

École polytechnique de Louvain

Non-Fourier Heat conduction: The Cattaneo Equation

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Abstract

This document introduces the subject of non-Fourier heat conduction. In particular, infinite speed of heat propagation associated with Fourier's law is explained. The Cattaneo law is introduced to correct this paradox. An analysis of this new heat equation is proposed to build a good understanding of its properties: discontinuities, modal analysis, variational formulation and numerical methods are discussed. The new heat model is then applied to a thermokeratoplasty operation and solution profiles are explained. Finally, a step toward other laws and applications is given with the introduction to fractional derivative heat conduction models.

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Chapter 1

Introduction

Fourier's law is known to many and is of current usage in several engineering applications. Fluid dynamics, thermoelasticity, civil engineering are fields where the classical heat equation has been used for a while with satisfying results.

However, since Joseph Fourier proposed this law two centuries ago, it has known some critics. First, it was discovered that it leads to an infinite speed of propagation. It is accepted that heat travels fast, but it's not physical that temperature perturbations at some position could be felt instantaneously everywhere. Also, it was observed that Fourier's law was not able to represent correctly the heat transfer phenomena in some particular cases. These observations motivated the interest to find more advanced models for heat transport, and opened up the extended area of non-Fourier heat conduction. In the present document, we aim to give a first introduction to this subject.

A brief history of non-Fourier heat conduction is first proposed, with the milestones of the domain. Then, a comparative study is made on the Fourier and Cattaneo equations. The paradox of the propagation speed is explained. Subjects like discontinuities, modal decomposition, variational formulation and numerical methods are also addressed. Since Cattaneo law was the first alternative suggested to Fourier, it seems important to understand its properties before studying other models. Then an application of Cattaneo equation for biological tissues is explained in detail. Finally a direction to continue the non-Fourier conduction exploration is given, with models using fractional derivatives.

1.1 Microscopic heat transfer

The heat transfer phenomenon can be described from a microscopic point of view. First consider a gas. It can be modeled as a cloud of particles that interact only through collisions. Each particle has a velocity and an associated kinetic energy, that can be translated into a temperature. If some particles have more energy than others, they can transfer it through collisions. The heat transfer phenomenon is thereby achieved.

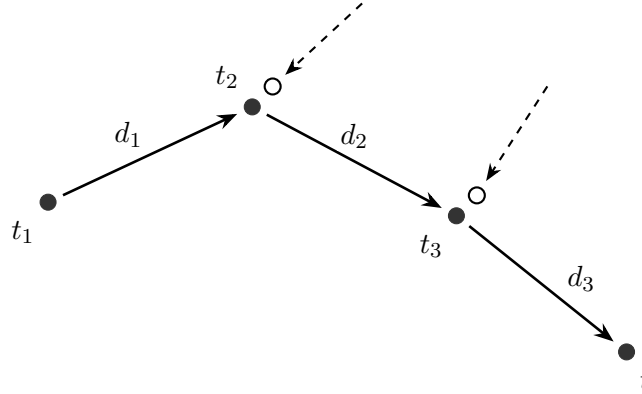


Figure 1.1: Illustration of particles collisions

In non-metallic rigid bodies, like dielectric materials or semiconductors, the concept of cloud of massive particles is no longer valid as molecules are arranged in a lattice. The local energy is then associated to the vibrations of the particles of the lattice around their equilibrium point. However, the complicated task to consider the whole lattice for heat transfer can be bypassed by the concept of a phonon. These are the quasiparticles associated with lattice vibrations. They represent a quantum of energy, in the same spirit as photons for light:

$$E = \nu h \quad (1.1)$$

where ν is the lattice frequency and h the Planck constant.

Now we can consider that the transport of heat in solids operates through phonon-phonon collisions, in the same spirit as for gases.

For metallic rigid bodies, the electrons play an important role. They will first absorb and propagate heat through electrons-electrons collisions, and then heat the lattice through electron-phonon collisions. Nevertheless, the mechanism is the same: collisions among heat carriers, represented as a cloud of particles.

Two important quantities related to these collisions are the mean free time

$$\tau_{mf} = \frac{t - t_1}{3} \quad (1.2)$$

which represents the average time elapsed between two collisions, and the mean free path

$$l = \frac{d_1 + d_2 + d_3}{3} \quad (1.3)$$

which represents the average length between two collisions [1]. It is interesting to keep this microscopic vision in mind when considering the heat transport phenomena. It offers a clearer vision of what occurs compared to macroscopic variables, and it's a key point for the microscale applications discussed further.

Chapter 2

Historical milestones of non-Fourier heat transfer

We present a brief history of non-Fourier heat conduction: important dates, names, and discoveries. The idea is that we are able to place the events on a temporal axis so that we can have a better understanding of the reasons why the different models are proposed and the links between them. Some names will appear often and are to be remembered for the area of heat transfer. The following is not expected to be exhaustive, but it will give enough so that we can understand the general history of non-Fourier heat conduction. Some of the models briefly cited here will be explained in more details in further sections, with an associated application.

This history is inspired in part by [2].

2.1 Heat transfer paradox and second sound

In 1807, Joseph Fourier proposes a law for heat transfer in his memoir "Théorie de la propagation de la chaleur dans les solides"

$$q = -k \frac{\partial T}{\partial x} \quad (2.1)$$

with k the thermal conductivity.

His work, presented in front of the "Académie des sciences", is first criticised by his fellows. It's only after some years that it will be published officially in his book "Théorie analytique de la chaleur", in 1822. Fourier's approach is purely phenomenological: it's based on observations, without strong theoretical foundations [3][4].

In 1867, Maxwell, one of the founders of kinetic theory of gases, published an article "On the dynamical theory of gases". He proposes a microscopic derivation of Fourier's law, from collisions among the particles of the gas. In fact, the complicated derivation of Maxwell already contained a term associated to a finite speed of propagation for heat. However, he wasn't aware of this drawback of Fourier's law and he simplified the term, writing "The first term of this second equation may be neglected, as the rate of conduction will rapidly establish itself" [5].

In 1931, Onsager clearly established that Fourier's law is in contradiction with thermodynamics reversibility. He says that using this law, we neglect the time for the heat flux

to establish. During this period, some research was carried out on liquid helium, which shows strange behavior at very low temperatures. At ambient temperature Helium is in gaseous form but when reaching 4.2K, it is in liquid form. When decreasing more the temperature, below 2.17K, we get helium II. In this range close to the absolute zero, we observe that Helium is able to climb vertical surfaces to flow outside a container, showing viscosity-free behavior, but at the same time a pendulum oscillating in the fluid will finally stop due to friction.

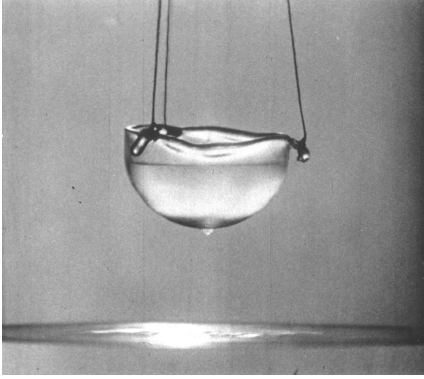


Figure 2.1: Liquid helium flowing outside the container from the walls

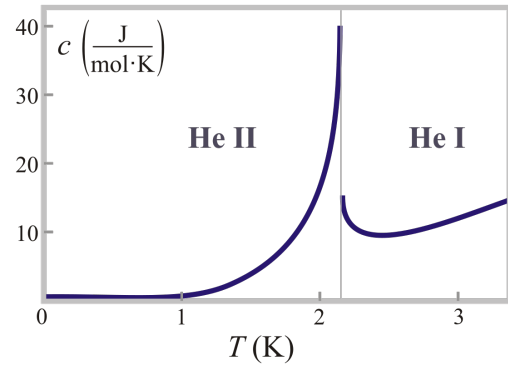


Figure 2.2: Molar heat capacity of Helium. Under the peak at 2.17K, we get Helium II

A theory for He II behavior was developed by Tisza and Landau around 1940. They propose a two-fluid model, where one fluid carries all the entropy and has viscosity. The other one has no entropy and no viscosity, it's the superfluid. All the properties of He II are then computed as follows:

$$\rho = \rho_s + \rho_n \quad (2.2)$$

where ρ is the density and the subscripts s and n denote the superfluid and normal parts of the fluid. Their model explains all the behaviors of He II, but with another surprising result. As their equations predict fluctuations of the local pressure (density), the well-known sound waves, they also predict local fluctuations in temperature and entropy: thermal waves. This kind of behavior is clearly non-Fourier. Landau called these "second sound" in reference to the "first sound" we are used to. In fact, the second sound is really close to first sound in the sense that these fluctuations in temperature can be seen as fluctuations of density in the phonon gas associated to the media. In that sense, the principle is the same. They find a velocity for the first sound, nearly constant with the temperature, and a velocity for second sound, which shows great influence from the temperature. At this moment, these phenomena were considered of quantum nature, limited to He II and it was not expected to find such waves in other materials [6].

In 1944, Peshkov observed second sound through experiments at 1.2K. He measures the velocity of the thermal waves and confirmed the validity of the two fluid theory proposed earlier. He will continue his experiments to measure the velocity of the waves up to 0.5K in 1960, assessing the theoretical curves. An interesting suggestion by Peshkov is the possibility to observe second sound in solids. Indeed, since heat propagates also through phonons there, we should also be able to observe second sound there.

In 1948, Cattaneo used arguments from kinetic gas theory to correct Fourier's paradox. He takes into account the time for the particles to move and transfer heat. This allows him to get a new term in the constitutive equation. The system he obtains is the following

$$\rho c \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = 0, \quad (2.3)$$

$$\tau \frac{\partial q}{\partial t} + q = -k \frac{\partial T}{\partial x}. \quad (2.4)$$

with c the specific heat capacity and τ the thermal relaxation time. He also explicitly mention the related hyperbolic heat equation (HHE),

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (2.5)$$

where α is the thermal diffusivity, and the fact that the propagation speed is finite [7]. The same result was also obtained independently by Vernotte in 1958. From the independent derivation of this result by Maxwell, Cattaneo and Vernotte, (2.4) is sometimes called the Maxwell-Cattaneo-Vernotte equation (MCV). At this moment, no reference to second sound is made: it is still considered as a side subject of quantic nature. It is also worth mentioning that if the work from Cattaneo and Vernotte was widely accepted, it did not change the use of Fourier equation as the time for the heat flux to establish was considered much shorter than any engineer application timescale.

In 1960, Nettleton shows that Cattaneo law is thermodynamically admissible. This is a contrast with Fourier laws which wasn't. Soon after that, Tevernier proposes a more fundamental derivation of Cattaneo equation from Boltzmann transport equation (BTE).

If it was already attempted to explain some results of second sound by a form of the telegraph equation, the first usage of Cattaneo law with it's associated physical parameters in this context is due to Chester in 1963. First, he introduces a thermal oscillations frequency window for the observation of second sound. Indeed, if the period is too long, we will be in a diffusive regime. If it's too short, the concept of temperature is no longer well defined. He expressed this as a criterion

$$w_c = \frac{1}{2\pi\tau} \quad (2.6)$$

To compute τ , he postulates the HHE equation to be valid for the phonon gas involved in second sound, and relates his velocity to the one of second sound at very low temperature

$$\frac{\alpha}{\tau} = v^2 = \frac{c_s^2}{3} \rightarrow \tau = \frac{3\alpha}{c_s^2} \quad (2.7)$$

where v is the velocity of the thermal wave and c_s is the speed of sound. This is the first formula proposed for the computation of the thermal relaxation time [8].

In 1966, second sound in solids is finally observed by Ackerman. He explains that from the limitations of the frequency window, the number of materials in which we could expect to observe the phenomenon is limited. But by taking solid crystals of He^4 at a temperature of 0.6 Kelvins (the pressure is set to 55 bars as Helium would stay liquid up to absolute zero at atmospheric pressure), they could observe the propagation of temperature waves [9]. This confirms the hypothesis that second sound is not limited to liquid Helium. It

was also observed later in other materials like sodium fluoride or bismuth [10]. The same year, Guyer and Krumhansl solve the Boltzmann's transport equation for a pure phonon field. This equation allows a good description of heat transfer in low temperature dielectric crystals by phonon. The system they obtain is

$$\begin{cases} \rho c \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = 0, \\ \tau_{mf} \frac{\partial q}{\partial t} + q = -k \frac{\partial T}{\partial x} + l^2 \frac{\partial^2 q}{\partial x^2}. \end{cases} \quad (2.8)$$

It corresponds to a hydrodynamic formulation for the phonon gas, and leads to strange thermal behaviors, like Poiseuille-type profile for the heat flux, in total disaccord with Fourier expectations [11].

2.2 Microscale length and time scales

Up to now, the interest for non-diffusive regimes was limited to very particular cases at low temperature and the philosophical need to correct the infinite speed of propagation. A new interest for alternative models emerged with modern applications at the microscale. In 1974, Anisimov was interested in ultrashort laser pulses over a metallic surface. In metals, the heat is carried first by electrons and then transmitted to phonons. So a single temperature, as well as Fourier's law, can't be used to describe the medium and he proposes the application of a two-temperature model: when using high-intensity and short-duration laser pulse on metallic surfaces, we need a temperature for the electrons, T_e and a temperature for phonons T_l . Later, this work is refined and extended by Qiu & Tien to get a hyperbolic two temperature model for metals [12].

In 1993, with the explosion of microelectronics, new models are needed for very thin dielectric films. For a range of thickness, Fourier law is no longer valid. Majumdar proposes a radiative transfer model, in the same spirit as for light. The novelty is that it allows to describe heat transfer in length scales such that temperature is no longer well defined, from meso-scale equations. The idea is to decompose, at any point, the heat carried by the phonons in the different directions. [13]. His work will be precised and extended by Chen in 2000, by introducing a decomposition of the heat flux in two parts, q_b and q_m for the heat transport that is due to ballistic phonons (without collisions) and by diffusion, respectively. If Majumdar derivation is closer to the BTE, Chen formulation is more in the continuity of Fourier and Cattaneo, with a more realistic computation time [14].

