definition 13** *The operator norm is defined as*

$$||T||_{\mathcal{L}(U;V)} := \sup_{||x||_U \leq 1} ||Tx||_V \,.$$

The $\mathcal{L}$ space is complete with respect to the operator norm $|| \cdot ||_{\mathcal{L}(U;V)}$ and thus is a Banach space, if $V$ is a Banach space. One get the operator norm delivered when you test an operator for limitedness, where $C$ is then equal to the operator norm. Examples of such operators are the integral operator[6] and the multiplication operator.

### Functionals

As the name functional analysis is suggesting, the main object of study is the functional, respectively the linear functional. A linear functional is a special linear operator, which is declared by the following definition:

**Definition 14** *A linear functional is a linear operator which maps into the underlying body* $\mathbb{K}$.

Because a linear functional is an linear operator, therefore continuity can be shown by showing limitedness as well.

An example of a linear functional is the integral functional which is the map $T : C^0(]0,1[) \longrightarrow \mathbb{R}$:

$$Tf = \int_0^1 f(x)\,\mathrm{d}x \,.$$

If we compare the integral functional with the integral operator, one can observe that an incarnation of the integral operator is the indefinite integral while an incarnation of an integral functional is the definite integral. Also with the derivation it behaves like this, the differential operator gives the derivation of the whole function $f'(x)$ while the differential functional gives the derivation at one point $f'(x_0)$.

[6] Operator norm of the integral operator: $||T||_{\mathcal{L}(C^0(]0,1[);C^1(]0,1[))}$.

### Dual Space

Analog to the space of the continuous linear operators (Def. 12), the space of the continuous linear functionals can be defined, this one will be given a special name:

**Definition 15** *The space of the continuous linear functionals is called the dual space and is denoted by*

$$U' := \mathcal{L}(U; \mathbb{R})\,.$$

This space is immediately equipped with a norm, which is defined quite analogously to the operator norm Def. 13:

**Definition 16** *The operator norm is defined as*

$$||T||_{U'} := \sup_{||x||_U \leq 1} |Tx|\,.$$

The dual space is complete with respect to this norm and thus is a Banach space, if V is a Banach space. $U$ does not have to be a Banach space for this. As a remark it is pointed out that the norm on the right is the $\mathbb{R}$-norm, i.e. the Euclidean norm, therefore the simple absolute value lines. As you can see $x$ is supposed to come from the unit sphere.

The tools to formally define distributions have now been worked out. Let us look at the dual space of test functions:

**Definition 17** *The dual space of the test functions $C_C^\infty$ with $\mathcal{D}'(\Omega)$ is called the **space of the distributions** and is given by*

$$(C_C^\infty(\Omega))' := \mathcal{D}'(\Omega) = \{T : \mathcal{D} = C_C^\infty(\Omega) \longrightarrow \mathbb{R} \mid T \text{ is linear and continuous}\}\,.$$

$\Leftrightarrow$ *A distribution is a continous linear functional on the space of the test functions.*

An important subspace of the distributions are the regular distributions, which are generated by locally integrable functions:

**Definition 18** *Be $f \in L^1_{loc}(\Omega)$ a locally integrable function*[7] *and $\varphi \in \mathcal{D}(\Omega)$. If*

[7] See App. B for the definition of a locally integrable function.

*there exist a representation*

$$Tf(\varphi) := T_f(\varphi) := \int_\Omega f(x)\varphi(x)\,\mathrm{d}x$$

*generated by $f$, then this distribution is called a **regular distribution**.*

The opposite of a regular distribution are non-regular or **singular distributions**, which are distributions for which there is no generating function $f$ in the sense of Def. 18.

Another special subspace of distributions is the space of tempered distributions. Tempered distributions are continous linear functinals on the Schwartz space, so the dual space of the Schwartz space $\mathcal{S}$:

**Definition 19** *The dual space of the fast falling functions $\mathcal{S}(\mathbb{R}^n)$ with $\mathcal{S}'(\mathbb{R}^n)$ is called the **space of the tempered distributions** and is given by*

$$\mathcal{S}'(\mathbb{R}^n) = \{T : \mathcal{S}(\mathbb{R}^n) \longrightarrow \mathbb{R} \mid T \text{ is linear and continuous}\}\,.$$

*⇔ A tempered distribution is a continous linear functional on the space of the fast falling functions.*

Another theorem shall be stated immediately:

**Theorem 3** *Every Polynomial function $P(x)$ generates a regular tempered distribution.*

Concerning the hierarchy of function spaces and their dual spaces the following theorem is still very illustrative:

**Theorem 4** *The inclusion chain*

$$\mathcal{D}(\mathbb{R}^n) \overset{\text{dense}}{\subseteq} \mathcal{S}(\mathbb{R}^n) \overset{\text{dense}}{\subseteq} L^p(\mathbb{R}^n) \subseteq \mathcal{S}' \subseteq \mathcal{D}'$$

*shows the hierarchy of the different function spaces and their dual spaces.*

This testifies to a certain symmetry, the smaller a space is, the larger is its dual space. The space of test functions $\mathcal{D}$ is very small because the constraints, compact support and infinity continuous differentiable, are very rigoros. Its dual space $\mathcal{D}'$ is very large.
So much for the theory about PDE, now it is time for a constructive preparation of the distributions, which will lead to Green's Functions. In concrete terms, delta distribution, which is fundamental in physics, is presented.

### 2.2.5. Distributions

The space of distributions $\mathcal{D}'(\Omega)$ was recognised in Def. 17 as the dual space of the test functions. Such as the weak derivation in Ch. 2.2.3, the derivation in the distributional sense is still motivated in the integration by parts. Be $f \in C^1(\mathbb{R})$ and $\varphi \in \mathcal{D}(\mathbb{R})$, then

$$\langle f', \varphi \rangle := \int_{\mathbb{R}} f'(x)\varphi(x) \,\mathrm{d}x = -\int_{\mathbb{R}} f(x)\varphi'(x) \,\mathrm{d}x = -\langle f, \varphi' \rangle$$

applies[8]. The derivative of a distribution is then defined as follows:

**Definition 20** *For $\varphi \in \mathcal{D}(\Omega)$ and $T \in \mathcal{D}'(\Omega)$, ones define the* ***derivation of a distribution****, so $\partial_x T \in \mathcal{D}'(\Omega)$, with*

$$\langle \partial_x T, \varphi \rangle := -\langle T, \partial_x \varphi \rangle \,.$$

*or represented differently*

$$T' : \mathcal{D}(\Omega) \longrightarrow \mathbb{R} \quad \text{with} \quad T'(\varphi) = -T(\varphi') \,.$$

This can be very easily generalized to higher derivatives, with only a sign change. Thus, the derivation is rolled over again to the test functions. The only difference to the weak derivation is that you do not take a function from $L^p(\Omega)$ but a distribution $T \in \mathcal{D}'(\Omega)$.

[8]The notation on the left side of the equation is a is a shorthand notation for the so called dual pairing.

