

3D hydrodynamic analysis of Cepheid star pulsations

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3D Hydrodynamic Analysis of Cepheid Star Pulsations

Under the supervision of

Prof. Marc-Antoine Dupret

Master's thesis submitted in fulfilment of the requirements for the
Master of Science in Engineering Physics

by

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Abstract

Asteroseismology is a rapidly growing field dedicated to the study of stellar pulsations. Among the various classes of pulsating stars, Cepheids occupy a particularly important place owing to their astrophysical significance. At the same time, one of the major challenges in stellar physics remains the modelling of turbulent convection. Consequently, understanding the interaction between convection and pulsations in Cepheid stars is an important and still largely unresolved problem.

This thesis presents a comprehensive analysis of this interaction through the study of a high-resolution three-dimensional numerical simulation of a Cepheid convective envelope exhibiting self-excited pulsations. Particular emphasis is placed on identifying and understanding the physical mechanisms responsible for driving these pulsations.

The analysis begins with an examination of the radial profiles of the main thermodynamic quantities, together with a study of the horizontal structure of the flow. This first investigation reveals a strongly asymmetric convective pattern, characterised by narrow, intense downflows surrounded by broader and smoother upflows. Such an asymmetry limits the relevance of horizontally averaged radial profiles, as they combine regions exhibiting very different behaviours.

To overcome this limitation, the flow is separated into upflow and downflow regions and analysed independently. This decomposition highlights a clear dominant role of the downflows in the transport of convective energy.

The thermodynamic cycle associated with the pulsations is then investigated through the study of the work of oscillation and of the heat exchanges occurring during the pulsation cycle. While the work diagram does not allow any firm conclusion to be drawn, the analysis of the heat supply demonstrates the existence of heat gains during the hot phase and heat losses during the cold phase, resulting in a driving thermodynamic cycle. This behaviour is driven by the downflows, which are more numerous during the hot phase as a consequence of the stronger convective instability and enhanced turbulence. Concerning the upflows, signatures of the classical κ -mechanism can be identified, but its contribution is completely dominated by other processes.

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Nomenclature

Acronyms

Acronym	Definition
CLÉS	Code Liégeois d'Évolution Stellaire
CO5BOLD	Conservative Code for the Computation of Compressible Convection in a Box of L Dimensions
DNS	Direct Numerical Simulation
HR	Hertzsprung-Russell
LES	Large Eddy Simulation
MLT	Mixing-Length Theory
RANS	Reynolds-Averaged Navier-Stokes

Latin Symbols

Symbol	Definition	CGS Unit
a	Radiation constant	$\text{erg cm}^{-3} \text{K}^{-4}$
c	Speed of light	cm s^{-1}
c_p	Specific heat at constant pressure	$\text{erg g}^{-1} \text{K}^{-1}$
c_v	Specific heat at constant volume	$\text{erg g}^{-1} \text{K}^{-1}$
dW	Work per unit mass	erg g^{-1}
Dq/Dt	Calorific exchanges	Same as q
e_{tot}	Specific energy of the gas	erg g^{-1}
E_{box}	Total energy of the box	erg
E_{conv}	Turbulent kinetic energy of the box	erg
E_i	Total internal energy of the box	erg
E_{kin}	Total kinetic energy of the box	erg
E_m	Energy of the mode	erg
E_{puls}	Pulsational kinetic energy of the box	erg
F	Radial energy flux	$\text{erg cm}^{-2} \text{s}^{-1}$
$\mathbf{F}$	Vector energy flux	$\text{erg cm}^{-2} \text{s}^{-1}$
F_{conv}	Convective flux	$\text{erg cm}^{-2} \text{s}^{-1}$
F_{rad}	Radiative flux	$\text{erg cm}^{-2} \text{s}^{-1}$
f_{buoy}	Archimedes force per unit volume	dyn cm^{-3}
G	Gravitational constant	$\text{cm}^3 \text{g}^{-1} \text{s}^{-2}$