An important advance in the non-Fourier conduction field is the law proposed by Tzou in 1995. His constitutive law allows for a generalization of diverse cases encountered before. This universal form covers both the classical diffusion regime, phonon wave regime, electron-phonon interactions, and short length scales. He introduces the concept of dual phase lag, with a delay introduced in both the heat flux and the temperature gradient

$$q(x, t + \tau_q) = -k \frac{\partial T}{\partial x}(x, t + \tau_T) \quad (2.9)$$

where τ_q and τ_T are the lag on the heat flux and the temperature, respectively [15].

2.3 Modern applications

Another interesting field over which non-Fourier heat conduction spread out is biology. For a while, Penne's bioheat equation was the commonly used model for heat transfer in the human body. It is essentially the heat equation plus a term linear in the temperature to account for the blood flow.

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + \rho_b c_b w_b (T_b - T) + Q \quad (2.10)$$

where the subscript b refers to blood physical properties and Q is a source term.

The experiments led by Mitra in 1995 aimed to show that in some cases heat conduction in biological tissues can be of hyperbolic nature. They postulate (2.5) for meat samples and compute the parameter τ by measuring the time for a heat pulse to propagate in the sample. When comparing the temperature profiles from the thermocouples and the HHE, they see good agreement, while the solution of the parabolic heat equation (PHE) totally fails. They also observe addition of waves, which emphasizes the hyperbolic nature of heat conduction [16]. However, some criticism about the experimental procedure are mentioned in [17] and it doesn't seem that the results are easily reproducible. Nevertheless, this result is important as it is the first step to the application of non-Fourier heat laws to heterogeneous materials of many types. The equations are often admitted, and the parameters determined experimentally.

More recently, the field of phononics emerged with great developments. The idea of this area is to apply the concepts of electronics, where energy is carried by electrons, to heat, where energy is transported by phonons. The interest is in developing components such as thermal diodes, thermal transistor or memory devices, where the working particle is the phonon. Of course, such small devices should be modelled by microscopic equations, without usage of classical Fourier's law. Despite the difficult task to work with phonons which have neither mass nor charge and interact in complicated ways, a step toward thermal circuits was made in 2006 with the first experimental validation of a thermal diode.

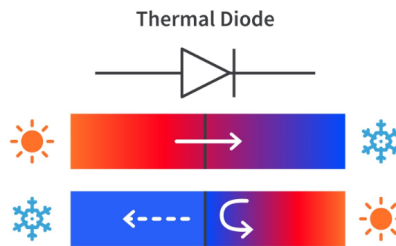


Figure 2.3: Operating principle of a thermal diode from [18]

This component can be a thermal conductor if a temperature gradient is applied in a direction, or an insulator if it is submitted to a temperature gradient in the opposite direction. It is based on the concept of symmetry-breaking, using two different materials with different thermal properties. The first thermal rectifier (diode) was made with carbon nanotube and mass added to one end. Differences in heat flows depending on the direction were observed. The phononics area is a very promising field for the future [19] [20].

Very recently, in 2019 and 2022, new observations of second sound were made in graphite at 100K and 200K. This is important because for a very long time, second sound was considered to be limited to very low temperatures around absolute zero. This indicated thus the possibility to observe thermal waves at ambient temperatures and motivates further research [21].

2.4 Summary

In conclusion, we have seen that non-Fourier heat conduction has known a great evolution over the last century. First motivated by liquid helium around absolute zero and the need for a finite speed of propagation, it experienced a boom when the time scales and length scales in which the transient effects of non-diffusive nature were expected to be observed could finally be reached by modern engineering. The field of alternative laws also extended to the wide area of heterogeneous materials, and it is still today a topic of great interest and research.

Chapter 3

Fourier and Cattaneo: a comparative study

After Fourier established his law in rigid bodies, Cattaneo was the first to suggest an alternative to correct Fourier's paradox. Here, we clearly explain why the classical heat equation (PHE) leads to an infinite speed of propagation for heat and how the hyperbolic heat equation corrects this. Since both equations are very close to each other, we also try to compare them in some aspects like modal analysis or numerical methods to clearly establish the consequences of using one law over another. Building a good understanding on how the MCV law differs from Fourier law is a first step toward more advanced models of non-Fourier heat conduction.

Working in the frame of continuum mechanics, we will assume the local conservation of energy to be the basis of each model (no source term), with different constitutive laws for the heat flux to close the problem.

$$\rho c \frac{\partial T}{\partial t} = - \frac{\partial q}{\partial x} \quad (3.1)$$

3.1 Fourier law

Heat flux formulation

Fourier law states a relation between the heat flux and the temperature gradient as follows

$$q = -k \frac{\partial T}{\partial x} \quad (3.2)$$

We see that when there is a temperature gradient, heat is instantaneously conducted at that point.

Temperature equation

Substituting (3.2) in (3.1), we obtain the parabolic heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (3.3)$$

Solving this equation in an infinite domain with initial condition $T(x, 0) = N\delta(x)$, the solution is

$$T(x, t) = \frac{N}{\sqrt{4\pi\alpha t}} e^{-x^2/4\alpha t} \quad (3.4)$$

which is a Gaussian function that spreads out over time, corresponding to the general idea of a diffusion process. But we see that from this initial condition of finite support, the expression (3.4) gives nonzero values for any x , at any time $t > 0$. So it's clear that a perturbation at the origin is felt instantaneously at any point of the domain, and that information travels at an infinite speed. This is what we call the paradox of Fourier law. However note the decaying exponential that will quickly decrease to very small values close to 0 when x is increased. Thus this can also be accepted as a small error.

In fact, (3.4) corresponds to the Green function, also called fundamental solution of the parabolic heat equation, and it allows to write an explicit form for the solution of equation (3.3) with any initial condition in unbounded domain.

Define $G(x, t)$ as the solution to a Dirac function of the PHE. Then for any initial condition $g(x, 0)$, the solution is written in a convolution form

$$T(x, t) = \int_{\mathbb{R}} G(x - y, t) g(y) dy = \frac{1}{\sqrt{4\pi\alpha t}} \int_{\mathbb{R}} e^{-\frac{(x-y)^2}{4\alpha t}} g(y) dy \quad (3.5)$$

So each point of the initial condition will diffuse like a Gaussian function, and each point influences the whole domain since the beginning.

3.2 Maxwell-Cattaneo-Vernotte law

Heat flux formulation

MCV law states a relation between the heat flux and the temperature gradient as follows

$$\tau \frac{\partial q}{\partial t} + q = -k \frac{\partial T}{\partial x} \quad (3.6)$$

We see that a new term appears from (3.2) containing the time derivative of the heat flux. Also, if τ is set to zero, we recover Fourier law. This constitutive law totally changes the dynamic of heat transfer. To understand this, we can first observe that (3.6) can be obtained as follows

$$\begin{aligned} q(x, t + \tau) &= -k \frac{\partial T}{\partial x}(x, t) \\ \downarrow \end{aligned} \quad (3.7)$$

$$q(x, t) + \tau \frac{\partial q}{\partial t}(x, t) \simeq -k \frac{\partial T}{\partial x}(x, t)$$

which means that with this equation, the heat flux is not instantaneous with respect to the temperature gradient. There is a delay related to the parameter τ that expresses some latency for the heat to flow. In fact, we can obtain a more involved expression for the heat flux. First, assume the temperature gradient to be constant in (3.6). Then it reduces to a first order non-homogeneous differential equation. For a fixed point x and an initial heat flux $q(0)$, the solution is as follows:

$$q(t) = -k \frac{\partial T}{\partial x} + \left(q(0) + k \frac{\partial T}{\partial x} \right) e^{-t/\tau} \quad (3.8)$$

So the heat flux relaxes to that of Fourier in a characteristic time τ . This is why τ is called the thermal relaxation time. Now we still consider a fixed point x but we allow

the temperature gradient to change over time. The solution of the differential equation is now written (using the integrating factor method)

$$q(t) = q(0)e^{-t/\tau} + \int_0^t \frac{e^{(\gamma-t)/\tau}}{\tau} \left(-k \frac{\partial T}{\partial x}(\gamma) \right) d\gamma \quad (3.9)$$

So the heat flux can be seen as an average sum over all the previous temperature gradients. So we introduce memory effects using the MCV law and as time goes to infinity, the effect of the initial condition $q(0)$ is forgotten.

Temperature equation

Now we take the divergence of (3.6) and substitute (3.1) in the obtained expression. This allows us to get the hyperbolic heat equation (HHE) describing the temperature evolution only

$$\frac{\partial^2 T}{\partial t^2} + \frac{1}{\tau} \frac{\partial T}{\partial t} = \frac{\alpha}{\tau} \frac{\partial^2 T}{\partial x^2} \quad (3.10)$$

This form of the equation corresponds to a telegraph equation or damped wave equation. We note that since we have a second time derivative, we need to specify the initial temperature velocity $\frac{\partial T}{\partial t}(x, 0)$ or the final temperature $T(x, F)$, where F denotes the final time, in addition to the initial condition for the problem to be well posed.

We can identify the speed of propagation

$$v = \sqrt{\frac{\alpha}{\tau}} \quad (3.11)$$

which already introduces the notion of finite speed of propagation. To make it clearer and to build a better understanding of (3.10), it's interesting to show the resolution by the method of characteristics. Since it will be useful later for numerical simulations and also to be more general, we propose a resolution for the system

$$\begin{cases} \frac{\partial q}{\partial x} + \rho c \frac{\partial T}{\partial t} = 0, \\ \tau \frac{\partial q}{\partial t} + q + k \frac{\partial T}{\partial x} = 0. \end{cases} \quad (3.12)$$

With $T(x, 0)$ and $q(x, 0)$ specified, and in the case of a bounded domain $q(x, t)$ or $T(x, t)$ specified on the boundaries (and independence of specification between the boundaries).

We introduce the dimensionless variables

$$T^* = \frac{T - T_0}{T_{\text{ref}} - T_0}, \quad q^* = \frac{qL}{k(T_{\text{ref}} - T_0)}, \quad t^* = \frac{t\alpha}{L^2}, \quad x^* = \frac{x}{L} \quad (3.13)$$

to get the dimensionless system

$$\begin{cases} \frac{\partial q^*}{\partial x^*} + \frac{\partial T^*}{\partial t^*} = 0, \\ \varepsilon \frac{\partial q^*}{\partial t^*} + q^* + \frac{\partial T^*}{\partial x^*} = 0. \end{cases} \quad (3.14)$$

with

$$\varepsilon = \delta^2 = \frac{\alpha\tau}{L^2} \quad (3.15)$$

a dimensionless parameter. The superscripts are omitted for the rest of the derivation. Combining the system with the differential forms of q and T , we finally obtain

$$\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & \varepsilon & 1 & 0 \\ dx & dt & 0 & 0 \\ 0 & 0 & dx & dt \end{pmatrix} \begin{pmatrix} \frac{\partial q}{\partial x} \\ \frac{\partial q}{\partial t} \\ \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial t} \end{pmatrix} = \begin{pmatrix} 0 \\ -q \\ dq \\ dT \end{pmatrix} \quad (3.16)$$

We can then set the determinant to zero to find the characteristic curves. The compatibility relations can be found by substituting one column of the matrix by the right-hand side of (3.16) and setting the determinant to zero again. We find

$$\delta dq + dT + q dx = 0 \quad \text{for} \quad \frac{dx}{dt} = \frac{1}{\sqrt{\varepsilon}} = \frac{1}{\delta} \quad (3.17)$$

$$\delta dq - dT - q dx = 0 \quad \text{for} \quad \frac{dx}{dt} = \frac{-1}{\sqrt{\varepsilon}} = \frac{-1}{\delta} \quad (3.18)$$

These relations can then be integrated to find the temperature field $T(x, t)$ and the heat flux $q(x, t)$ at any point in the domain.

These expressions make clear the concept of finite speed of propagation. The information travels along the characteristic curves and is limited. The heat flux propagates over a finite range for a given period. There is a finite time for a point to be influenced by other points.

When going back to the dimensional form we have for the characteristic curves

$$v = \frac{dx}{dt} = \pm \sqrt{\frac{\alpha}{\tau}} \quad (3.19)$$

And we see that as τ goes to zero and we recover the PHE associated to Fourier, the characteristic curves tend to horizontal lines. This corresponds to an infinite speed of propagation, as expected.

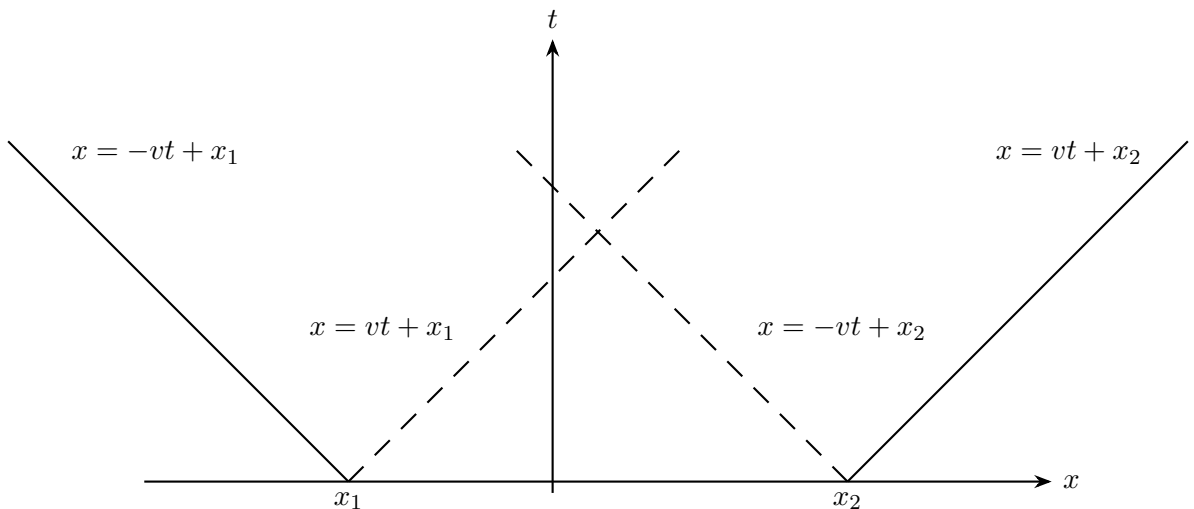


Figure 3.1: Characteristic curves propagating information in the (x, t) plane

Another interesting aspect of the damped wave equation (3.10) can be observed from the analytical solution in unbounded domain.