With the help of the weak derivation, the example with the derivative of the absolute value function (2.32) could be solved. The weak derivative there has turned out to be the signum function (2.33), which itself is no longer weakly differentiable. However, it has already been noted that the signum function will be differentiable in the distributive sense, so let's see. The sign function

$$f : \mathbb{R} \longrightarrow \mathbb{R}\,, \quad \operatorname{sgn}(x) = \begin{cases} 1 & , \quad x > 0\,, \\ 0 & , \quad x = 0\,, \\ -1 & , \quad x < 0 \end{cases}$$

can also be thought of as a constant polynomial function with a jump point at $x = 0$. According to Theorem 3, every polynomial function generates a tempered distribution, so the sign function generates the tempered distribution

$$\mathcal{S}(\Omega) \ni \varphi \longrightarrow \operatorname{sgn}[\varphi] = \int_\Omega \operatorname{sgn}(x)\varphi(x)\,\mathrm{d}x \in \mathcal{S}'(\Omega)\,.$$

The derivation in the distributional sense is then

$$\begin{aligned} \langle \partial_x \operatorname{sgn}, \varphi\rangle(x) &= \operatorname{sgn}'[\varphi] \\ &= \int_\Omega \operatorname{sgn}'(x)\varphi(x)\,\mathrm{d}x \overset{\text{Def.20}}{=} -\int_\Omega \operatorname{sgn}(x)\varphi'(x)\,\mathrm{d}x \\ &= -\langle \operatorname{sgn}, \partial_x\varphi\rangle(x) \\ &= \int_a^0 \varphi'(x)\,\mathrm{d}x - \int_0^b \varphi'(x)\,\mathrm{d}x = 2\varphi(0) =: 2\delta[\varphi] \end{aligned} \tag{2.34}$$

A distribution that can do the last step $\delta[\varphi] = \varphi(0)$ is the delta distribution, which will be introduced in the next section. What does all this bring us for PDE?

With the help of Def. 20 the distributional solution of PDE can now be defined:

**Definition 21** *Be $L$ a linear differential operator (Def. 2) and $T \in \mathcal{D}'(\Omega)$ a given distribution, then the distribution $u \in \mathcal{D}'(\Omega)$ is the* ***distributional solution of the PDE***

$$Lu = T\,,$$

*if*

$$\langle Lu, \varphi \rangle = \langle T, \varphi \rangle$$

*for all* $\varphi \in \mathcal{D}(\Omega)$.

The functional analytical foundations for solving PDE are thus outlined, culminating in Def. 21. With the help of this definition, the fundamental solution and Green's function can now be defined. Why these are so helpful is then shown in Ch. 2.2.6 about the convolution.

Before that, the Delta distribution and its properties should be briefly introduced. This special distribution is essential for finding the fundamental solution and the Green's function of a PDE.

### Delta Distribution

Let us assume that we want to describe a mass point, i.e. mass that is unified at a zero-dimensional point. Trying to describe this situation with classical functions, one will quickly come up against an insurmountable limit. If you try to integrate over the mass density, i.e. to calculate the mass, this mass density is zero everywhere, except at the point where the mass is concentrated, where the density diverges.
Another situation, which is important in this thesis, arises when snow falls to the ground. In general, the falling snow will have a different temperature than the ground. As soon as the snow reaches the ground, according to the heat equation, the average temperature between the snow and the ground is instantaneously adjusted. Both facts, the point concentration in space or time, cannot be modelled with the help of classical functions. The delta distribution models such a circumstance. Thus, one can intuitively define the Delta Distribution through its properties. It must be noted that this definition is only symbolic and the exact definition is already contained in Def. 17, noting that the delta distribution is a singular distribution. The intuitive definition is therefore

$$\delta(x) = 0 \quad \text{when} \quad x \neq 0\,, \quad \text{and} \quad \int_{-\infty}^{\infty} \delta(x) = 1\,,$$

where $x$ here represents the time and space coordinate. This models the very properties of a point concentration that are not inherent in a classical function. The rigid definition over the space of the test functions is then as follows:

**Definition 22** *Let $\varphi \in \mathcal{D}$. The mapping*

$$\delta : \mathcal{D} \longrightarrow \mathbb{R}\,, \;\; \varphi \longmapsto \varphi(0)$$

*is called the* ***Delta distribution****.*

With this definition, the last step in (2.34) also becomes immediately clear. It should be noted that the Delta distribution is not a regular distribution. In (2.34) one can see, that the derivation of the Heaviside function results in the delta distribution. The Heaviside function is a regular distribution. The derivative of it, so the Delta distribution, is a singular distribution, as mentioned. With the derivative of a distribution the regularity can change, this price must be paid[9].

A very appropriate physical definition of the Delta distribution can be achieved with the help of the Fourier transformation:

$$\delta(x) = \mathcal{F}^{-1}(1)\,.$$

With this approach the physical content of the Delta distribution becomes a descriptive meaning, namely that the delta distribution contains all frequencies at the same magnitude. This is an ideal pulse.

With the help of the Delta distribution, the fundamental solution of a PDE can now be defined.

### Fundamental Solution

With the help of the Delta distribution (Def. 22), the fundamental solution is defined by:

[9] In mathematics one cannot simply define away problems.

**Definition 23** *Be $L$ a linear differential operator as defined in Def. 2. A distribution $F \in \mathcal{D}'(\mathbb{R})$, which fullfills the equation*

$$LF = \delta \quad \text{in} \quad \mathcal{D}'(\mathbb{R}) \,,$$

*is called the* ***Fundamental solution*** *of the linear differential operator $L$.*

The theorem 5 of Malgrange-Ehrenpreis is ensuring a greens function of a linear differential operator with constant coefficient for the associated PDE, so in particular also the existence of a fundamental solution.

Fundamental solutions are not uniquely determined. For example, let $F_0 \in \mathcal{D}'$ be a solution of the homogeneous equation

$$LF_0 = 0 \,,$$

so $F + F_0$ is also a fundamental solution of $L$. If additional boundary value conditions are applied to $F$, one speak of the Green's function $G$.

### Green's Function

The Green's function is a fundamental solution with homogenous boundary conditions on a bounded domain with border $\partial D$, so:

**Definition 24** *Be $L$ a linear differential operator as defined in Def. 2 and $0 \le j \le k$. A distribution $G \in \mathcal{D}'(\Omega \subset \mathbb{R})$, which fullfills the equations*

$$\begin{aligned} LG &= \delta \quad \text{in} \quad \mathcal{D}'(\Omega \subset \mathbb{R}) \,\text{and} \\ \partial^j G &= 0 \quad \text{on the border} \quad \partial D \end{aligned}$$

*is called the* ***Green's Function*** *of the boundary value problem with the linear differential operator $L$.*

In the case of $j = 0$ these are Dirichlet boundary conditions and in the case of $j = 1$ these are Neumann boundary conditions. As already indicated in the case of the fundamental solution, the existence of such a Green's function is ensured by the theorem of **Malgrange-Ehrenpreis**:

**Theorem 5** *Let $L$ be a linear partial differential operator with constant coefficients. Then the associated PDE has a Green's function.*

This Theorem together with the boundary conditions defines Green's Function well, unlike the fundamental solution. In the following, the equation

$$LG = \delta \tag{2.35}$$

will called the auxiliary equation to the PDE (2.25).
In summary, we can say that Green's function is the solution to the inhomogeneous auxiliary equation (2.35), where the inhomogeneity, or forcing term, is a point source.

The PDE (2.25) with arbitrary inhomogenity, can than constructed by superposition this point sources[10]. The convolution in the next section carries out this construction.

### 2.2.6. Convolution

The convolution smears a function $f$ and forms its moving average, it is defined by means of integration:

**Theorem 6** *Be $f, g : \mathbb{R} \to \mathbb{C}$, than the **convolution** is defined by*

$$(f * g)(x) := \int f(x')g(x - x')\, \mathrm{d}x' \,.$$

Now back to the auxiliary equation (2.35). If we multiply this equation by a function $f$ and integrate over $x'$, the following results:

$$\int LG(x, x')f(x')\, \mathrm{d}x' = \int \delta(x - x')f(x')\, \mathrm{d}x' = f(x)\,.$$

[10]This only works for linear differential operators.