g	Gravity	cm s^{-2}
h	Specific enthalpy	erg g^{-1}
H_P	Pressure scale height	cm
I	Radiation intensity	$\text{erg cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1}$
k_B	Boltzmann constant	erg K^{-1}
L	Luminosity	erg s^{-1}
L_r	Radiative luminosity	erg s^{-1}
l_{conv}	Mixing length	cm
ℓ	Photon mean free path	cm
m, m_b	Mass functions	g
M	Total mass	g
m_u	Atomic mass unit	g
P	Pressure	dyn cm^{-2}
q	Generic physical quantity	Variable
R	Total radius	cm
r	Radial coordinate	cm
$\mathbf{r}$	Radial position vector	cm
R_g	Universal gas constant	$\text{erg mol}^{-1} \text{ K}^{-1}$
s	Specific entropy	$\text{erg g}^{-1} \text{ K}^{-1}$
S	Surface	cm^2
S_I	Source function	$\text{erg cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1}$
t	Time	s
T	Temperature	K
T_{eff}	Effective temperature	K
u	Specific internal energy	erg g^{-1}
v	Specific volume	$\text{cm}^3 \text{ g}^{-1}$
$\mathbf{v}$	Velocity vector	cm s^{-1}
v_{conv}	Characteristic convective velocity	cm s^{-1}
v_r	Radial velocity	cm s^{-1}
$v_{z,\rho}$	Mass-weighted radial velocity	cm s^{-1}
V	Volume	cm^3
W	Work	erg
x, y, z	Cartesian coordinates	cm
z_0	Lagrangian radius coordinate	cm

Greek Symbols

Symbol	Definition	CGS Unit
α	Thermal expansion coefficient	K^{-1}
α_{conv}	Mixing-length parameter	—
χ	Thermal diffusivity	$\text{cm}^2 \text{ s}^{-1}$
δ	Expansion coefficient	—
ε_g	Gravitational energy generation rate	$\text{erg g}^{-1} \text{ s}^{-1}$

ε_n	Nuclear energy generation rate	$\text{erg g}^{-1} \text{ s}^{-1}$
η	Growth rate	s^{-1}
Γ_1	First adiabatic exponent	—
Γ_3	Third adiabatic exponent	—
κ	Rosseland mean opacity	$\text{cm}^2 \text{ g}^{-1}$
κ_λ	Monochromatic opacity	$\text{cm}^2 \text{ g}^{-1}$
κ_T, κ_ρ	Sensitivity coefficients of the opacity	—
λ	Photon wavelength	cm
μ	Mean molecular weight	—
∇	Real temperature gradient	—
∇_{ad}	Adiabatic temperature gradient	—
∇_{rad}	Radiative temperature gradient	—
∇_e	Temperature gradient of a convective element	—
ν	Kinematic viscosity	$\text{cm}^2 \text{ s}^{-1}$
Ω	Solid angle	sr
ω	Angular pulsation frequency	s^{-1}
ϕ	Phase shift	rad
ψ	Gravitational potential	erg g^{-1}
ρ	Density	g cm^{-3}
σ	Complex eigenfrequency	s^{-1}
σ_B	Stefan-Boltzmann constant	$\text{erg cm}^{-2} \text{ s}^{-1} \text{ K}^{-4}$
τ	Optical depth	—
τ_{conv}	Convective timescale	s
τ_{diff}	Thermal diffusion timescale	s
τ_{dyn}	Dynamical timescale	s
τ_{th}	Thermal relaxation time	s
θ	Polar angle	rad