We use the following dimensionless variables

$$\hat{t} = \frac{t}{2\tau}, \quad \hat{x} = \frac{x}{\sqrt{4\tau\alpha}} \quad (3.20)$$

(3.10) is now in the form

$$\frac{\partial^2 T}{\partial \hat{t}^2} + 2 \frac{\partial T}{\partial \hat{t}} = \frac{\partial^2 T}{\partial \hat{x}^2} \quad (3.21)$$

with initial conditions $T(\hat{x}, 0) = F(\hat{x})$ and $\frac{\partial T}{\partial \hat{t}}(\hat{x}, 0) = G(\hat{x})$. In this form, the characteristic curves have a slope of one. Then the solution to (3.21) is [10]

$$T(\hat{x}, \hat{t}) = \frac{e^{-\hat{t}}}{2} \left[F(\hat{x} + \hat{t}) + F(\hat{x} - \hat{t}) + \int_{\hat{x}-\hat{t}}^{\hat{x}+\hat{t}} I(s, \hat{x}, \hat{t}) ds \right] \quad (3.22)$$

$$I(s, \hat{x}, \hat{t}) = \left[F(s) + G(s) \right] \Psi(\hat{t}^2 - (s - \hat{x})^2) - 2\hat{t} F(s) \Psi'(\hat{t}^2 - (s - \hat{x})^2), \quad (3.23)$$

$$\Psi(y) = J_0(\sqrt{y}) \quad (3.24)$$

Where J_0 is the Bessel function of zeroth order.

We observe that a part of this solution corresponds to the usual wave equation with half of the initial condition going to the left and to the right (d'Alembert formula), but a damping factor associated to the term $\frac{\partial T}{\partial \hat{t}}$ causes an exponential decay. We will come back later on this damping. Also observe the integral term that is limited to the interval $[\hat{x} - \hat{t}, \hat{x} + \hat{t}]$ reflecting the fact that the value at that point only depends on those whose characteristic curves have reached this point. The finite speed of propagation is also highlighted by this expression.

3.3 Discontinuities

Now we discuss the propagation of thermal discontinuities. For the PHE, expression (3.5) shows that the solution is infinitely differentiable for all times $t > 0$, thus preventing the propagation of thermal fronts. We can start with a discontinuity in the initial condition but it will be instantaneously erased by the diffusion. This well-known property of the heat equation is called the smoothing effect.

On the contrary, the hyperbolic heat equation allows the propagation of damped discontinuities provided that they are introduced by the initial condition or the boundary conditions. Indeed, the emergence of a discontinuity in the domain is caused by the intersection of characteristic curves from the same family which cannot occur for a linear hyperbolic equation of the form (3.10).

Illustrative example

An analytical example of discontinuity propagation is obtained by considering a semi-

infinite domain with

$$\left\{ \begin{array}{l} \frac{\partial^2 T^{cv}}{\partial t^2} + \frac{1}{\tau} \frac{\partial T^{cv}}{\partial t} = v^2 \frac{\partial^2 T^{cv}}{\partial x^2} \\ T^{cv}(0, t) = H(t), \\ T^{cv}(\infty, t) = 0, \\ T^{cv}(x, 0) = 0, \\ \frac{\partial T^{cv}}{\partial t}(x, 0) = 0. \end{array} \right. \quad (3.25)$$

with v is the speed of propagation and $H(t)$ the unit step function.

The solution is then (obtained by Laplace transform [22])

$$T^{cv}(x, t) = H(vt - x) \left[e^{-x/\chi} + \frac{x}{\chi} \int_x^{vt} e^{-\xi/\chi} \frac{I_1 \left(\chi^{-1} \sqrt{\xi^2 - x^2} \right)}{\sqrt{\xi^2 - x^2}} d\xi \right] \quad (3.26)$$

$$\chi = 2v\tau$$

where I_1 is the modified Bessel function of first order.

Evaluating this expression along the path $\gamma(y) : y \rightarrow (vy, y)$ gives

$$T(vy, y) = H(0) \exp \left(-\frac{y}{2\tau} \right) \quad (3.27)$$

and we clearly see the discontinuity that is propagating along the curve (vt, t) , which is also the characteristic curve emanating from the origin. We need to wait for some time for the information that a unit value has been imposed on the left boundary to reach a point before we observe a change in the zero value. We also have the damping of the discontinuity by the exponential.

For comparison, the corresponding PHE problem is

$$\left\{ \begin{array}{l} \frac{\partial T^f}{\partial t} = \alpha \frac{\partial^2 T^f}{\partial x^2} \\ T^f(0, t) = H(t) \\ T^f(\infty, t) = 0 \\ T^f(x, 0) = 0 \end{array} \right. \quad (3.28)$$

and the solution is the error function

$$T^f(x, t) = 1 - \operatorname{erf} \left(\frac{x}{2\sqrt{\alpha t}} \right) \quad (3.29)$$

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\eta^2} d\eta \quad (3.30)$$

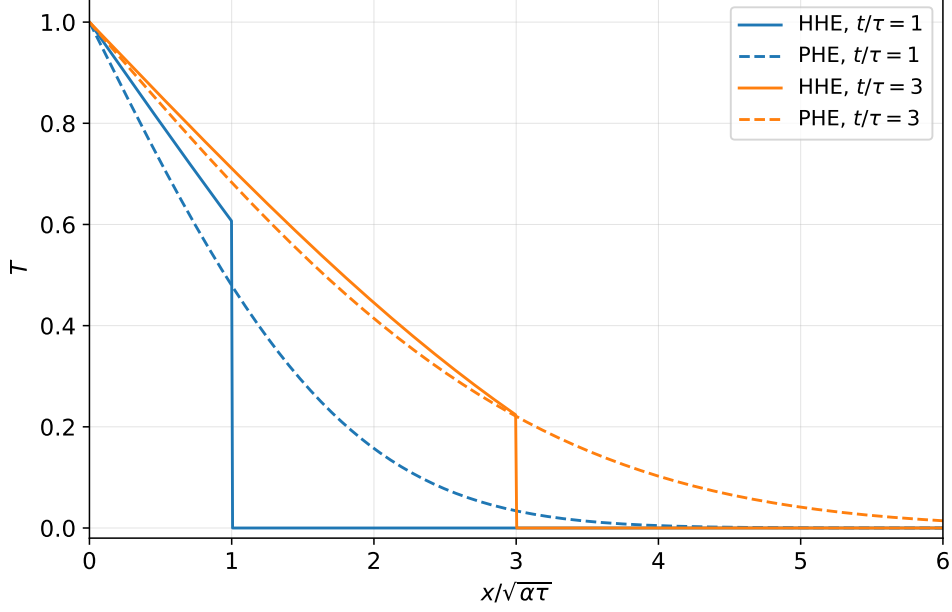


Figure 3.2: Solution to problem (3.25) and (3.28) for different dimensionless times

We clearly see Figure 3.2 the front propagation and its damping. This illustrates well the finite speed of propagation. Also, the heat equation gives a smooth profile with nonzero values everywhere, as expected for the infinite propagation speed of this equation.

Jump conditions

Motivated by the previous example, we derive the Rankine-Hugoniot jump conditions across the thermal wave front.

We start from system (3.12) written

$$\frac{\partial}{\partial t} \begin{pmatrix} T \\ q \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \frac{1}{\rho c} q \\ \frac{k}{\tau} T \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{1}{\tau} q \end{pmatrix}. \quad (3.31)$$

In compact form:

$$\frac{\partial Y}{\partial t} + \frac{\partial F(Y)}{\partial x} = S(Y) \quad (3.32)$$

where $Y = \begin{pmatrix} T \\ q \end{pmatrix}$. We identify in (3.32) a space-time divergence. To derive the relations across the jump, we consider a discontinuity propagating in the (x, t) plane and integrate the equations over a control volume (see Figure 3.3).

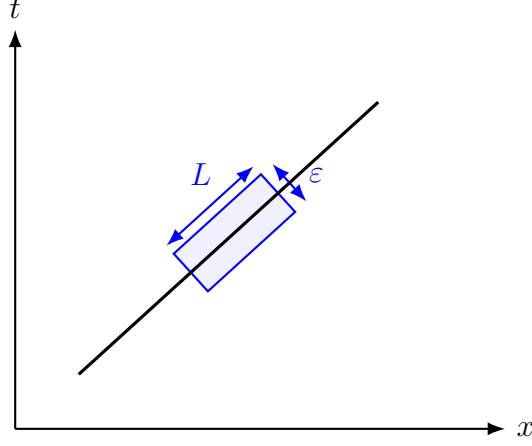


Figure 3.3: Control volume across a moving discontinuity in the (x, t) plane.

$$\int_{\Omega} \nabla_{x,t} \cdot (F(Y), Y) d\Omega = \int_{\Omega} S(Y) d\Omega \quad (3.33)$$

Using the Gauss-Ostrogradsky theorem, we find:

$$\int_{\partial\Omega} (F(Y), Y) \cdot n d\Omega = \int_{\Omega} S(Y) d\Omega \quad (3.34)$$

Now we let the small box shrink to zero volume. Since $S(Y)$ is bounded, and $L\varepsilon \rightarrow 0$, this term goes to 0. We also separate the integration on the part along the discontinuity curve and perpendicular to

$$\int_{\parallel} (F(Y), Y) \cdot n d\Omega + \int_{\perp} (F(Y), Y) \cdot n d\Omega = 0 \quad (3.35)$$

But as $\varepsilon \rightarrow 0$, the box sticks to the discontinuity and the fluxes on the segments perpendicular to the discontinuity reduce to 0. We are left with

$$\int_{\parallel} (F(Y), Y) \cdot n d\Omega = 0 \quad (3.36)$$

Since it's true for every control volume, we get

$$[(F(Y), Y)] \cdot n = 0 \quad (3.37)$$

If we write the normal vector in the form $n = (-1, v)$ with v the propagation velocity of the discontinuity, we obtain the relations across the jump

$$v[[Y]] = [[F(Y)]] \quad (3.38)$$

In full form

$$\begin{cases} v[[T]] = \frac{1}{\rho c} [[q]] \\ v[[q]] = \frac{k}{\tau} [[T]] \end{cases} \quad (3.39)$$

To verify both conditions, the velocity of propagation can be computed

$$v = \pm \sqrt{\frac{\alpha}{\tau}} \quad (3.40)$$

And we recover the propagation speed found from the method of characteristics. The discontinuity indeed propagates along the characteristic curves.

3.4 Modal analysis

It is interesting to solve the HHE and the PHE from the separation of variables technique. This allows us to see how the solutions decompose in modes and it describes the features well of both equations. It also suggests the approximation of the solution by truncated sums.

We work on the domain $[0, L]$ and we assume homogeneous Dirichlet or Neumann boundary conditions. We can also easily tackle the case with non-homogeneous boundary conditions and a related example is shown below.

PHE decomposition

Starting with the PHE, we want to find solutions of the form $T^f(x, t) = X(x)\Gamma(t)$.

Inserting this into the equation, we find:

$$X\Gamma' = \alpha\Gamma X'' \quad (3.41)$$

$$\frac{1}{\alpha} \frac{\Gamma'}{\Gamma} = \frac{X''}{X} = -k^2 \quad (3.42)$$

Solving the ordinary differential equation with respect to x we find

$$X(x) = A \cos(kx) + B \sin(kx) \quad (3.43)$$

and with respect to t we get

$$\Gamma(t) = C e^{-\alpha k^2 t} \quad (3.44)$$

Combining both results gives

$$T^f(x, t) = T_s(x) + \sum_n [A_n \sin(k_n x) + B_n \cos(k_n x)] \exp(-\alpha k_n^2 t) \quad (3.45)$$

where $T_s(x)$ is the stationary solution and the constants A_n , B_n , and k_n are determined to satisfy the boundary and initial conditions. From the form of (3.43), the admissible values of k_n are typically given by

$$k_n = \frac{n\pi}{L} \quad \text{or} \quad k_n = \frac{(2n-1)\pi}{2L}, \quad n = 1, 2, \dots$$

depending on the type of boundary conditions. The expression (3.45) shows a feature of the PHE, which is that the highly oscillating modes, associated to high values of k_n , will be quickly reduced by the exponential. Thus the details in the initial condition are erased to give a smoother profile for the function. This also justifies the absence of discontinuities

which contain all frequencies, here dissipated too quickly.

HHE decomposition

Now, looking at the HHE, we want to find solutions of the form $T^{cv}(x, t) = X(x)\Gamma(t)$. Inserting in the equation we find:

$$\tau X\Gamma'' + X\Gamma' = \alpha X''\Gamma \quad (3.46)$$

$$\frac{\tau}{\alpha} \frac{\Gamma''}{\Gamma} + \frac{1}{\alpha} \frac{\Gamma'}{\Gamma} = \frac{X''}{X} = -k^2 \quad (3.47)$$

The ordinary differential equation in x also gives

$$X(x) = A \cos(kx) + B \sin(kx) \quad (3.48)$$

and in t we get

$$\Gamma(t) = Ce^{r_1 t} + De^{r_2 t} \quad (3.49)$$

$$r_1 = \frac{-1 + \sqrt{1 - 4\alpha\tau k^2}}{2\tau} \quad r_2 = \frac{-1 - \sqrt{1 - 4\alpha\tau k^2}}{2\tau} \quad (3.50)$$

Now we highlight the cases where $4\alpha\tau k^2 > 1$ (underdamped modes)

$$\Gamma^{ud}(t) = \exp\left(-\frac{t}{2\tau}\right) [C \cos(\omega_k t) + D \sin(\omega_k t)] \quad (3.51)$$

$$\omega_k = \frac{\sqrt{4\alpha\tau k^2 - 1}}{2\tau} \quad (3.52)$$

The solution can now be written in an overdamped and underdamped part:

$$\begin{aligned} T^{cv}(x, t) = T_s(x) + \sum_{od} [A_n \sin(k_n x) + B_n \cos(k_n x)] [C_n \exp(r_1^n t) + D_n \exp(r_2^n t)] \\ + \sum_{ud} [A_n \sin(k_n x) + B_n \cos(k_n x)] \exp\left(-\frac{t}{2\tau}\right) [C_n \sin(\omega_n t) + D_n \cos(\omega_n t)]. \end{aligned} \quad (3.53)$$

Where A_n, B_n, C_n, D_n and k_n are determined to satisfy the boundary and initial conditions. In view of (3.48), the admissible values for k_n are the same as before. The particularity of solution (3.53) is that all the under damped modes decay at the same rate $\exp(-t/2\tau)$. This means that we don't have a hierarchy of decay for high modes, and the presence of all modes associated to an oscillating behavior is limited to a few τ before the solution presents only a diffusive behavior. It also allows the propagation of discontinuities as the high oscillating modes are kept for some time. This also implies the need of these terms in a truncated series that approximates well the solution.