As we know, the operator $L$ is linear and is operating just on $x$, so $L = L(x)$. Therefore the operator can be taken out of the integral

$$L\left(\int G(x,x')f(x')\,\mathrm{d}x'\right) = f(x)\,.$$

From this then follows that

$$u(x) = \int G(x,x')f(x')\,\mathrm{d}x' = (G * f)(x) \tag{2.36}$$

is a solution of the inhomogen PDE (2.25). So once Green's function is found, the problem can be considered solved. By convolution with the inhomogeneity $f$ a solution $u$ is constructed, thus by superposition. This is guaranteed by the linearity of the differential operator $L$. As shown in Carslaw and Jaeger (1947, Ch. 1.14, p. 30), using Duhamel's principle, one can switch back and forth between inhomogeneity in the PDE and inhomogeneity of a boundary value condition.

In Ch. 3 the Green's function will be derived.

# 3. Green's Function to the Problem

First of all the problem is posed. The problem is an initial value problem with an inhomogeneous boundary condition of the second kind, also known as the Neumann boundary condition. The first step will now be to find the fundamental solution in the whole space. With the help of the mirror charge principle, the Green's function can be found based on the fundamental solution.

## 3.1. The Problem

The Problem of heat flux in the soil is described by the initial boundary value problem in the semi infinite domain $0 \leq x < \infty$ and is given by

$$ku_{xx} - u_t = 0 \tag{3.1a}$$
$$u(x, 0) = u_0 \tag{3.1b}$$
$$-u_x(0, t) = f(t) \tag{3.1c}$$
$$-u_x(x \to \infty, t) = const.. \tag{3.1d}$$

The diffusion constant $k$ is set, without loss of generality, to 1 for the time being. It was exploited that according to Wang (2012) for short integration times the initial condition does not have much effect on the solution, so one can simplify $u(x, 0) = const. = u_0$.

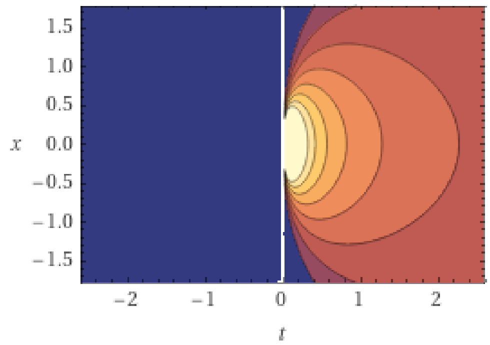


Figure 3.1.: Contour plot of the Fundamental solution (3.5) of the problem (3.2) at the time $\tau = 0$ and for $\xi = 0$. One can see the propagation of the heat very well.

## 3.2. Fundamental Solution to the Problem

First of all, the fundamental solution to the Problem shall be found. The corresponding auxiliary equation to (3.1) for the whole domain respectively the whole space $-\infty < x < \infty$ is given by

$$u_{xx} - u_t = \delta(x-\xi)\delta(t-\tau) \tag{3.2a}$$

$$u(x, t < \tau) = 0 \tag{3.2b}$$

$$-u_x(|x| \to \infty, t) \to 0\,, \tag{3.2c}$$

where the boundary condition is homogenous. Without of loss of generality, it's appropriate to transform the ordinate segment to $\xi = 0 = \tau$. The Laplace transformed (Appendix A) of the problem (3.2) is than given by

$$U_{xx} - sU = \delta(x) \tag{3.3a}$$

$$U_x(s, |x| \to \infty) \to 0\,, \tag{3.3b}$$

which is an ODE with $\delta$-inhomogenity and is bounded at infinity. The homogenous solution reads than

$$U(s,x) = A(s)e^{-\sqrt{s}x} + B(s)e^{\sqrt{s}x}\,.$$

This solution will diverge if $|x| \to \infty$ and is therefore not bounded as the boundary condition (3.3b) requires. To fulfill the boundary condition, the solution have to be split at $x = 0$

$$U(s,x) = \begin{cases} A(s)e^{-\sqrt{s}x} & , \quad x > 0\,, \\ B(s)e^{\sqrt{s}x} & , \quad x < 0\,. \end{cases}$$

Continuity at the origin $x = 0$, with $x$ coming from the left and from the right, gives the coefficients $A(s) = B(s) = \frac{1}{2\sqrt{s}}$. The Laplace transformed of the fundamental solution is then given by

$$U(s,x) = \frac{1}{2\sqrt{s}} e^{-\sqrt{s}|x|}\,. \tag{3.4}$$

The **Fundamental solution** respectively the heat kernel is therefore

$$F(x-\xi, t-\tau) := u(x,t) = \Theta(t-\tau)\frac{1}{2\sqrt{\pi(t-\tau)}} e^{-\frac{(x-\xi)^2}{4(t-\tau)}} \tag{3.5}$$

in general, with a unit heat source at $x = \xi$ at the time $t = \tau$. The contour of the Fundamental solution is shown in Fig. 3.1.

## 3.3. Green's Function

With the concern to find the Green's function to the Problem (3.1), the first step was taken by finding the fundamental solution (3.5), because symmetry considerations will lead to the goal. What exactly is meant by this will become clear later in this section. In view of the Green's function, the problem is limited to the half space $0 \le x < \infty$ and the boundary condition (3.1c) has to be taken into account, which is an inhomogenous boundary condition of the second kind respectively a Neumann boundary condition.

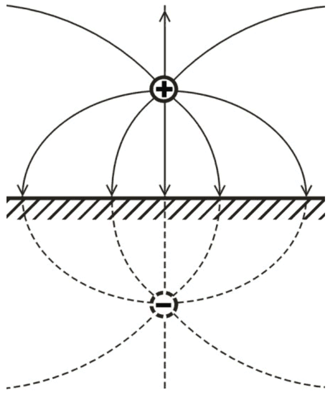

Figure 3.2.: Method of mirror images. The unit heat source in the soil (negative sign) is compensated at the surface by an opposite unit heat source, which was placed in the opposite position. Figure from Pepper (2007).

### 3.3.1. Homogenous Neumann Boundary Condition

The auxiliary equation to the initial value boundary condition problem (3.1) with $\tau = 0$ is given by

$$u_{xx} - u_t = \delta(x-\xi)\delta(t) \tag{3.6a}$$

$$u(x,0) = 0 \tag{3.6b}$$

$$-u_x(0,t) = 0 \quad \text{for} \quad t > 0 \tag{3.6c}$$

$$-u_x(x \to \infty, t) = const.. \tag{3.6d}$$

The solution $u$ of this PDE can be intepreted as the temperature in the semi infinite soil in response to a unit heat source at $x = \xi$ and $t = 0$. The boundary condition at $x \to \infty$ means that the soil at this end is coupled to an infinite heat bath.