Perturbations and Operators

Symbol	Definition	CGS Unit
d/d	Derivative operator	—
$\partial/\partial t$	Eulerian time derivative	s^{-1}
D/Dt	Lagrangian (material) derivative	s^{-1}
∇	Gradient operator	—
$\nabla \cdot$	Divergence operator	—
$'$	Eulerian perturbation	Same as variable
δ	Lagrangian perturbation	Same as variable
δ_{rel}	Relative Lagrangian perturbation	—
Δ	Horizontal/spatial fluctuation operator	Same as variable
Δ_{rel}	Relative horizontal/spatial fluctuation	—
$\langle \rangle$	Horizontal/spatial average	—
—	Time average	—

Chapter 1

Introduction

1.1 Context and motivations

Asteroseismology is a growing branch of stellar physics that aims to understand the internal structure of stars through the study of their oscillations. These pulsations provide a unique probe of stellar interiors and offer valuable constraints on the physical processes governing stellar structure and evolution. This kind of oscillation is observed in a variety of pulsating stars, which constitute an important class of objects in stellar astrophysics. Among them, Cepheid variables represent one of the most prominent and historically significant types of pulsating stars.

Alongside pulsations, energy transport plays a fundamental role in modelling the internal structure of stars and their evolution. While radiative transport is relatively well understood and can be described with a high degree of accuracy, convection remains one of the major challenges of stellar physics due to its intrinsically nonlinear and turbulent nature.

In this context, the interaction between convection and pulsations represents an even more complex problem. While significant progress has been made in the study of each phenomenon separately, many aspects of their coupling remain poorly understood. Understanding this interaction is one of the key challenges in modern stellar physics.

Over the past three decades, three-dimensional hydrodynamical simulations have emerged as a powerful tool for investigating stellar convection. They have significantly improved the understanding of turbulent flows in stellar interiors and provide a much more realistic description than traditional one-dimensional models. Recent advances in computational capabilities now allow simulations at increasingly high resolutions, opening new perspectives for the study of stellar dynamics. In particular, the application of such simulations to pulsating stars remains largely unexplored. At the same time, they remain computationally demanding and numerically challenging because of the extreme physical conditions encountered in stars.

1.2 Objectives

This study aims to provide a comprehensive analysis of a high-resolution three-dimensional numerical simulation of a self-excited Cepheid envelope. Particular emphasis is placed on the

detailed description of convective motions and, more importantly, on the identification and understanding of the underlying physical mechanisms that drive these stellar pulsations.

This work is of a preliminary nature and is not intended for direct comparison with observational constraints, owing to several intrinsic limitations that will be addressed later. It however provides a particularly insightful first step towards understanding the complex convection-pulsation dynamics.

1.3 Study overview

The first part of this work is devoted to the theoretical background required to properly understand this study. It includes a general presentation of the astrophysical context as well as a detailed description, both in physical and mathematical terms, of the basic equations of stellar structure. It also presents several simplified models that will be used for comparison with the results, in particular for convection and pulsations.

The second part presents the numerical framework used to conduct this study. It includes a detailed description of the analysed simulation and the presentation of the code used to perform it, as well as an overview of other codes used for comparison.

Finally, the third part constitutes the main part of this work, in which a comprehensive analysis of the simulation is performed. After some necessary preliminary considerations, it provides an overview of the simulation before presenting a first analysis of basic quantities. It then moves on to a more detailed study of the convective flow before concluding with an analysis of the thermodynamic cycle and the associated physical mechanisms responsible for stellar pulsations.

Chapter 2

Theoretical framework for Cepheid variables

This chapter aims to provide a complete physical and mathematical description of Cepheid variables. It begins by presenting them in a general context and highlighting the conditions under which they exist. Subsequently, the main equations governing stellar structure are introduced. The important question of energy transport is then addressed, with particular emphasis on convection, as it plays a key role in this work. Finally, the theory of stellar pulsations is presented.

This chapter provides the necessary foundation for the remainder of this work, both in terms of the equations used in the codes presented in Ch. 3 and the physical understanding required to interpret the results in Ch. 4. It also introduces key concepts that will be used throughout.