Abstract problem

The developments thereafter are based on [23].

The truncated sum of (3.53) has a nice property that we explain. First we make a short digression and consider the following abstract problem, called a second order hyperbolic problem

For given Hilbert spaces V and W , find u such that for each $t > 0$, $u(t) \in V$, $u'(t) \in V$, $u''(t) \in W$ and

$$c(u''(t), v) + a(u'(t), v) + b(u(t), v) = c(f(t), v) \quad \text{for each } v \in V \quad (3.54)$$

satisfying $u(0) = u_0$ and $u'(0) = u_1$. We define the energy norm $\|\cdot\|_V$ and the inertia norm $\|\cdot\|_W$ as the norms induced by the forms $b(\cdot, \cdot)$ and $c(\cdot, \cdot)$ respectively.

If u is solution of (3.54) and it can be written in modes, assuming also $f(t) = 0$ and initial conditions $u(0) \in V$ and $u'(0) = 0$, the truncated sum

$$u^N(t) = \sum_{k=1}^N y_k(t) w_k \quad \text{of} \quad u(t) = \sum_{k=1}^{\infty} y_k(t) w_k \quad (3.55)$$

where w_k are orthogonal eigenfunctions with respect to the spaces V and W , satisfies

$$\|u(t) - u^N(t)\|_V^2 + \|u'(t) - (u^N)'(t)\|_W^2 \leq \|u(0) - u^N(0)\|_V^2 \rightarrow 0 \quad \text{if } N \rightarrow \infty \quad (3.56)$$

The inequality (3.56) means that the accuracy of the approximated solution only depends on the approximation of the initial condition computed with the energy norm. The error at any time $t > 0$ is bounded by the error on the initial condition. This ensures that we will not observe an increase on the error over time provided the initial condition was well represented by the truncated sum. Of course we expect that the form $b(\cdot, \cdot)$ is such that the norm $\|\cdot\|_V$ is interesting.

Now we return to equation (3.10) and write its weak formulation (working on the interval $[0, 1]$)

$$\int_0^1 v \frac{\partial^2 T}{\partial t^2} dx + \frac{1}{\tau} \int_0^1 v \frac{\partial T}{\partial t} dx + \frac{\alpha}{\tau} \int_0^1 \frac{\partial v}{\partial x} \frac{\partial T}{\partial x} dx = 0 \quad (3.57)$$

with $v(0) = 0$ or $v(1) = 0$ if we don't have Neumann conditions on these points. We also define the spaces

$$V = \{v \in H^1(0, 1) : v(0) = 0 \text{ and/or } v(1) = 0\}; \quad W = L^2(0, 1) \quad (3.58)$$

and we can identify the form (3.54) by

$$c(u, v) = \int_0^1 uv dx \quad a(u, v) = \frac{1}{\tau} c(u, v) \quad b(u, v) = \frac{\alpha}{\tau} \int_0^1 u'v' dx \quad (3.59)$$

which means that (3.57) presents the properties of the abstract problem. So in view of the form $b(\cdot, \cdot)$, (3.56) allows a good control on the oscillations for times $t > 0$ if it is small on the approximation of the initial condition.

Illustrative example

Now we illustrate the modal composition with an example. We consider the case of a step function imposed on the left boundary $T(0, t) = H(t)$, an isolated boundary on the right $\frac{\partial T}{\partial x}(1, t) = 0$ and initial conditions $T(x, 0) = 0$ and $\frac{\partial T}{\partial t}(x, 0) = 0$. Since the boundary condition on the left is not homogeneous, we set $U(x, t) = 1 - T(x, t)$ and solve the

modified problem

$$\left\{ \begin{array}{l} \frac{\partial^2 U^{cv}}{\partial t^2} + \frac{1}{\tau} \frac{\partial U^{cv}}{\partial t} = \frac{\alpha}{\tau} \frac{\partial^2 U^{cv}}{\partial x^2} , \\ U^{cv}(0, t) = 0, \\ \frac{\partial U^{cv}}{\partial x}(1, t) = 0, \\ U^{cv}(x, 0) = 1, \\ \frac{\partial U^{cv}}{\partial t}(x, 0) = 0. \end{array} \right. \quad (3.60a)$$

$$\left\{ \begin{array}{l} \frac{\partial U^f}{\partial t} = \alpha \frac{\partial^2 U^f}{\partial x^2} , \\ U^f(0, t) = 0, \\ \frac{\partial U^f}{\partial x}(1, t) = 0, \\ U^f(x, 0) = 1. \end{array} \right. \quad (3.60b)$$

For the HHE and PHE, respectively.

Then using formulas (3.53) and (3.45) we have $A_n = 0$ and $k_n = (2n-1)\frac{\pi}{2}$ for $n = 1, 2, \dots$

The remaining coefficients can be computed from the initial conditions and we get

$$U^{cv}(x, t) = \sum_n \sin(k_n x) [A_n \exp(r_1^{k_n} t) + B_n \exp(r_2^{k_n} t)] \quad (3.61)$$

$$A_n = \frac{2}{Lk_n(1 - r^n)} \quad B_n = \frac{-2r^n}{Lk_n(1 - r^n)} \quad r^k = \frac{r_1^n}{r_2^n}$$

and

$$U^f(x, t) = \sum_n A_n \sin(k_n x) \exp(-\alpha k_n^2 t) \quad (3.62)$$

$$A_n = \frac{2}{Lk_n}$$

ε	Number of overdamped modes
10^{-1}	1
10^{-2}	2
10^{-3}	5
10^{-4}	16
10^{-5}	50

Table 3.1: Number of overdamped modes for different values of ε .

A criterion for the identification of the underdamped modes is the parameter $\varepsilon = \frac{\alpha\tau}{L^2}$, easily identified in (3.50) (see 3.1). The result for $\varepsilon = 10^{-4}$ is shown in 3.4. We see that with the 1000 first terms we can already obtain a good approximation of the solution

profile. A better insight into the HHE decomposition is shown in Figure 3.5. We clearly see the overdamped part of the solution diffusing and the underdamped part associated to the discontinuity.

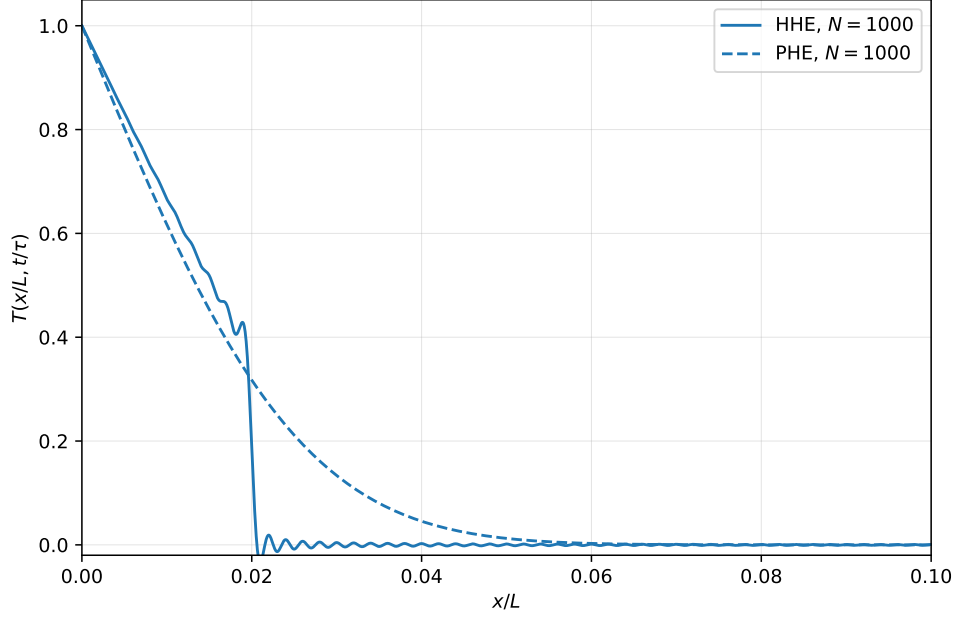


Figure 3.4: Finite sum approximation of modal solution of (3.60a) and (3.60b), $\varepsilon = 10^{-4}$

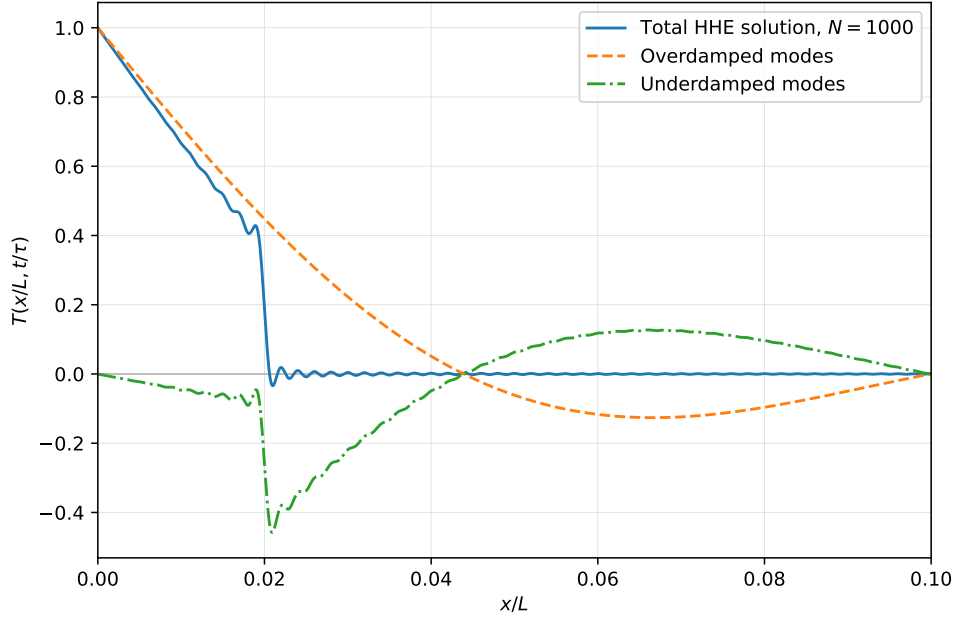


Figure 3.5: Separation of overdamped and underdamped modes in the solution of (3.60a), $\varepsilon = 10^{-4}$

3.5 Variational framework

We can find a variational principle for the hyperbolic heat equation (3.10), but there is no such formulation for the parabolic heat equation. This is a great advantage for the HHE because many features can be used when we study an equation in this framework. For example, it is very useful for the finite element method as we can work with the functional to compute the coefficients of the form functions. It also allows to optimize the positions of the nodes for a mesh. Furthermore, we can obtain conserved quantities.

Lagrangian

We consider functions ϕ

$$\phi : \Omega \times [0, T] \rightarrow \mathbb{R} \quad (3.63)$$

An action is a functional of the form

$$S[\phi] = \int_{\Omega \times [0, T]} \mathcal{L} \left(\phi, \frac{\partial \phi}{\partial x^\mu}, x^\mu \right) d^n x dt \quad (3.64)$$

where $x^\mu = (t, x_1, \dots, x_n)$ and $\mathcal{L}$ is the Lagrangian density.

Action stationarity

$$\delta S[\phi] = 0 \quad (3.65)$$

can be obtained from the Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi}{\partial x^\mu} \right)} \right) = 0 \quad (3.66)$$

We say that an equation has a variational formulation if it corresponds to the stationarity of an action of the form (3.66) with an associated Lagrangian.

The HHE has a Lagrangian [24],

$$\mathcal{L} \left(t, x, T, \frac{\partial T}{\partial t}, \frac{\partial T}{\partial x} \right) = \frac{1}{2} e^{t/\tau} \left[\tau \left(\frac{\partial T}{\partial t} \right)^2 - \alpha \left(\frac{\partial T}{\partial x} \right)^2 \right]. \quad (3.67)$$

Indeed, we first compute

$$\frac{\partial \mathcal{L}}{\partial T} = 0, \quad \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial T}{\partial t} \right)} = e^{t/\tau} \tau \frac{\partial T}{\partial t}, \quad \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial T}{\partial x} \right)} = -e^{t/\tau} \alpha \frac{\partial T}{\partial x}. \quad (3.68)$$

and from (3.66) we get

$$-\frac{1}{\tau} e^{t/\tau} \tau \frac{\partial T}{\partial t} - e^{t/\tau} \tau \frac{\partial^2 T}{\partial t^2} + e^{t/\tau} \alpha \frac{\partial^2 T}{\partial x^2} = 0. \quad (3.69)$$

Rearranging the terms we recover the HHE

$$\frac{\partial T}{\partial t} + \tau \frac{\partial^2 T}{\partial t^2} = \alpha \frac{\partial^2 T}{\partial x^2}. \quad (3.70)$$

From expression (3.67) we may be tempted to take the limit $\tau \rightarrow 0$ to obtain a Lagrangian for the parabolic heat equation. However, we see that

$$e^{t/\tau} \rightarrow +\infty \quad (3.71)$$

and

$$\left[\tau \left(\frac{\partial T}{\partial t} \right)^2 - \alpha \left(\frac{\partial T}{\partial x} \right)^2 \right] \rightarrow -\alpha \left(\frac{\partial T}{\partial x} \right)^2 \quad (3.72)$$

so the product goes to infinite negative values and we can't recover an expression.