In principle, the problem does not seem to be much different from (3.2), except that it is limited to the half space. Already for the problem (3.2) the so called mirror image method was implicitly used to find the fundamental solution. What this method means exactly will be explained briefly using the Poisson equation of electrostatics.
A common boundary value problem in electrostatics is a point charge near a grounded metal plate. The potential of the point charge at the plate disappears

in this case ($\Phi = 0$ at the metal plate). The Poisson equation satisfies such an electrostatic boundary value problem. To solve this problem, often mirror charges are used. In this case, an opposite charge of the same amount is simply placed opposite the metal plate. Thus the boundary value ($\Phi = 0$ at the plate) is guaranteed and the problem remains mathematically the same.
In finding Green's function for the problem (3.6), most of the work has already been done, with finding the fundamental solution (3.5). To ensure the boundary condition (3.6c) a mirrored unit heat source is placed at the point $x = -\xi$, what is schematic shown in Fig. 3.2. Due to symmetry considerations, the solution to (3.6) is simply given by

$$G(x - \xi, t) = F(x - \xi, t) + F(x + \xi, t)\,, \tag{3.7}$$

where $F$ is the fundamental solution (3.5). With the help of (2.36) this gives the solution

$$u(x,t) = \int_0^t \int_0^\infty G(x - \xi, t - \tau) f(\xi, \tau)\, \mathrm{d}\xi \mathrm{d}\tau\,. \tag{3.8}$$

### 3.3.2. Inhomogeneous Neumann Boundary Condition

Back to the Problem (3.1), with inhomogeneous Neumann boundary condition (3.1c). The Problem now is, that the Green's function Def. 24 is just defined for homogenous boundary conditions and not for inhomogenous boundary conditions at all, this fact is shown in Kerner and Wahl (2013, ch. 12.5, p. 358). To overcome this problem, the solution $u$ have to be transformed to become homogenous. The homogenizing transformation can be given by

$$w(x,t) = u(x,t) - x f(t)\,. \tag{3.9}$$

The transformed solution $w$ solves

$$w_{xx} - w_t = x\dot{f}(t) \tag{3.10a}$$
$$w(x,0) = x f(0) \tag{3.10b}$$
$$-w_x(0,t) = 0 \tag{3.10c}$$

and has homogenous boundary condition, what can be easily verified by recalculation. With the help of (3.8), the solution for $w$ is calculated by

$$\begin{aligned} w(x,t) = u(x,t) - xf(t) = &- \int_0^t \dot{f}(\tau) \underbrace{\int_0^\infty \xi G(x-\xi, t-\tau)\,\mathrm{d}\xi}_{=:I} \,\mathrm{d}\tau \\ &- f(0) \int_0^\infty \xi G(x-\xi, t)\,\mathrm{d}\xi \end{aligned} \tag{3.11}$$

where the second summand takes the initial value into account and is not important for the time being. The Green's function $G$ for the homogenous problem is known and is given by (3.7). The next step is to calculate the inner integral

$$I = \int_0^\infty \xi G(x-\xi, t-\tau)\,\mathrm{d}\xi\,.$$

This integral is again split into the antisymmetric parts of the fundamental solution

$$I = \underbrace{\frac{1}{\sqrt{\pi}} \int_0^\infty \xi \frac{\exp\left(\frac{-(x-\xi)^2}{4(t-\tau)}\right)}{2\sqrt{t-\tau}}\,\mathrm{d}\xi}_{=:J} + \underbrace{\frac{1}{\sqrt{\pi}} \int_0^\infty \xi \frac{\exp\left(\frac{-(x+\xi)^2}{4(t-\tau)}\right)}{2\sqrt{t-\tau}}\,\mathrm{d}\xi}_{=:K}\,.$$

Let's take a look on the Integral $J$. This must be split into two parts, namely into the intervals $0 \le \xi \le x$ and $x \le \xi < \infty$. Let's make the substitution $\nu(\xi) = \frac{x-\xi}{2\sqrt{t-\tau}}$ which gives the new integration variable $\mathrm{d}\xi = -2\sqrt{t-\tau}\,\mathrm{d}\nu$ and the conversion rule for $\xi$ with $\xi = x - 2\nu\sqrt{t-\tau}$. The interval limits transform to $\nu(0) = \frac{x}{2\sqrt{t-\tau}}$, $\nu(x) = 0$ and $\nu(\xi \to \infty) = -\infty$. All inserted then results in

$$\begin{aligned} J &= -\frac{1}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{t-\tau}}}^0 \left(x - 2\nu\sqrt{t-\tau}\right) e^{-\nu^2}\,\mathrm{d}\nu - \int_0^{-\infty} \left(x - 2\nu\sqrt{t-\tau}\right) e^{-\nu^2}\,\mathrm{d}\nu \\ &= \frac{1}{\sqrt{\pi}} \int_0^{\frac{x}{2\sqrt{t-\tau}}} \left(x - 2\nu\sqrt{t-\tau}\right) e^{-\nu^2}\,\mathrm{d}\nu + \int_0^{\infty} \left(x - 2\nu\sqrt{t-\tau}\right) e^{-\nu^2}\,\mathrm{d}\nu \\ &= x\mathrm{erf}\left(\frac{x}{2\sqrt{t-\tau}}\right) - \sqrt{\frac{t-\tau}{\pi}}\left(1 - e^{-\frac{x^2}{4(t-\tau)}}\right) - \sqrt{\frac{t-\tau}{\pi}} \\ &= x - \frac{x}{2}\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right) - 2\sqrt{\frac{t-\tau}{\pi}} + \sqrt{\frac{t-\tau}{\pi}} e^{-\frac{x^2}{4(t-\tau)}}\,. \end{aligned}$$

The function $\mathrm{erf}(\cdot)$ in the second last line respectively the function $\mathrm{erfc}(\cdot)$ in the last line are the error function respectively the complementary error function who are explained in App. B.3.
Now to the integral $K$, the procedure is the same here, except that the integration interval does not have to be split. The integral is therefore

$$\begin{aligned} K &= \frac{1}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{t-\tau}}}^{\infty} \left(2\nu\sqrt{t-\tau} - x\right) e^{-\nu^2} \,\mathrm{d}\nu \\ &= 2\sqrt{\frac{t-\tau}{\pi}} \int_{\frac{x}{2\sqrt{t-\tau}}}^{\infty} \nu e^{-\nu^2} \,\mathrm{d}\nu - \frac{x}{\sqrt{\pi}} \int_{\frac{x}{2\sqrt{t-\tau}}}^{\infty} e^{-\nu^2} \,\mathrm{d}\nu \\ &= \sqrt{\frac{t-\tau}{\pi}} e^{-\frac{x^2}{4(t-\tau)}} + \frac{x}{2}\left[\mathrm{erf}\left(\frac{x}{2\sqrt{t-\tau}}\right) - 1\right] \\ &= \sqrt{\frac{t-\tau}{\pi}} e^{-\frac{x^2}{4(t-\tau)}} - \frac{x}{2}\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right) . \end{aligned}$$

Thus $I$ is calculated to

$$\begin{aligned} I(x-\xi, t-\tau) &= J + K \\ &= 2\sqrt{\frac{t-\tau}{\pi}} e^{-\frac{x^2}{4(t-\tau)}} - x\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right) - 2\sqrt{\frac{t-\tau}{\pi}} + x\,. \end{aligned}$$

If we put $I$ into (3.11), we get

$$\begin{aligned} w(x,t) &= -\int_0^t \dot{f}(\tau) I(x, t-\tau) \mathrm{d}\tau - f(0) I(x,t) \\ &= -\frac{2}{\sqrt{\pi}} \int_0^t \dot{f}(\tau)\sqrt{t-\tau} e^{-\frac{x^2}{4(t-\tau)}} \mathrm{d}\tau + x \int_0^t \dot{f}(\tau)\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right) \mathrm{d}\tau \\ &+ \frac{2}{\sqrt{\pi}} \int_0^t \dot{f}(\tau)\sqrt{t-\tau}\mathrm{d}\tau - x \underbrace{\int_0^t \dot{f}(\tau)\,\mathrm{d}\tau}_{=f(t)} - f(0) I(x,t) = u(x,t) - x f(t)\,. \end{aligned}$$