2.1 General presentation

In astrophysics, Cepheid variables, more commonly referred to as Cepheids, denote a specific class of pulsating variable stars characterised by regular variations in luminosity caused by radial oscillations of their outer layers. The term Cepheid does not refer to a permanent stellar classification but only to a transient evolutionary phase during which the star exhibits this type of pulsational behaviour. The existence of this type of star is thus strictly defined by its position within the Hertzsprung–Russell (HR) diagram, shown in Fig. 2.1, which constitutes the fundamental framework used to classify stars according to their luminosity and surface temperature. Within this diagram, Cepheids occupy a specific region known as the instability strip. This narrow, nearly diagonal region corresponds to stellar parameters for which the physical conditions lead the outer envelope to behave as a heat engine driving pulsations.

On a concrete physical level, Cepheids are massive objects, typically ranging from 4 to 20 solar masses, with radii that extend to dozens or even hundreds of times that of the Sun. Their most striking characteristic is their high luminosity, which can reach up to 10^5 times that of the Sun. Their pulsational behaviour is characterised by regular radial oscillations, with typical periods ranging from about 1 to 50 days.

As for every star, its life begins with the gravitational contraction of a molecular gas cloud, leading to the formation of a protostar. This contraction results in a continuous increase in temperature and pressure within the stellar interior. At a critical stage, these conditions become

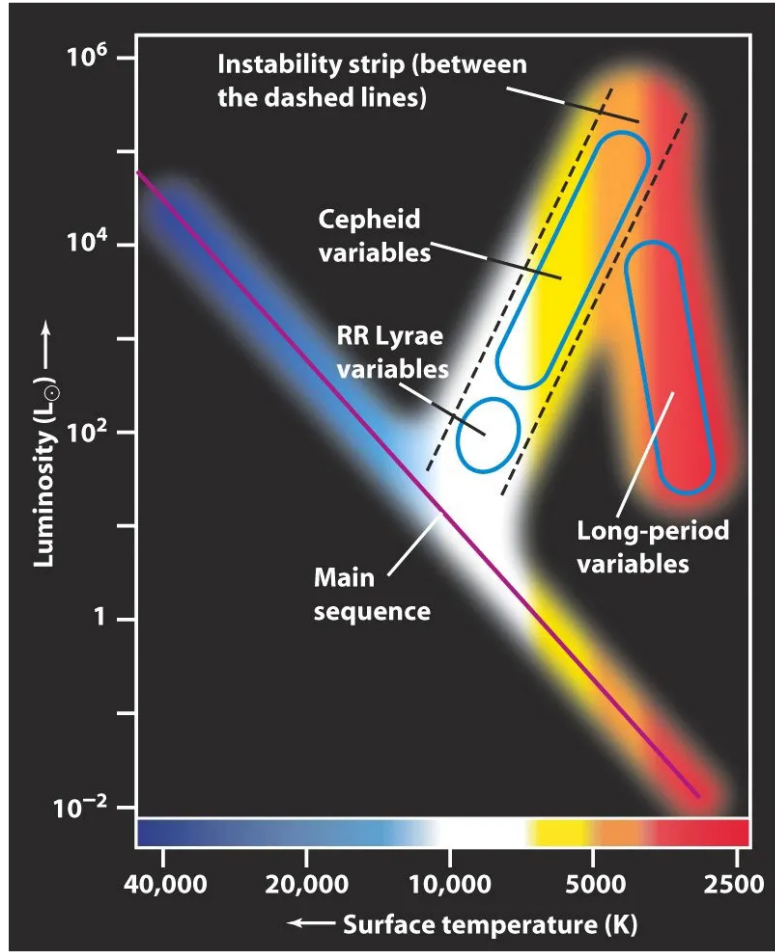


Figure 2.1: Hertzsprung-Russell diagram showing the classification of stars in terms of luminosity (in solar units $L_{\odot}$) and surface temperature. The main sequence is also indicated. The instability strip, where Cepheid variables are located, is clearly highlighted. Credit: Portland Community College.