Energy-momentum tensor

Now we derive conserved quantities associated to the HHE. If the Euler-Lagrange equations were obtained by the stationarity of the action from small perturbations on the field, now we fix the field and we look at the stationarity from changes of coordinates. This introduces the energy-momentum tensor defined as

$$T_\nu^\mu = \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi}{\partial x^\mu} \right)} \frac{\partial \phi}{\partial x^\nu} - L \delta_\nu^\mu \quad (3.73)$$

Conserved quantities are then obtained by taking the divergence

$$\frac{\partial T_\nu^\mu}{\partial x^\mu} = \frac{\partial \mathcal{L}}{\partial X^\nu} \quad (3.74)$$

In our case we find

$$T_\nu^\mu = e^{t/\tau} \begin{pmatrix} \frac{1}{2} \left[\tau \left(\frac{\partial T}{\partial t} \right)^2 + \alpha \left(\frac{\partial T}{\partial x} \right)^2 \right] & -\alpha \frac{\partial T}{\partial t} \frac{\partial T}{\partial x} \\ \tau \frac{\partial T}{\partial t} \frac{\partial T}{\partial x} & -\frac{1}{2} \left[\tau \left(\frac{\partial T}{\partial t} \right)^2 + \alpha \left(\frac{\partial T}{\partial x} \right)^2 \right] \end{pmatrix} \quad (3.75)$$

and

$$\frac{\partial T_0^\mu}{\partial x^\mu} = \frac{\mathcal{L}}{\tau} \quad \frac{\partial T_1^\mu}{\partial x^\mu} = 0 \quad (3.76)$$

The "momentum" part is conserved, but as the Lagrangian explicitly depends on t , the "energy" part is not conserved.

Hamiltonian

Another interesting quantity that can be computed is the Hamiltonian $\mathcal{H}$. It is the Legendre transform of the Lagrangian with respect to the velocity $\frac{\partial T}{\partial t}$. The Hamiltonian is expressed as a function of the momentum p .

$$\mathcal{H} = p \frac{\partial T}{\partial t} - \mathcal{L} \quad (3.77)$$

where

$$p = \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial T}{\partial t} \right)} \quad (3.78)$$

In our case,

$$p = e^{t/\tau} \tau \left(\frac{\partial T}{\partial t} \right) \quad (3.79)$$

and

$$\mathcal{H} = \frac{1}{2} e^{t/\tau} \left[\tau \left(\frac{\partial T}{\partial t} \right)^2 + \alpha \left(\frac{\partial T}{\partial x} \right)^2 \right] \quad (3.80)$$

And we see that we recover the first component of (3.75)

3.6 Numerical simulation

We propose schemes for the numerical resolution of the hyperbolic and parabolic heat equations. Simulation results for both Dirichlet and Neumann boundary conditions are presented so that we can see the behavior of the solution and highlight some properties.

3.6.1 Parabolic heat equation

We use the finite difference method to compute the numerical solution.

Solving a partial differential equation for $u(x, t)$ on domain $[0, L]$, we first discretize the space domain with $N + 1$ equally spaced points

$$x_i = i\Delta x, \quad \Delta x = \frac{L}{N}, \quad i = 0, \dots, N \quad (3.81)$$

Now discretize in space and continuous in time, we want to find $u_i(t)$. We approximate the spatial derivatives with finite differences and we get a system for the u_i

$$\frac{d\mathbf{u}}{dt} = A\mathbf{u} \quad (3.82)$$

We can then discretize in time

$$t^n = n\Delta t, \quad n = 0, \dots \quad (3.83)$$

and choose a temporal integrator that is stable to find u_i^n , the discrete-in-space-and-time approximation of solution $u(x, t)$.

We apply this procedure to equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad (3.84)$$

where we kept the notation u for the temperature as it is more convenient in what follows.

Space discretization

We consider a discretization of the form (3.81) and use second order finite differences for the second derivative

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + O(\Delta x)^2 \quad (3.85)$$

Thus for each $u_i(t)$ we have from (3.84) and (3.85)

$$\frac{du_i}{dt}(t) = \alpha \left(\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} \right) + O(\Delta x)^2 \quad (3.86)$$

Depending on the boundary conditions we obtain different systems (3.82):

Dirichlet case

With conditions in the form $u(0, t) = g_1(t)$ and $u(L, t) = g_2(t)$, the system is

$$\frac{d\mathbf{u}}{dt} = A\mathbf{u} + \mathbf{b}(t) \quad (3.87)$$

where

$$A = \frac{\alpha}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \\ & & 1 & -2 \end{bmatrix} \quad \text{and} \quad \mathbf{b}(t) = \frac{\alpha}{(\Delta x)^2} \begin{bmatrix} g_1(t) \\ 0 \\ \vdots \\ g_2(t) \end{bmatrix} \quad (3.88)$$

The eigenvalues of the matrix A are (useful for stability)

$$\lambda_k = -\frac{4\alpha}{(\Delta x)^2} \sin^2 \left(\frac{\pi k}{2N} \right), \quad k = 1, \dots, N-1 \quad (3.89)$$

Neumann case

With conditions in the form $\frac{\partial T}{\partial x}(0, t) = h_1(t)$ and $\frac{\partial T}{\partial x}(L, t) = h_2(t)$ the system is

$$\frac{d\mathbf{u}}{dt} = A\mathbf{u} + \mathbf{b}(t) \quad (3.90)$$

Where

$$A = \frac{\alpha}{(\Delta x)^2} \begin{bmatrix} -2 & 2 & 0 & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & 2 & -2 \end{bmatrix} \quad \text{and} \quad \mathbf{b}(t) = \frac{\alpha}{\Delta x} \begin{bmatrix} -2h_1(t) \\ 0 \\ \vdots \\ 2h_2(t) \end{bmatrix} \quad (3.91)$$

For the second derivative approximation at the boundary points we need values that are not in the domain, so we used second-order approximations of the condition on the derivative to obtain an expression:

From

$$h_1(t) = \frac{u_1 - u_{-1}}{2\Delta x} + O(\Delta x)^2 \quad h_2(t) = \frac{u_{N+1} - u_{N-1}}{2\Delta x} + O(\Delta x)^2 \quad (3.92)$$

we get

$$u_{-1} \approx -2h_1(t)\Delta x + u_1 \quad u_{N+1} \approx 2h_2(t)\Delta x + u_{N-1} \quad (3.93)$$

and we can substitute these values in the expression of the second derivative approximation at the boundaries.

The eigenvalues of the matrix A are (useful for stability)

$$\lambda_k = -\frac{4\alpha}{(\Delta x)^2} \sin^2 \left(\frac{k\pi}{2N} \right), \quad k = 0, 1, \dots, N \quad (3.94)$$

Time integration

Using a temporal integrator for systems (3.87) or (3.90), we expect to find a form

$$\mathbf{u}^{n+1} = B\mathbf{u}^n \quad (3.95)$$

where B is the amplification matrix. To limit growth of the error, we need the eigenvalues of B to have modulus lower than one such that we can control the evolution of the function:

$$\|\mathbf{u}^n\| = \|B^n \mathbf{u}^0\| \leq \|X\| \|D^n\| \|X^{-1}\| \|\mathbf{u}^0\| = \kappa(X) \left(\max_j |d_j| \right)^n \|\mathbf{u}^0\| \quad (3.96)$$

where $XD X^{-1}$ is the diagonalisation of B , d_j the eigenvalues of D and $\kappa(X) = \|X\| \|X^{-1}\|$ is the condition number.

The stability region of an integrator expresses the allowed eigenvalues λ_i of the matrix A such that using this scheme, the eigenvalues d_j of B have modulus lower than one. We consider two temporal schemes:

Explicit Euler

for $\frac{du}{dt}(t) = f(u, t)$, the general formula of the Euler scheme (first-order global) is

$$\frac{u^{n+1} - u^n}{\Delta t} = f(u^n, t^n) \quad (3.97)$$

In our case, it reduces to

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = A\mathbf{u}^n \quad (3.98)$$

Rearranging the terms we obtain the form (3.95)

$$\mathbf{u}^{n+1} = (\Delta t A + I)\mathbf{u}^n = X^{-1}(\Delta t \Lambda + I)X\mathbf{u}^n \quad (3.99)$$

and we see that the stability region for this scheme is obtained from the condition (see also 3.6a)

$$|\lambda \Delta t + 1| \leq 1 \quad (3.100)$$

From the expressions of the eigenvalues (3.89) and (3.94) we obtain

$$r \leq \frac{1}{2}, \quad r = \frac{\alpha \Delta t}{(\Delta x)^2} \quad (3.101)$$

where r is the Fourier number, a dimensionless numerical parameter. This condition should be verified for the scheme to be stable.

Crank-Nicolson

For $\frac{du}{dt} = f(u, t)$, the general formula of the Crank-Nicolson scheme (second-order global) is

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}(f(u^{n+1}, t^{n+1}) + f(u^n, t^n)) \quad (3.102)$$

In our case, it reduces to

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \frac{1}{2}(A\mathbf{u}^{n+1} + A\mathbf{u}^n) \quad (3.103)$$

Rearranging the terms we get the form (3.95)

$$\mathbf{u}^{n+1} = \left(I - \frac{\Delta t}{2}A\right)^{-1} \left(I + \frac{\Delta t}{2}A\right) \mathbf{u}^n = X^{-1} \left(I - \frac{\Delta t}{2}\Lambda\right)^{-1} \left(I + \frac{\Delta t}{2}\Lambda\right) X\mathbf{u}^n \quad (3.104)$$

and we see that the stability region for this scheme is obtained from the condition (see also 3.6b)

$$\left| \frac{1 + \frac{\lambda \Delta t}{2}}{1 - \frac{\lambda \Delta t}{2}} \right| \leq 1. \quad (3.105)$$

In this case the scheme is unconditionally stable, which means that we can choose the time step, but the drawback is that a system has to be solved at each time step in (3.104) (as we do not invert the matrix).

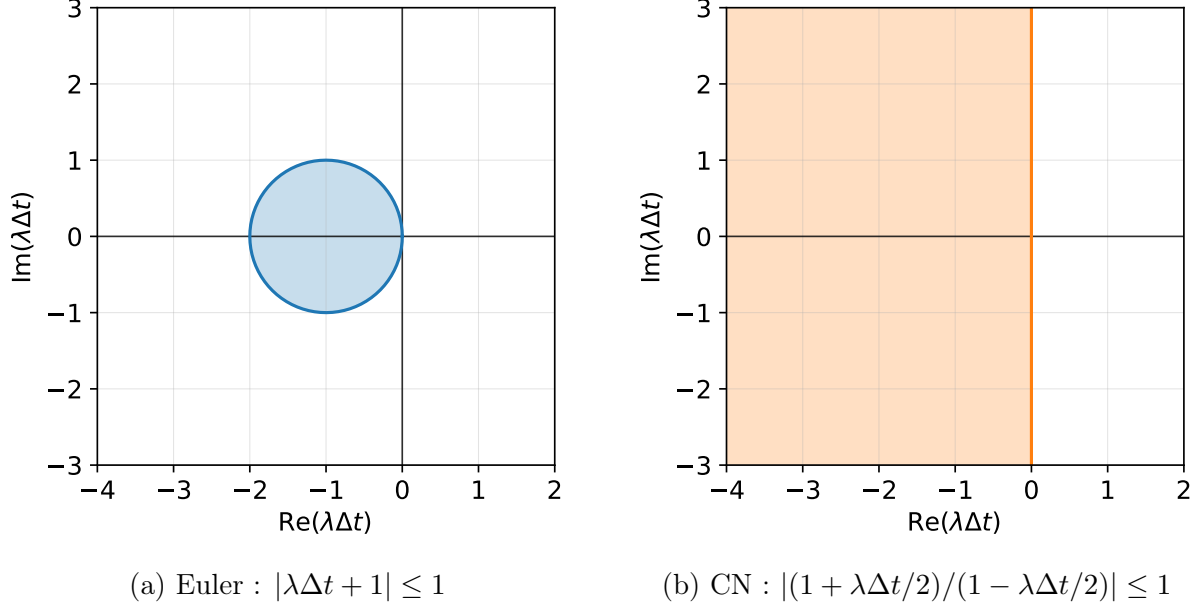


Figure 3.6: Stability region of the Euler and Crank-Nicolson (CN) schemes in the complex plane

3.6.2 Hyperbolic heat equation

We integrate the compatibility relations along the characteristic curves to compute the numerical solution.

Solving a partial differential equation for $u(x, t)$ on domain $[0, L]$, we discretize the space domain with $N + 1$ points equally spaced

$$x_i = i\Delta x, \quad \Delta x = \frac{L}{N}, \quad i = 0, \dots, N \quad (3.106)$$

and the time domain

$$t^n = n\Delta t, \quad \Delta t = \frac{\Delta x}{v}, \quad n = 0, \dots \quad (3.107)$$

where v is the velocity of propagation. We can then integrate the two compatibility relations from each discrete point to the next left and right discrete points to construct the solution. We can approximate the integral terms if needed.

We apply this procedure to equations (3.17) and (3.18) [25]. We also go back to the notation T for the temperature. See Figure 3.7 for the points A, B and P and a visual interpretation.

First we integrate the compatibility relations

$$\delta \int_{q_A}^{q_P} dq + \int_{T_A}^{T_P} dT + \int_{x_A}^{x_P} q dx = 0 \quad \text{along} \quad \frac{dx}{dt} = \frac{1}{\delta} \quad (3.108)$$

$$\delta \int_{q_B}^{q_P} dq - \int_{T_B}^{T_P} dT - \int_{x_B}^{x_P} q dx = 0 \quad \text{along} \quad \frac{dx}{dt} = -\frac{1}{\delta} \quad (3.109)$$

The first integral terms can be computed exactly but the last one is approximated (second order global)

$$\delta(q_P - q_A) + (T_P - T_A) + \frac{1}{2}(q_P + q_A)\Delta x = O(\Delta x^3) \quad (3.110)$$

$$\delta(q_P - q_B) - (T_P - T_B) + \frac{1}{2}(q_P + q_B)\Delta x = O(\Delta x^3) \quad (3.111)$$

An explicit expression for T_P and q_P can then be derived:

$$q_P = \left[(q_A + q_B) \left(\delta - \frac{1}{2}\Delta x \right) + (T_A - T_B) \right] \left[2 \left(\delta + \frac{\Delta x}{2} \right) \right]^{-1} \quad (3.112)$$

$$T_P = \frac{1}{2} \left[T_A + T_B + \left(\delta - \frac{\Delta x}{2} \right) (q_A - q_B) \right] \quad (3.113)$$

So, starting from points A and B where (T, q) are known, we can compute at point P the values (T, q) .