The last term sums to 0 and we can state the solution $u(x,t)$ to be

$$\begin{aligned} u(x,t) &= -\frac{2}{\sqrt{\pi}} \int_0^t \dot{f}(\tau)\sqrt{t-\tau} e^{-\frac{x^2}{4(t-\tau)}} \mathrm{d}\tau + x \int_0^t \dot{f}(\tau)\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right) \mathrm{d}\tau \\ &+ \frac{2}{\sqrt{\pi}} \int_0^t \dot{f}(\tau)\sqrt{t-\tau}\mathrm{d}\tau - f(0) I(x,t)\,. \end{aligned}$$

The second last term depends only on $t$ and not on $x$, so this integral should still be calculated, twice partial integration leads here to the goal.

$$\begin{aligned}\frac{2}{\sqrt{\pi}}\int_0^t \dot{f}(\tau)\sqrt{t-\tau}\mathrm{d}\tau &= \frac{2}{\sqrt{\pi}}\left\{\left[f(\tau)\sqrt{t-\tau}\right]_0^t + \frac{1}{2}\int_0^t f(\tau)\frac{1}{\sqrt{t-\tau}}\,\mathrm{d}\tau\right\}\\ &= \frac{2}{\sqrt{\pi}}\left\{-f(0)\sqrt{t} + \frac{1}{2}\int_0^t f(\tau)\frac{1}{\sqrt{t-\tau}}\,\mathrm{d}\tau\right\} \overset{*}{=} .\end{aligned}$$

The last integral evaluated again with partial integration yields

$$\int_0^t f(\tau)\frac{1}{\sqrt{t-\tau}}\,\mathrm{d}\tau = 2\int_0^t \dot{f}(\tau)\sqrt{t-\tau}\,\mathrm{d}\tau - 2f(0)\sqrt{t}\,.$$

Substituting this into the equation before gives a total of

$$\overset{*}{=} -\frac{1}{\sqrt{\pi}}f(0)\sqrt{t} + \frac{2}{\sqrt{\pi}}\int_0^t \dot{f}(\tau)\sqrt{t-\tau}\,\mathrm{d}\tau\,.$$

The total chain of equations is then

$$\frac{2}{\sqrt{\pi}}\int_0^t \dot{f}(\tau)\sqrt{t-\tau}\mathrm{d}\tau = \frac{2}{\sqrt{\pi}}\int_0^t \dot{f}(\tau)\sqrt{t-\tau}\,\mathrm{d}\tau - \frac{1}{\sqrt{\pi}}f(0)\sqrt{t}\,.$$

From this it follows immediately that for this term $t = 0$ must be valid and therefore disappears. The solution $u(x,t)$ thus results in

$$\begin{aligned}u(x,t) = &-\frac{2}{\sqrt{\pi}}\int_0^t \dot{f}(\tau)\sqrt{t-\tau}e^{-\frac{x^2}{4(t-\tau)}}\mathrm{d}\tau + x\int_0^t \dot{f}(\tau)\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right)\mathrm{d}\tau\\ &- f(0)I(x,t)\\ &= -\int_0^t \dot{f}(\tau)\left\{\frac{2}{\sqrt{\pi}}\sqrt{t-\tau}e^{-\frac{x^2}{4(t-\tau)}} - x\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right)\right\}\mathrm{d}\tau\\ &- f(0)I(x,t)\,.\end{aligned}$$

If we compare this with (2.36), we finally get the searched **Green's function of the problem** (3.1)

$$G(x,t-\tau) = \frac{2}{\sqrt{\pi}}\sqrt{t-\tau}e^{-\frac{x^2}{4(t-\tau)}} - x\mathrm{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right)\,. \tag{3.12}$$

This function coincides with the Green's function given in Wang (2012).

Now that Green's function has been found, the next chapter will be about calculating the soil heat flux from the measured point temperature data time series. Once this has been found, the entire ground heat flux and temperature profile can be reconstructed as will be shown.

# 4. Reconstruction of the Ground Heat Flux

For the purpose of clarity and simpler calculation, all parameters are still normalised to 1, the parameters will only be reintroduced later if necessary.

The solution $u(x,t)$ of the problem (3.1) is in our case the temperature $T(x,t)$, so $T(x,t) := u(x,t)$. It's noted in Wang (2012) that $T(x,t)$, so the convolution (2.36), is given by a Stieltjes Integral

$$\Theta(x,t) := T(x,t) - u_0 = \int_0^t f(t-\tau)\,\mathrm{d}G(x,\tau)\,, \tag{4.1}$$

where $G(x,t)$ is the Green's function (3.12) of the problem. The soil heat flux is then simply calculated using Fourier's law (2.13) to be

$$B(x,t) = -\frac{\partial T}{\partial x} = \int_0^t f(t-\tau)\,\mathrm{d}\tilde{G}(x,\tau)\,, \tag{4.2}$$

where for the Green's function derived according to $x$

$$\tilde{G} = \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right) \tag{4.3}$$

holds. As one can easily see, $f(t-\tau) = B(0,t-\tau)$ applies at the surface, where $B(0,t-\tau) =: B_0(t-\tau)$ is the ground heat flux as given in (1.1). Already in Ch. 2.2.6 it was mentioned that the Duhamel's principle allows an exchange of the inhomogenuity between the boundary condition and the PDE. Therefore (4.1) can be written as

$$T(x,t) - u_0 = \int_0^t B(0,t-\tau)\,\mathrm{d}G(x,\tau) \tag{4.4}$$

and (4.2) as

$$B(x,t) = \int_0^t B(0, t-\tau)\, \mathrm{d}\tilde{G}(x,\tau)\,. \tag{4.5}$$

As can be seen from (4.4) and (4.5), only the soil heat flux $B_0(t-\tau)$ is needed to have all information together for a complete temperature and heat flux profile of the soil. However, the existing time series are discrete temperature data at a certain soil depth. The soil heat flux can now be calculated from this time series.

## 4.1. Numeric

The temperature time series are available in discretised form, so the first step to calculate the soil heat flux $B_0$ is the discretisation of time $\{t_j = j\Delta t \mid j = 0, 1, 2, \ldots, N\}$.

Following Wang (2012), the discretised form of the convolution (4.4) by numerical integration respectively Trapezoidal rule results in

$$\Theta(x,n) = \frac{1}{2}\sum_{j=1}^{n-1} \{B_0(n-j) + B_0(n-j+1)\}\, \Delta G(x,j)\,, \tag{4.6}$$

where

$$\Delta G(x,j) := G(x,j) - G(x,j-1)\,. \tag{4.7}$$

With $\tilde{\Theta}(x,n) := 2\Theta(x,n)$ the sum in (4.6) reads

$$\begin{aligned}
\tilde{\Theta}(x,n) = \sum_{j=1}^{n-1} &\{B_0(n-j) + B_0(n-j+1)\}\,\Delta G(x,j) \\
&= \{B_0(n-1) + B_0(n)\}\Delta G(x,1) \\
&+ \{B_0(n-2) + B_0(n-1)\}\Delta G(x,2) \\
&+ \{B_0(n-3) + B_0(n-2)\}\Delta G(x,3) \\
&+ \{B_0(n-4) + B_0(n-3)\}\Delta G(x,4) \\
&+ \dots \\
&+ \{\underbrace{B_0(n-n+2)}_{=B_0(-2)} + \underbrace{B_0(n-n+2+1)}_{=B_0(3)}\}\Delta G(x,n-2) \\
&+ \{\underbrace{B_0(n-n+1)}_{=B_0(1)} + \underbrace{B_0(n-n+1+1)}_{=B_0(2)}\}\Delta G(x,n-1)\,.
\end{aligned}$$

This can now be rearranged to the ground heat flux

$$\begin{aligned}
B_0(n) &= B(0,n) \\
&= \frac{1}{\Delta G(x,1)}\{2\Theta(x,n) - B_0(n-1)\Delta G(x,1) \\
&- \sum_{j=2}^{n-1} [B_0(n-j) + B_0(n-j+1)]\,\Delta G(x,j)\} \\
&= \frac{1}{\Delta G(x,1)}\{2\Theta(x,n) \\
&\underbrace{- \left[B_0(n-1)\Delta G(x,1) + \sum_{j=2}^{n-1} [B_0(n-j) + B_0(n-j+1)]\,\Delta G(x,j)\right]}_{=:J_{n-1}(B_0,\Delta G_x)}\}
\end{aligned} \tag{4.8}$$

So the ground heat flux can be given in the compact form

$$B(0,n) = \frac{2\Theta(x,n) - J_{n-1}(B_0,\Delta G_x)}{\Delta G(x,1)}\,. \tag{4.9}$$

It is noteworthy that the input variable for (4.9), namely the temperature $\Theta(x,n)$, does not have to be measured at the surface, but can be measured at any depth. This underlines again the great advantage of this method.

Now the implementation for calculating the soil heat flux $B(0,t)$ can be specified.

## 4.2. Implementation

With (4.9) a problem arises at the beginning, for $j = 1, 2$ respectively $n = 1, 2$ the Green's function (3.12) diverges because of $\Delta G(x, j) = G(x, j) - G(x, j-1)$. This problem could possibly be solved with the help of the residual theorem, but it is not worth the effort, since the Green's function converges to the correct value after a certain integration time anyway, due to the constantly new incoming temperature data.

Anyway, values for $j = 1, 2$ respectively $n = 1, 2$ must be specified, otherwise the numerical quadrature cannot start. A possibility for calculating the initial values is shown in Sadeghi et al. (2021, Eq. (A15)). The two initial values for $n = 1$ and $n = 2$ and the calculation for $n > 2$ are implemented by

$$
\begin{aligned}
B(0,1) &= \frac{\Theta(x,1)}{G(x,1)} \\
B(0,2) &= B(0,1) + \frac{\Theta(x,2) - B(0,1)G(x,2)}{G(x,1)} \\
B(0,n) &= B(0,n-1) + \frac{1}{G(x,1)}\{\Theta(n) - B(0,1)G(x,n+1) \\
&\quad - \sum_{j=3}^{n} \left[B(0,j-1) - B(0,j-2)\right] G(x,n-j+2)\Delta t\} \, .
\end{aligned}
\tag{4.10}
$$

Let's summarize again, with the help of (4.9) respectively (4.10), the soil heat flux at the surface can be calculated numerically from the temperature measurements at any depth.

Once the ground heat flux $B_0(t) = B(0,t)$ is available, (4.4) respectively (4.5) can be used to calculate the total temperature profile respectively the total heat flux profile of the entire soil.

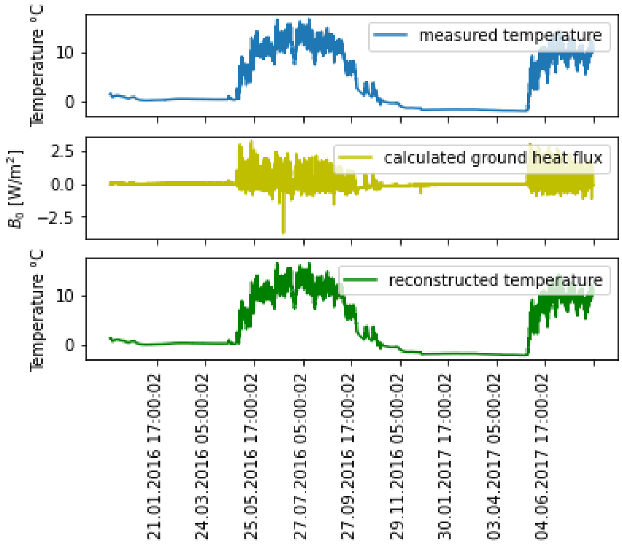


Figure 4.1.: The top plot shows a long-term measurement of the soil temperature, whereby the data were obtained from a temperature logger. The middle plot shows the soil heat flux calculated using (4.10). The bottom plot shows the reconstructed temperature, which was calculated using (4.4).

## 4.3. Temperature and Flux Profiles

As in Ch. 1.1, the data from the Gscheideggkogel measuring station are presented here as representative of all other measuring stations. For the time series that now follow, the two model parameters, diffusion constant[1] $D$ and depth $x$ of the buried temperature loggers, were set to identical 1, without loss of generality. Furthermore, the two parameters are unitless.

So far, Green's function to the problem could be found. Furthermore, the numerical implementation for the calculation of $B_0$ was shown. The validation of the method is still outstanding.

In Fig. 4.1 the time series of the soil temperature and the ground heat flux is plotted over a time of approximately one and a half year. The top plot shows

[1]An extra application arises with the following consideration. If one knew the heat flux $B(x,t)$ from another method, one could determine the diffusion constant of the soil using the method presented here.

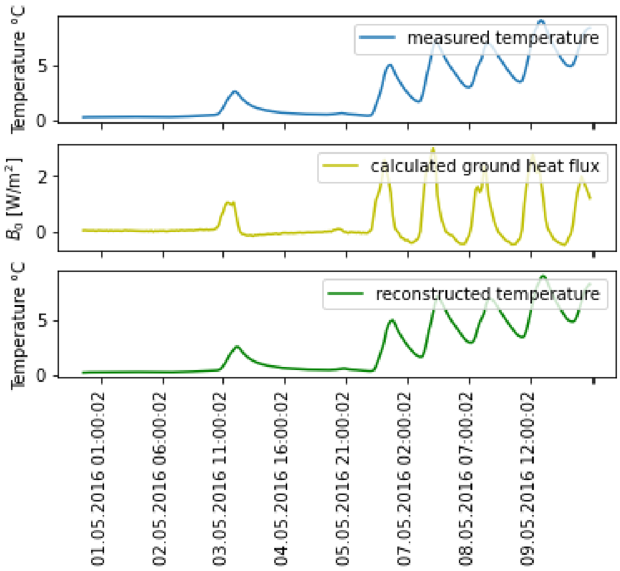


Figure 4.2.: Same as in Fig. 4.1 but short-term time series over about a week within this likely the snowmelt occurs.

the time series as measured by the temperature loggers. the middle time series represents the ground heat flux $B_0$ where this was calculated using (4.10). Here we can already see that the ground heat flux decreases to zero in winter, which must be the case because of the insulating snow cover. The lowest time series validates the method. It is a calculated time series that reconstructs the measured temperature using $B_0$ and (4.4). It coincides exactly with the time series in the top plot.

Fig. 4.2 then shows the same data over a shorter period of time. One could assume that within this week the snowmelt starts. Note again the exact agreement of the measured temperature with the reconstructed temperature.