On the left boundary, we have only one characteristic curve but using boundary conditions we have

$$q_P = \left[(f(t_P) - T_B) + q_B \left(\delta - \frac{\Delta x}{2} \right) \right] \left[\delta + \frac{\Delta x}{2} \right]^{-1} \quad (3.114)$$

if the temperature is specified, or

$$T_P = T_B + f(t_P) \left(\delta + \frac{\Delta x}{2} \right) + q_B \left(\frac{\Delta x}{2} - \delta \right) \quad (3.115)$$

if the heat flux is specified.

On the right boundary also,

$$q_P = \left[(T_A - f(t_P)) + q_A \left(\delta - \frac{\Delta x}{2} \right) \right] \left[\frac{\Delta x}{2} + \delta \right]^{-1} \quad (3.116)$$

if the temperature is specified, or

$$T_P = T_A - f(t_P) \left(\delta + \frac{\Delta x}{2} \right) + q_A \left(\delta - \frac{\Delta x}{2} \right) \quad (3.117)$$

if the heat flux is specified.

So this scheme is fully explicit and the time step is constrained from a CFL type condition with equality

$$\Delta t = \delta \Delta x \quad (3.118)$$

or

$$\Delta t = \sqrt{\frac{\tau}{\alpha}} \Delta x \quad (3.119)$$

In dimensional variables.

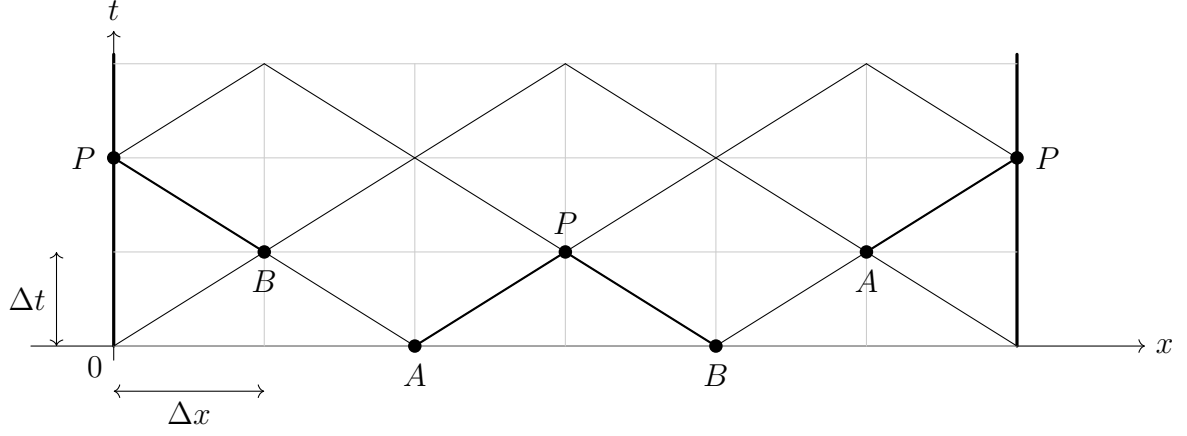


Figure 3.7: Operating principle of numerical integration along the characteristic curves: from point A and B, we compute solution at point P

3.6.3 Results

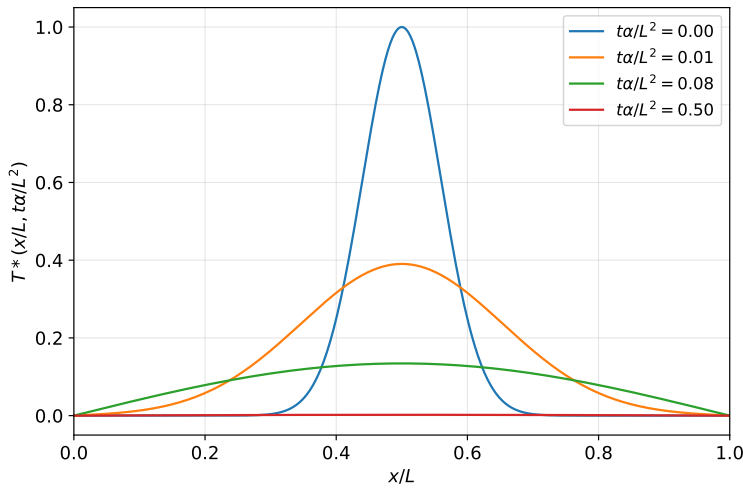
We used the numerical methods aforementioned to compute the temperature field of two test cases with homogeneous Dirichlet and Neumann boundary conditions. The heat flux is also presented, calculated from Fourier's law for the PHE and calculated directly from the scheme for the HHE. We highlight the features of the solution profiles.

Dirichlet test case

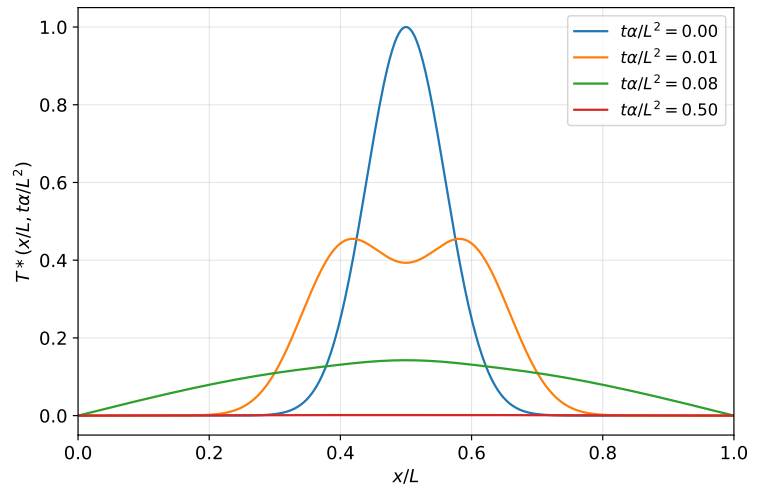
We solve the pulse of the form

$$T(x, 0) = \exp\left(-\frac{(x - x_0)^2}{2\sigma^2}\right) \quad (3.120)$$

with $x_0 = \frac{1}{2}$ and $\sigma = 0.06$. The boundary conditions are set to zero temperature and for the HHE, the initial heat flux is set to zero.



(a) PHE temperature solution for problem (3.120)



(b) HHE temperature solution for problem (3.120)

Figure 3.8: Comparison of the temperature profiles obtained with the parabolic and hyperbolic heat equations for initial condition (3.120), $\varepsilon = 0.008$

The classical heat equation shows the usual diffusive behavior. The steep peak is quickly reduced to a smoother curve. This corresponds to the high oscillating modes that are quickly removed from the series solution. After some time, only the lowest mode is kept, slowly decreasing toward zero value as imposed by the boundary conditions. The hyperbolic heat equation solution is more limited to the center of the domain, due to the finite velocity of propagation. We observe that the initial pulse is divided into two parts going to the left and the right. However after some time, the oscillating modes decayed and we are left with the diffusive part that tends to the same profile as the heat equation. After a sufficiently long time, the solution is zero everywhere as expected.

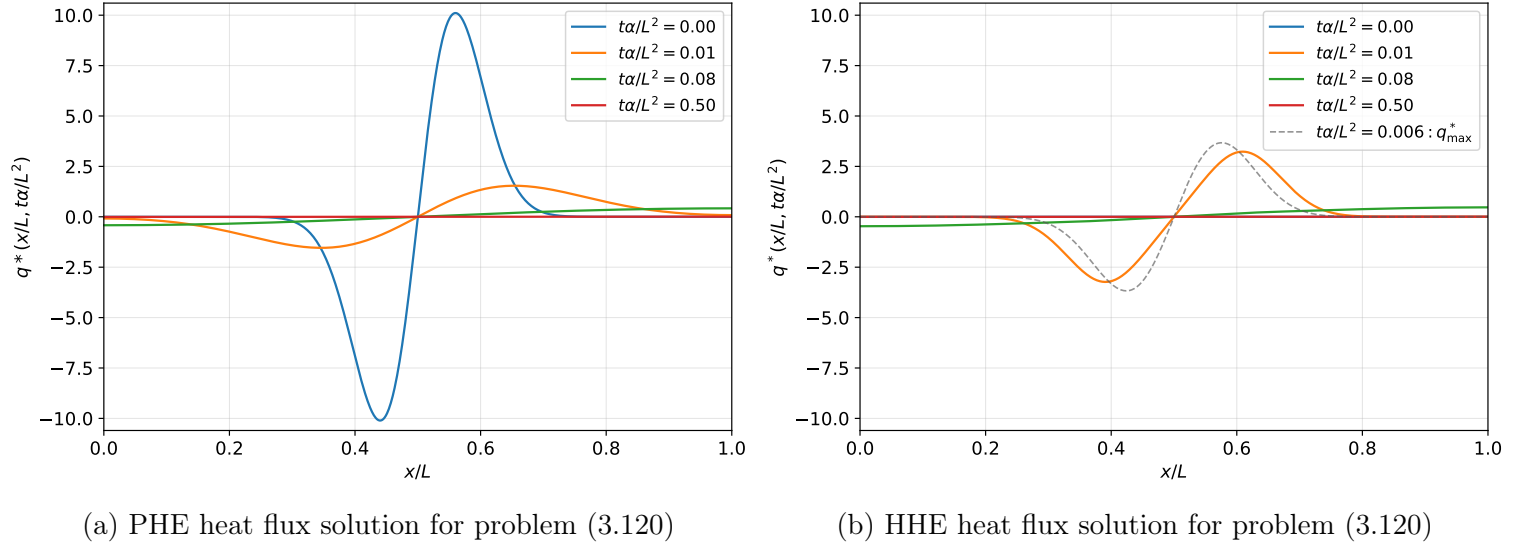


Figure 3.9: Comparison of the heat flux profiles obtained with the parabolic and hyperbolic heat equations for initial condition (3.120), $\varepsilon = 0.008$

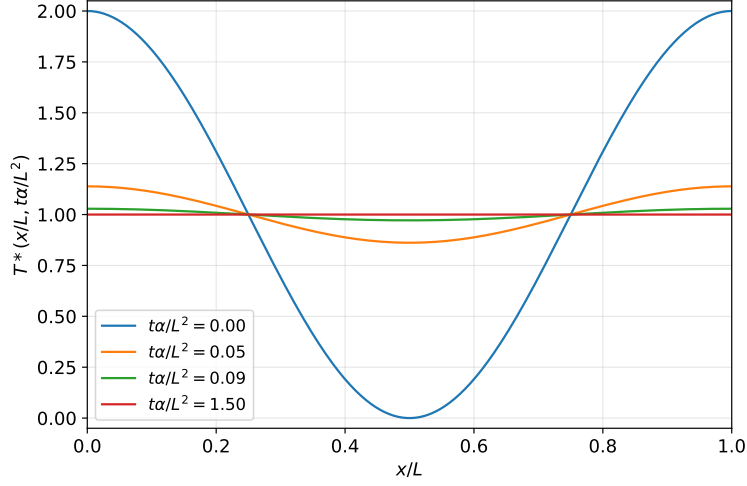
Looking at the heat flux, difference in the constitutive formulations is obvious. At time zero, the PHE shows large heat flux, corresponding to the highest values obtained over time. This also explains the quick decay of the temperature curve. On the contrary, the Cattaneo law leads to zero heat flux at initial time. Then it will grow, but to a lower value than Fourier, and then decrease to values similar to Fourier. The heat flux reflects the fact that the heat flux was zero at initial time, from memory effects, which explains this transitory behavior. We feel the inertia of the heat flux.

Neumann test case

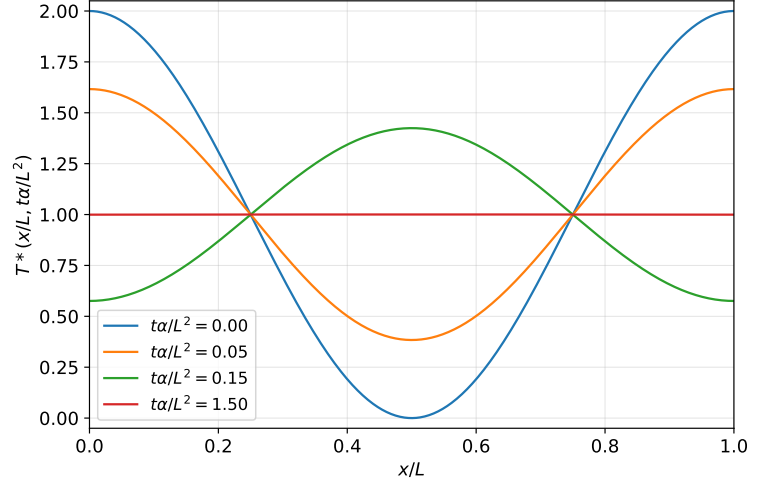
We solve an oscillating function of the form

$$T(x, 0) = 1 + \cos(2\pi x) \quad (3.121)$$

The boundary conditions are set to zero spatial temperature derivative and for the HHE, the initial heat flux is set to zero.