In Fig. 4.3 then, a different depth than that of the temperature logger was set to reconstruct the temperature, namely $x = 100$. One can see the warming trend into the summer. The strong dampening of the temperature trend in the soil is mirrored in the smoothness of the curve.

In Fig. 4.4 finally the depth parameter, for the reconstruction of the tem-

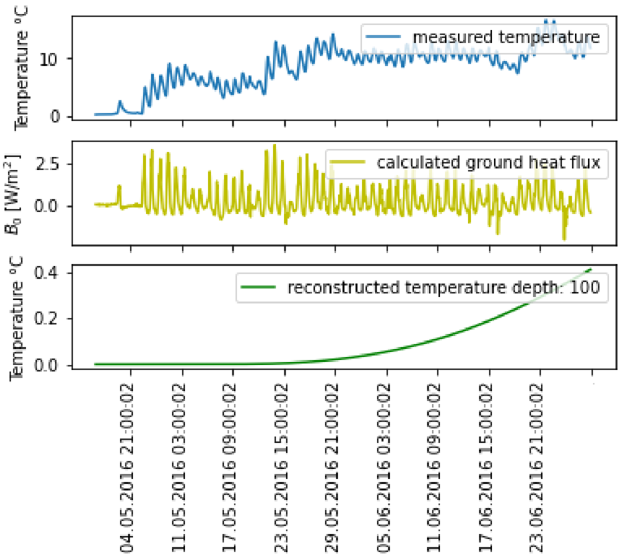


Figure 4.3.: Here the depth parameter, for the reconstruction of the temperature, was set to $x = 100$. One can see the warming trend into the summer. The strong dampening of the temperature trend in the soil is mirrored in the smoothness of the curve.

perature, was set to $x = 20000$. So quite a great depth. Here, the temperature has constantly dropped to zero, which must be so by construction (see. (3.6d)). A few more comments follow about this chapter.

When talking about exact agreement of the reconstructed temperature with the measured temperature, this only means that the method works perfectly in a mathematically and numerically sense. For the practical validation, further field tests would have to be undertaken, respectively more numerics would have to be implemented. However, the validation of the method is also shown in Wang (2012).

There is a numerical artifact in the implementation. For very small diffusion constants $D$ the solution function diverges and nonsensical values result. The application in App. C needs among other things also a debugging in this respect. As said, it is a numerical artifact, mathematically the method stands on very solid ground.

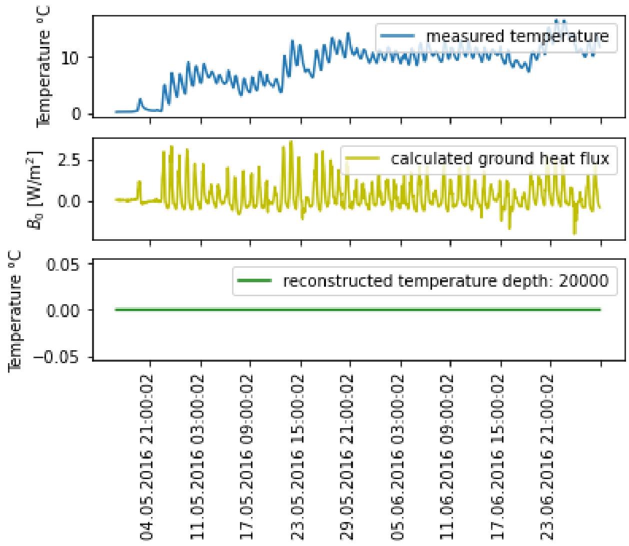


Figure 4.4.: Here the depth parameter, for the reconstruction of the temperature, was set to $x = 20000$. So quite a great depth. Here, the temperature has constantly dropped to zero, which must be so by construction (see. (3.6d)).

# 5. Conclusio

Note that some important issues have already been discussed in Ch. 4.3. It should also be noted that a Fourier analysis of the time series would certainly also be of interest.

The Gesäuse with its great biodiversity, high relief energy and broadly networked research complex, provides an ideal environment for basic research, especially in terms of climate and in terms of ecosystem research (one can guess the mentioned properties in Fig. 5.1). Earth system models can be considered as standard in numerical climate modelling. That is why there are common state variables for the climate system (ECV's) as well as for ecosystems (SO's). Two of these state variables, the surface temperature of the Earth and the soil heat flux, can be easily obtained from space-time temperature data using the method presented here. In contrast to the conventional temperature gradient method with heat flux plates, which is presented in H. Kraus (2008, Ch. 11), the method presented here is very easy to implement. You just have to bury ordinary temperature loggers in the ground. The only two parameters that need to be known are the diffusion constant of the soil and the depth at which the temperature loggers are buried. Anyway, first to the results of the work.

The main goal of the work was to get the essential climate variables (ECV's) respectively the standard observations (SO's) ground heat flux $B_0$ and the land surface temperature $T_0$ from the temperature data of the loggers. For this purpose, in chap. 2.2 the basics of Green's function method were presented. Therein, the concept of functions was generalised and the solution in the distributive sense was defined. The mathematical setting of this approach is provided by functional analysis. The framework was limited to linear operators and thus to linear PDE.

Figure 5.1.: Thunderclouds over the Planspitze. Here the north-east face seen from Gstatterboden. With kind permission of Mag. Verena Lewenhofer.

The Green's function (3.12) was found:

$$G(x, t-\tau) = \frac{2}{\sqrt{\pi}}\sqrt{t-\tau}e^{-\frac{x^2}{4(t-\tau)}} - x\text{erfc}\left(\frac{x}{2\sqrt{t-\tau}}\right) .$$

This is the Green's function solution to the problem (3.1). The problem can thus be considered solved. With the found Green's function, the ground heat flux $B_0$ is than defined by (4.4) and is well defined if temperature data from any depth in the soil are available. Once you know the ground heat flux $B_0$, you can use the convolution to calculate the entire temperature and heat flux profile with (4.4) and (4.5). In particular, the measured temperature can thus be reproduced. The two ECV's respectively SO's, land surface temperature and ground heat flux, are thus found. With the latter, the energy closure problem (1.1) is more accessible, which will become important for the outlook.
The implementation of the method was shown in Ch. 4. The python code can be seen in the appendix App. C. Anyway, the mathematical validation of the method was shown by restoring the originally measured temperature data with the help of (4.4). One more remark should be made at this point:

For the time series who are considered in Ch. 4.3 the two model parameters, diffusion constant $D$ and depth $x$ of the buried temperature loggers, were set to identical 1 without loss of generality. The latter parameter can be measured very easily and are available from the National Park. The approximate diffusion constant of the soils can also be determined relatively easily. An extra application arises with the following consideration. If one knew the heat flux $B(x, t)$ from another method, one could determine the diffusion constant of the soil using the method presented here.

At the end of Ch. 2.1 it was already mentioned that a more adequate description of the problem would have to include both, the advection-convection equation and the porous media equation. In general, the soil is not a a fluid-tight homogeneous body and the interface between soil and atmosphere is not an abrupt transition, there is both plant cover and fallen snow. Nevertheless, the treatment with the help of the diffusion equation is legitimate, if only because of the validation carried out in Wang (2012). Greater accuracy is then of course connected with greater effort. However, one has to take a closer look at the measurement sites anyway and set the framework for the particular location.