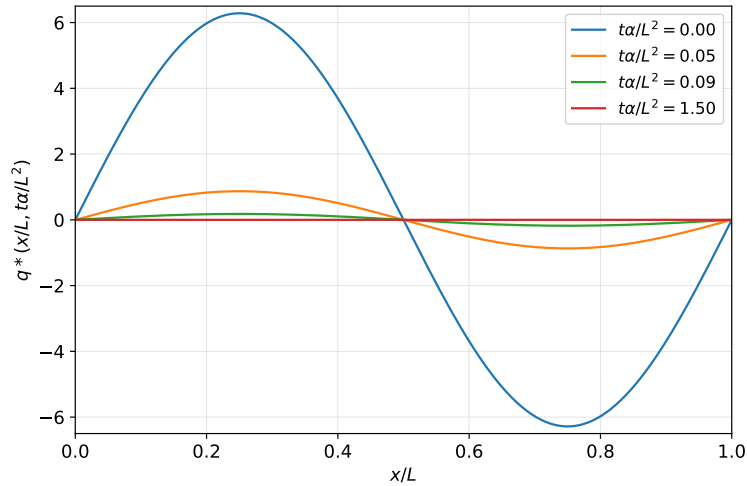
(a) PHE temperature solution for problem (3.121)



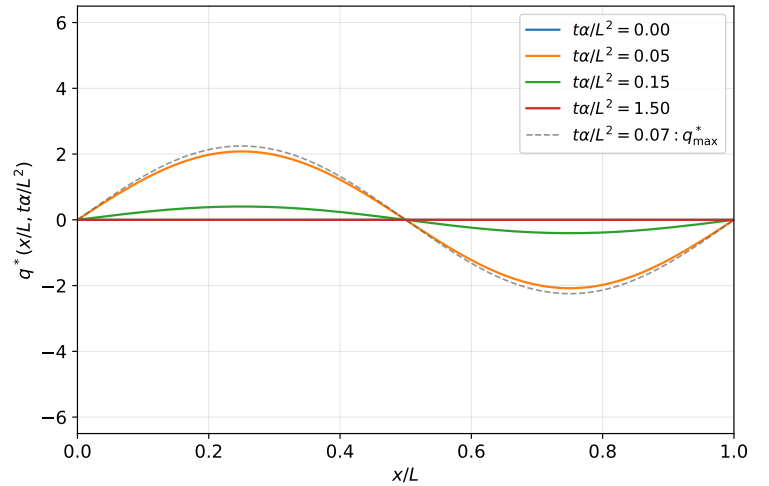
(b) HHe temperature solution for problem (3.121)

Figure 3.10: Comparison of the temperature profiles obtained with the parabolic and hyperbolic heat equations for initial condition (3.121), $\varepsilon = 0.1$

For the PHE, the temperature evolution is diffusive with a quick decrease of the initial condition from the instantaneous establishment of the heat flux. Since the boundaries are isolated, we see that all the heat is well conserved and we tend to a constant nonzero value after some time. For the damped wave heat equation, the decrease in temperature is much slower due to inertia of the heat flux. We observe also a reversal of the curvature of the profile, like an oscillating wire. Such behavior is forbidden with Fourier law, as the minimum should stay a minimum over time and it can't become a maximum. We verify that with isolated boundaries, the HHE conserves well the integral of the initial condition over time.



(a) PHE heat flux solution for problem (3.121)



(b) HHe heat flux solution for problem (3.121)

Figure 3.11: Comparison of the heat flux profiles obtained with the parabolic and hyperbolic heat equations for initial condition (3.121), $\varepsilon = 0.1$

For the heat flux, we also observe the inertia mentioned above. Interesting is the green curve for the PHE. From the temperature profile at this time, we would expect positive

heat flux on the right half of the boundary and negative heat flux on the left part of the boundary. Here, this is not the case, and it shows the memory of the heat flux from previous temperature profiles, causing a delay in the adaptation.

Chapter 4

Application of Cattaneo equation

4.1 Thermokeratoplasty

First addressed in the paper [16] for meat samples with good results, the idea of using a modified version of the heat flux for biological tissues expanded to more practical applications. The justification for using the MCV model does not come from microscopic modeling, such as phonon-phonon collisions, which do not exist in biological tissues. Here we consider the flux equation (3.9) as a postulate for its nice properties with the hope that it could model the complicated heterogeneous structure of the biological material.

We first give some explanation about radiofrequency heating and keratoplasty surgery, then we explain the model presented in [26] [27] and reproduce their analytical results (obtained by laplace transform on the temperature equation) with the numerical method of 3.6. Finally, a more complete explanation of the results is proposed as well as additional comments on the heat flux profiles.

4.1.1 Process explanation

The eye functions as follows: luminous rays reach its surface, and are deviated through the cornea and the crystalline lens to be concentrated on the back of the eye, the retina, where information is then sent to the brain for processing. The eye can undergo many disorders like keratoconus, hyperopia or astigmatism. In the case of hyperopia, the eye is not convergent enough: the cornea is too flat. The rays are sent behind the retina and the vision is blurred.

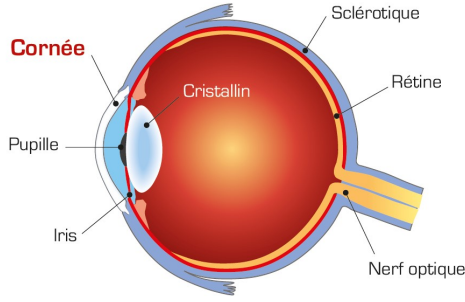


Figure 4.1: Diagram of the human eye

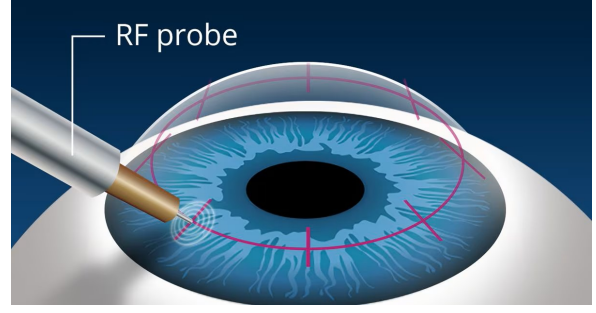


Figure 4.2: Illustration of the probe insertion in the cornea for heating of collagen

Thermokeratoplasty consists in a local heating of the cornea to change its curvature from shrinking of collagen, its main constituent. The conductive keratoplasty is when an electrode is inserted in the cornea and produces local heating by radiofrequency (RF). An alternative voltage of 330-350kHz is applied in the probe to create an oscillating electric field. The resulting displacement of the ions and free charges of collagen will dissipate heat because of the high electrical resistance of collagen and resulting Joule effect. So the probe itself is not warm, it just heats the collagen around. By applying several such local heatings in a circular shape, we can tighten the cornea and give it a more rounded shape. This makes it possible to correct where the rays are focused and recover clear vision. Nevertheless, this operation is very challenging from an engineer point of view. The collagen should be heated between 58 and 76°C, as exceeding this limit may results in damages. The thermally affected zone should also be limited to 300 μ m as the endothelium, closely located, should not be exposed to temperatures exceeding 45°C. In that sense, precise modelling of the intervention and control on the temperature profiles is mandatory to avoid eye damage [28] [29].

4.1.2 Keratoplasty model

The model geometry is as follows: a sphere representing the electrode is totally embedded and in close contact with the cornea, which is considered to fill the whole space, see 4.3.

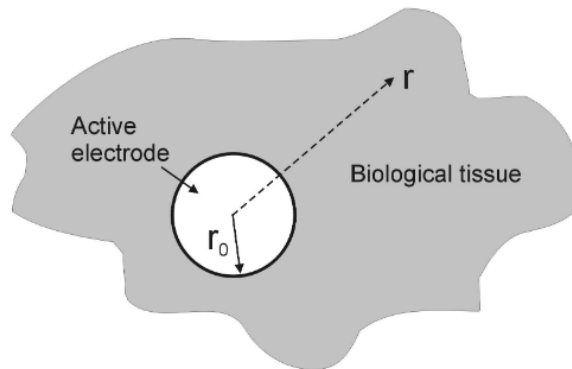


Figure 4.3: Simplified geometry for cornea heating by RF, from [27]

We can thus consider radial symmetry and the problem becomes 1D in the r direction. The governing equations for the hyperbolic model are the conservation of energy and the

heat flux constitutive law (working in spherical coordinates)

$$\begin{aligned}\rho c \frac{\partial T}{\partial t}(r, t) &= -\nabla \cdot (q(r, t) \mathbf{e}_r) + Q(r, t), \quad r \geq r_0, \quad t \geq 0, \\ q(r, t) + \tau \frac{\partial q}{\partial t}(r, t) &= -k \nabla T(r, t), \quad r \geq r_0, \quad t \geq 0.\end{aligned}\tag{4.1}$$

or, expanding the operators in spherical coordinates

$$\begin{aligned}\rho c \frac{\partial T}{\partial t} &= -\frac{\partial q}{\partial r} - \frac{2}{r}q + Q \\ q + \tau \frac{\partial q}{\partial t} &= -k \frac{\partial T}{\partial r}\end{aligned}\tag{4.2}$$

where

$$Q(r, t) = \frac{Pr_0}{4\pi r^4}\tag{4.3}$$

is the volumetric heat source from the probe generating radiofrequency heating, r_0 is the radius of the sphere embedded in the cornea (see 4.3) and P the total applied power.

The limit conditions are

$$\begin{cases} T(r, 0) = T_0, \\ q(r, 0) = 0, \\ T(\infty, t) = T_0, \\ q(r_0, t) = -\frac{\rho_0 c_0 r_0}{3} \frac{\partial T}{\partial t}(r_0, t). \end{cases}\tag{4.4}$$

where the boundary condition on the surface of the spherical probe comes from the fact that in the sphere, the conservation of energy is

$$\rho_0 c_0 \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{q}\tag{4.5}$$

where the subscript 0 refers to the physical parameters of the probe, and integration over the volume of the sphere gives

$$\rho_0 c_0 \frac{4}{3} \pi r_0^3 \frac{\partial T}{\partial t} = -4\pi r_0^2 \mathbf{q} \cdot \mathbf{e}_r\tag{4.6}$$

where we used Green-Ostrogradsky theorem and the fact that the sphere is small with high conductivity, resulting in approximately constant temperature inside. This condition simply means that the heat flux at the probe boundary is used to heat the probe. This corresponds well to one of the interests of using inserted probes rather than surface probes: part of the heat generated at the tip of the electrode is removed along the high conductivity metal part of the needle form, thus protecting the endothelium.

The associated PHE system is straightforward. We simply set τ to zero in (4.2), the initial condition on the heat flux is removed from (4.4) and the left boundary condition can be modified by substituting q using Fourier's law.

Table 4.1: Physical parameters involved in the thermokeratoplasty

Parameter	Symbol	Value	Unit
Corneal density	ρ	1060	kg m^{-3}
Corneal specific heat	c	3830	$\text{J kg}^{-1} \text{K}^{-1}$
Corneal thermal conductivity	k	0.556	$\text{W m}^{-1} \text{K}^{-1}$
Thermal relaxation time	τ	0.1	s
Probe density	ρ_0	21.5×10^3	kg m^{-3}
Probe specific heat	c_0	132	$\text{J kg}^{-1} \text{K}^{-1}$
Probe thermal conductivity	k_0	71	$\text{W m}^{-1} \text{K}^{-1}$
Probe radius	r_0	45	μm
Applied power	P	30	mW

All the physical values are summarized in table 4.1. It should be noted that the value for the relaxation time was guessed from existing data on biological tissues, and not computed precisely. Also, the power is typically one order of magnitude higher for the electrodes employed clinically but for the simplified geometry it was reduced here. The radius of the probe and its physical parameters correspond to platinum-iridium material.

4.1.3 Solution profiles

For the numerical resolution of (4.2) with conditions (4.4), we first put the system in dimensionless form with (3.13), then we develop the method of characteristics to obtain compatibility relations similar to (3.17) and (3.18). We can then integrate numerically these differential equations to obtain the solution. Since all the steps were already explained in detail in previous sections and the present model is very similar, we directly show the results for the sake of brevity.

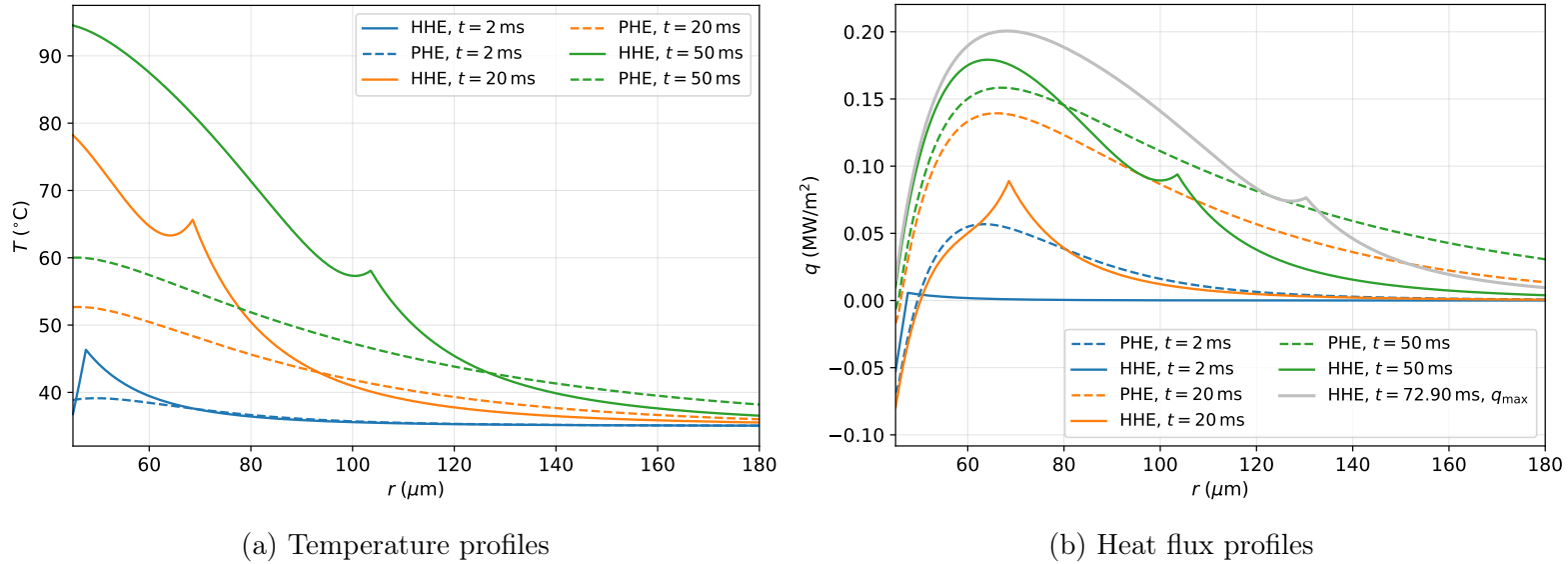


Figure 4.4: Solution profiles for the keratoplasty model, short times

The analysis of the results is interesting because both the source term and the heating of the electrode play an important role in the solutions dynamic. We see that just after

starting the heating, the PHE solution is smooth with a high heat flux toward the electrode and nonzero heat flux everywhere. Then the temperature grows from the RF heating with always the highest value at the left boundary, where the source term is the most important. The temperature and heat flux dynamics from the HHE totally differ. Since the heat flux is limited from memory of the zero initial value, the heat flux toward the electrode is limited, as well as the temperature increase at this point from the last condition in (4.4) which acts like a brake. This will result in a peak form that will propagate in the cornea over time. The velocity corresponds to propagation along the characteristics. After some time the flux has relaxed and we observe a high increase of temperature, far exceeding the temperature of the PHE at the boundary. From the limitation of propagation speed, the heat is more contained and the temperatures are much higher. The heat flux is limited and heat cannot flow toward larger distances. While looking further on the radial axis, we see that the PHE temperature is higher than that of the HHE. The heat flux of the HHE will finally exceed that of the PHE, resulting then in a decrease of temperature.