With the global radiation $Q_0$, which we get from standard meteorological measurements, and the ground heat flux $B_0$, the energy balance (1.1) is already 50 % closed. The latent and sensible heat, which are connected via the Bowen ratio (2.2), are still missing. Also shown in H. Kraus (2008, Ch. 11.5), there are some methods to parameterise the energy balance terms. But a new method is presented in Sadeghi et al. (2021) to determine the sensible heat $H$ via the ground heat flux $B_0$. Here, an analogy between the daily mean turbulent heat transport in the atmospheric boundary layer and the convective-advective heat transport in the soil is exploited as well as the temperature continuity at the soil-atmosphere interface. The correlation $H = H(G_0)$ can thus be shown, which finally solves the energy closure problem without any parameterisation.

# Appendix A.

# Laplace Transformation

The Laplace Transformation, as given in Arens et al. (2022, ch. 33.2), to a function $f : [0, \infty) \to \mathbb{C}$, is defined as the parameter integral

$$F(s) = \mathcal{L}f(s) = \int_0^\infty f(t)e^{-st}\,\mathrm{d}t\,, \quad s \in \mathbb{C}\,,$$

if the integral exist. The function $F(s)$ is called the laplace transform of the function $f(t)$ and the function $e^{-st}$ is the integral kernel of the transformation. It must be noted that only functions of the exponential type, i.e. functions that satisfy

$$|f(t)| \leq Ce^{s_0 t}\,,$$

where $t > 0$ and $C$ and $s_0$ are poitive constants , are transformable. If then additionally

$$\int_0^T |f(t)|\,\mathrm{d}t < \infty$$

applies, than the laplace transformation $\mathcal{L}f(s)$ exist. The integration condition $\int_0^T |f(t)|\,\mathrm{d}t < \infty$ is already fulfilled, if $f$ is piecewise continuous.

## Inverse Laplace Transform

To each laplace transform belongs a inverse laplace transform, one speaks also of transform pair. To find the original function again, the inverse laplace transform is given as

$$\mathcal{L}^{-1}\{F\}(t) = \frac{1}{2\pi i} \int_{s_0 - i\infty}^{s_0 + i\infty} e^{st} F(s)\,\mathrm{d}s = \Theta(t) f(t)\,.$$

Calculating the inverse is often the most difficult task when working with such a method. You often have to deal with singularities and have to use function theory to solve this problem. Fortunately, there are transformation tables where the transformation pairs are listed and you can easily look them up.

## Properties of the Laplace Transformation

Some calculation rules are given here, which are especially helpful for solving PDE. Be $f$ and $g$ functions of exponetial type, than applies:

(i) $\mathcal{L}(f+g) = \mathcal{L}f + \mathcal{L}g$,

(ii) $\mathcal{L}\lambda f = \lambda \mathcal{L} f$,

(iii) $\lim\limits_{Re(s)\to\infty} \mathcal{L}f(s) = 0$,

(iv) $\mathcal{L}f^{(n)}(s) = s^n \mathcal{L}f(s) - \sum_{k=1}^{n-1} f^{(k)}(0) s^{n-1-k}$,

(v) $\mathcal{L}t^n f(t)(s) = (-1)^n \frac{d^n}{ds^n} \mathcal{L}f(s)$,

(vi) $\mathcal{L}f(t-a)(s) = e^{-as}\mathcal{L}f(s)\,, \quad \forall a > 0$,

(vii) $\mathcal{L}e^{at} f(t)(s) = \mathcal{L}f(s-a)\,, \quad \forall a \in \mathbb{C}$,

(viii) $\mathcal{L}(f * g) = \mathcal{L}f\mathcal{L}g$.

# Appendix B.

# Notation and Definitions

## B.1. Locally Integrable Function

Locally integrable functions $f \in L^1_{loc}(\Omega)$, where $L^1_{loc}$ is the space of the locally integrable functions, are defined by the condition

$$\int_C |f(x)| \, \mathrm{d}x < \infty \, .$$

Here the integral is to be understood in the Lebesgue sense.

## B.2. Multiindices

A multi-index is a tuple of numbers

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n) \, ,$$

which are numbered with natural numbers from 1 to $n$.

## B.3. Error Function

The error function is defined by the integral

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\tau^2} \mathrm{d}\tau \, .$$

The complementary error function is defined by

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-\tau^2} \mathrm{d}\tau$$

at once.

# Appendix C.

# Code

## Reconstruction of Ground Temperature

It should be remarked that the following rough implementation is only for validation of the method. For quantitative results, the two parameters diffusion coefficient and depth of the temperature logger in the soil must be known.

```
import numpy as np
import math
import matplotlib.pyplot as plt

#initialize time steps
hours = 2500
skip_header = 7000

# loading date:
date = np.genfromtxt("Gscheidegg_A50258_20181106130608.
    csv", dtype=None, delimiter=',', skip_header=
    skip_header, usecols = (1), max_rows = hours)

#loading temperature measurement's:
temp = np.genfromtxt("Gscheidegg_A50258_20181106130608.
    csv", delimiter=',', skip_header=skip_header, usecols
     = (2), max_rows = hours)
```

```
plt.figure()
plt.xlabel("time (hours)")
plt.ylabel("Temperature  C ")
plt.plot(temp[50:hours])

#initialize Ground Heat flux array G_0(n):
G_0_n = np.zeros(1)

# greens function g(x,t):
def green(t, x=0.1, k=1, c=1): #set parameters to 1
    without loss of generality
    return (1/(k*c))*(((4*k*t)/(math.pi))**(1/2)*math.e
        **(-x**2/(4*k*t)) - x*math.erfc(x/(4*k*t)**(1/2))
        )

def ground_heat_flux_n_greater_2(n, G_0_n, temp):
    sum_J = 0
    for j in range(2, np.size(G_0_n)+1):
        sum_J = sum_J + (G_0_n[j-1] - G_0_n[j-2])*green(
            np.size(G_0_n) - j + 2)
    ground_n = G_0_n[-1] + (1/green(1))*(temp[n] -
        ground_1*green(n+1) - sum_J)
    return ground_n

# G_0(1):
ground_1 = (temp[0])/green(1)
G_0_n[0] = ground_1

# G_0(2):
ground_2 = ground_1 + (temp[1] - ground_1*green(2))/
    green(1)
G_0_n = np.append(G_0_n, ground_2)

# iterating calculation to get ground heat flux array
    G_0(n)
for n in range(2, hours): #np.size(temp)):
```

```python
    G_0_appendix = ground_heat_flux_n_greater_2(n, G_0_n
        , temp)
    G_0_n = np.append(G_0_n, G_0_appendix)

plt.figure()
plt.xlabel("time (hours)")
plt.ylabel("Ground Heat Flux")
plt.plot(G_0_n[50:hours])

#reconstruct temp:
def reconstructed_temp_at_time_n(n, G_0_n, x=0.1):
    theta_n = 0
    for j in range(1, n + 1):
        theta_n = theta_n + (G_0_n[j] - G_0_n[j - 1])*
            green(n - j + 1, x)
    theta_n = G_0_n[0]*green(n + 1, x) + theta_n
    return theta_n

reconstructed_temp = np.zeros(1)
reconstructed_temp[0] = reconstructed_temp_at_time_n(1,
   G_0_n)

for n in range(50, hours): #np.size(temp)):
    reconstructed_temp_appendix =
        reconstructed_temp_at_time_n(n, G_0_n)
    reconstructed_temp = np.append(reconstructed_temp,
        reconstructed_temp_appendix)

plt.figure()
plt.xlabel("time (hours)")
plt.ylabel("reconstructed Temperature C ")
plt.plot(reconstructed_temp)
```

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