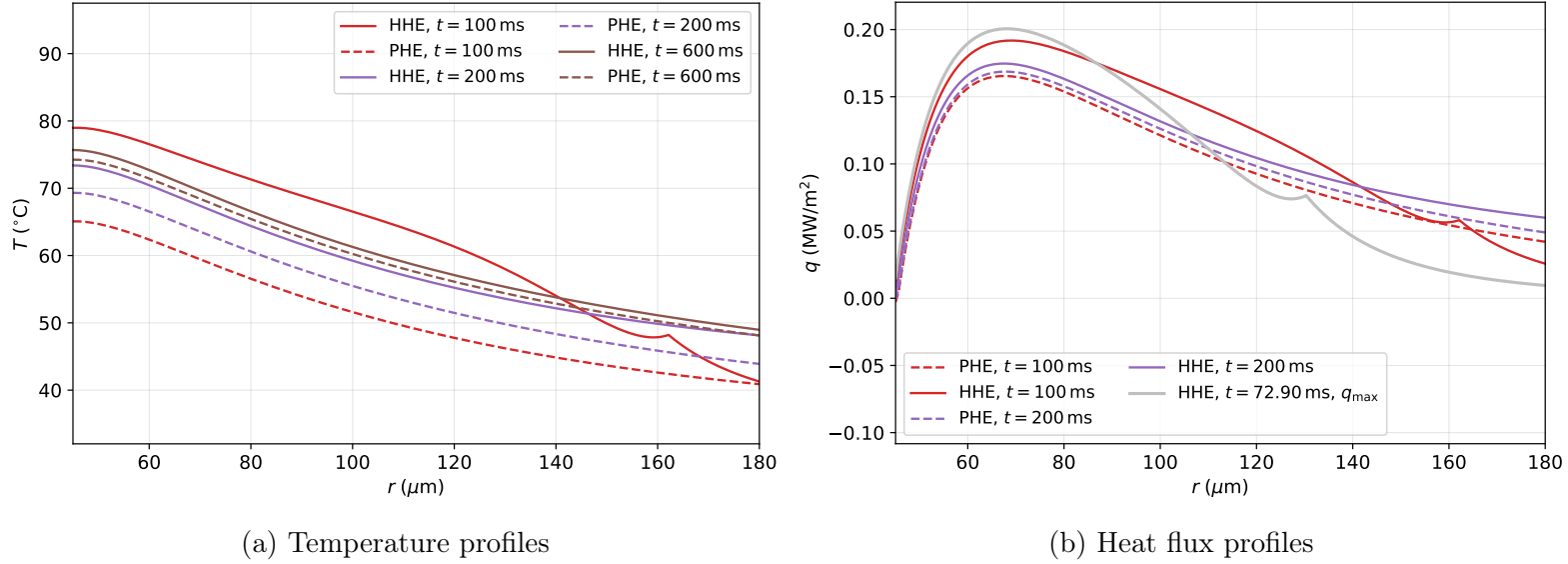


Figure 4.5: Solution profiles for the keratoplasty model, long times

As the high temperature gradients become more important in the memory kernel of heat flux, the heat flows toward external regions: the temperature close to the electrode decreases, and the temperature far away increases. Between 200ms and 600ms we observe a re-increase of the temperature. The underdamped modes will finally give way to a diffusive behavior around $t = 0.6s = 6\tau$. The classical heat equation doesn't show this oscillating behavior, with a regular increase in the temperature everywhere. We also note that the maximum heat flux from the HHE exceeded that of the PHE.

Remarks

In view of the temperature constraints for the thermokeratoplasty to avoid damage of the cornea, it is clear that the choice of the model is important. The HHE will result in much higher temperatures than the PHE. In the present study, there is a real lack of experimental data for comparing results with real temperature evolution to assess which model is better. Also, experiments or models should be developed to work with more accurate values for the parameter τ .

Chapter 5

Other models for non-Fourier heat conduction

5.1 Models using fractional derivatives

Another category of models is those using fractional derivatives. This allows memory effects to be presented and is widely used for non-standard structure like polymers, porous materials or composite materials. It can also be used for short-time laser pulse heat transfer modeling. We introduce the basics of fractional calculus and present the time-fractional Cattaneo law, its associated heat equation and resulting temperature profiles.

5.1.1 Fractional calculus

We know the usual differentiation and integration operators

$$(Df)(x) = \frac{d}{dx}f(x) \quad (If)(x) = \int_0^x f(s) ds \quad (5.1)$$

and we can easily define the composition of these operators

$$D^n(f) = (D \circ D \cdots \circ D)(f) \quad (5.2)$$

leading to integer-order differentiation or integration.

The question of fractional calculus is to generalize this notion to real- or complex-order differentiation or integration. For the integration, it can be introduced using Cauchy's formula for repeated integration

$$(I^n f)(x) = \frac{1}{(n-1)!} \int_0^x (x-s)^{n-1} f(s) ds \quad (5.3)$$

Using the gamma function for the generalization of the factorial, we can define an intuitive notion of real-order integration by

$$(I^p f)(x) = \frac{1}{\Gamma(p)} \int_0^x (x-s)^{p-1} f(s) ds \quad (5.4)$$

For the real-order differentiation, as many definitions are possible with different properties, the name of the formula should be specified. We give two definitions, the Caputo derivative

is

$$({}_a D_x^p f)(x) = \left({}_a I_x^{n-p} \left(\frac{d^n f}{dx^n} \right) \right) (x) = \frac{1}{\Gamma(n-p)} \int_a^x (x-s)^{n-p-1} f^{(n)}(s) ds \quad (5.5)$$

where $n = \lceil p \rceil$. It can be interpreted as first differentiating n times with n the closest integer above p . Then we correct the too high derivative with real value integration defined above. The advantage of this formula is that the fractional derivative of a constant is zero. We can also interpret formula (5.5) as power-law kernel looking over all the past values of the derivative with increasing importance for recent values.

Another definition is the Grünwald-Letnikov formula

$$({}_a D_x^\alpha f)(x) = \lim_{h \rightarrow 0^+} \frac{1}{h^\alpha} \sum_{r=0}^{\lfloor \frac{x-a}{h} \rfloor} (-1)^r \binom{\alpha}{r} f(x - rh). \quad (5.6)$$

This comes from a general form of the differential definition in integer calculus. This formula is very suitable for numerical methods [30] [31].

5.1.2 Fractional Cattaneo law

Now we introduce the fractional generalization of the MCV law (3.6) as presented in [32]

$$\tau^p {}_0 D_t^p q + q = -k \frac{\partial T}{\partial x} \quad 0 < p < 1 \quad (5.7)$$

where τ^p is such that dimensions are respected and ${}_0 D_t^p$ denotes the Caputo fractional derivative.

Combining this with the local conservation of energy results in

$${}_0 D_t^{1+p} T + \frac{1}{\tau^p} \frac{\partial T}{\partial t} = \frac{\alpha}{\tau^p} \frac{\partial^2 T}{\partial x^2} \quad (5.8)$$

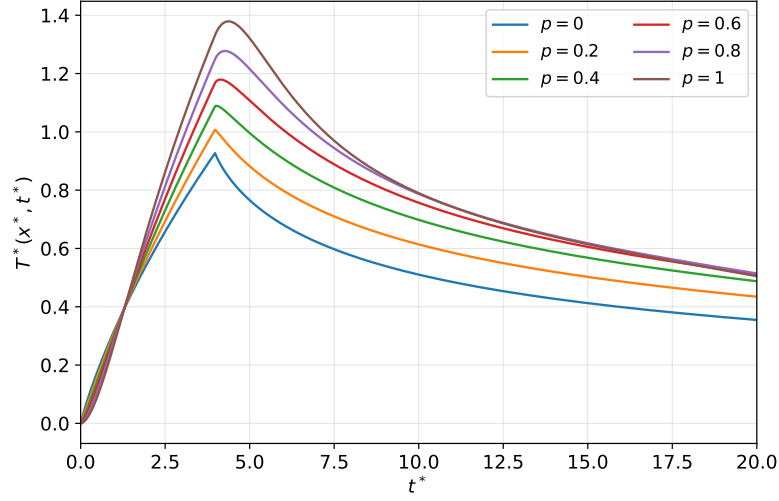
and we see that as $\tau \rightarrow 0$ we recover the PHE and as $p \rightarrow 1$ we recover the HHE. The fractional derivative allows us to introduce intermediate models.

To illustrate this heat equation, we present the case tackled in [32]. We consider a short-time laser pulse and we look at the temperature profiles in the material (in the direction of the pulse). The pulse is modeled as a source term, resulting in the system

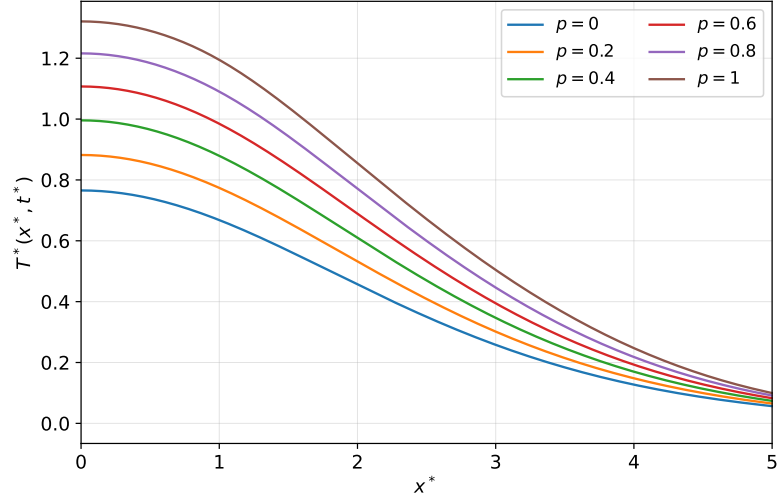
$$\left\{ \begin{array}{l} {}_0 D_t^{1+p} T + \frac{1}{\tau^p} \frac{\partial T}{\partial t} = \frac{\alpha}{\tau^p} \frac{\partial^2 T}{\partial x^2} + \frac{\alpha I_1 \delta}{k \tau^p} f(t) g(x), \\ T(x, 0) = 0, \\ \frac{\partial T}{\partial t}(x, 0) = 0, \\ T(\infty, t) = 0, \\ \frac{\partial T}{\partial x}(0, t) = 0. \end{array} \right. \quad (5.9)$$

where $I_1 = (1 - r_f) I_0$ with r_f the reflection coefficient, I_0 the power intensity of the laser pulse, δ the absorption coefficient, $f(t) = H(t) - H(t - t_d)$ with t_d the pulse duration, and $g(x) = e^{-\delta x}$.

We can then define dimensionless variables similar to (3.13) but using δ^{-1} as length scale and then solve the system for different parameters p . The presented results are for $t_d = 4$.



(a) Temperature evolution at $x^* = 0$ for values of p . $\tau = 1$



(b) Temperature evolution over x^* for $t^* = 5$ and $\tau = 1$

We see that for larger values of p , the temperature at the surface increases more, with the highest values for the HHE. We also see that for higher values of p , the drop in temperature when the pulse stops is steeper, from the high temperature gradients kept in memory. The temperature profiles along the depth are also given.

We observe from these plots that intermediate propagation speeds are proposed by the fractional heat equations. This new parameter p , with parameter τ^p , gives us more flexibility on the fitting of experimental data for propagation in heterogeneous media or laser-pulse applications. The fractional derivative has a wide range of applications and is a subject of research today.

Chapter 6

Conclusion

In this manuscript, the subject of Non-Fourier heat conduction was addressed. We first tried to give some context and historical milestones for the emergence of this field. The motivation for the search for new models beyond Fourier heat law was exposed. Then a deeper understanding of the Maxwell-Cattaneo-Vernotte law was proposed. The correction of the infinite speed of propagation was explained as well as subjects such as propagation of discontinuities, modal analysis, variational framework and numerical schemes. The aim of that chapter was to help build intuition about this new model and to give some related tools, like the finite sum approximation, the Lagrangian formulation or suitable numerical methods. The example of thermokeratoplasty was then worked out in detail. The model was presented and temperature fields with heat flux profiles were then obtained. The differences from the parabolic heat equation and hyperbolic heat equations were explained, with great differences in the temperature profiles justified by memory effects of the Maxwell-Cattaneo-Vernotte law. In the last chapter another step toward the large field of non-Fourier heat conduction is made with a short introduction to fractional models and laser-pulse applications. This presents a next direction that one could take to continue on the subject of heat modeling where Fourier's law is unable to explain the physics.

For future research, it could also be interesting to see if the transition from a parabolic equation with infinite speed of propagation for a physical quantity to a hyperbolic equation with a finite speed could be addressed in other fields than heat transfer. Parabolic equations are everywhere in physics; for example, one can consider momentum diffusion in hydrodynamics, and one may ask if the associated infinite speed of propagation is not an issue in some cases. This would certainly be an interesting topic to study and explore.

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Statement on the use of support tools

During the preparation of this work, support tools, including artificial intelligence tools, were used. The help from AI was limited to searching for information, understanding new concepts, helping with coding and correcting spelling. The present manuscript is my own writing and the content is always supported by sources that I read.

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