sufficient to ignite hydrogen nuclear fusion in the core, marking the beginning of the main sequence. For Cepheid-mass stars, the core is convective during this phase, which induces efficient mixing and leads to a more extended convective core. The main sequence constitutes the longest and most stable stage of stellar evolution, during which the hydrogen is burnt in its core. When all this hydrogen in the core is exhausted, the absence of nuclear reactions causes the core to contract under gravity. At the same time, hydrogen shell burning in the surrounding layers continues to release energy. This energy output drives the expansion and cooling of the outer envelope. The star then moves across the Hertzsprung–Russell diagram on a relatively short timescale, from left to right [1]. It is during this post-main-sequence evolution that the star may cross the instability strip and potentially become a Cepheid. The typical structure of a Cepheid during this phase is illustrated in Fig. 2.2.

Note that a Cepheid stage can be reached more than once during a star’s later evolutionary phases, as it may cross the instability strip again at more advanced stages. In any case, this work focuses on the stellar envelope, so the results are not sensitive to the exact evolutionary stage of the star. This comes from the fact that the core and the envelope evolve in a largely decoupled way, while the pulsational behaviour is almost entirely controlled by the envelope structure.

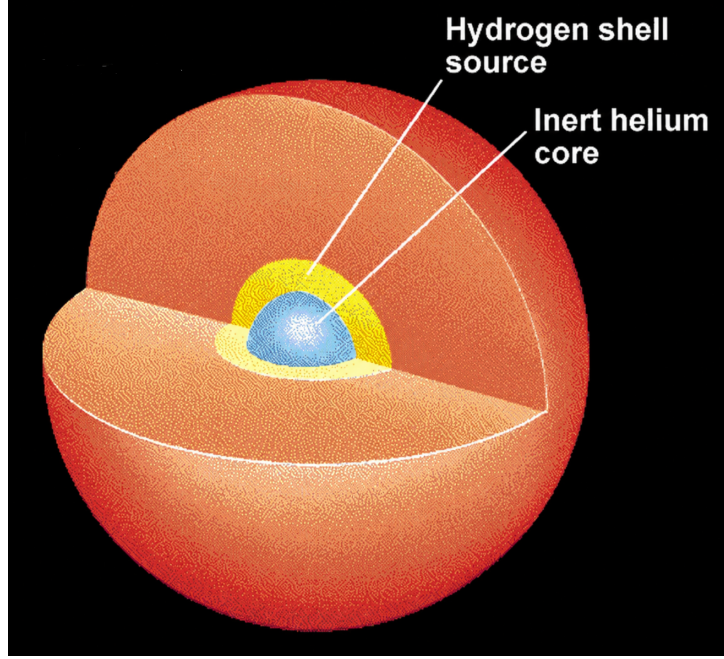


Figure 2.2: Typical structure of a Cepheid during its first crossing of the instability strip. Its interior consists of an inert helium core surrounded by a hydrogen-burning shell, while the envelope is predominantly composed of hydrogen. Diagram adapted from Ref. [2].

Historically, Cepheids have played a central role in the development of modern astrophysics and cosmology. Their systematic study began in the early 20th century with the discovery of the period–luminosity relation by Henrietta Swan Leavitt, which established a direct correlation between the pulsation period and the intrinsic luminosity of these stars [3]. This property allows Cepheids to be used as standard candles since their intrinsic brightness can be inferred from the observed period and thus compared to the apparent brightness to determine distances. This relation was later used by Edwin Hubble to measure extragalactic distances and to show that Cepheids observed in external systems are located at distances far greater than the size of the Milky Way, thereby demonstrating that these objects belong to entirely separate galaxies [4]. As a consequence, Cepheids became a cornerstone of the cosmic distance ladder and remain a key reference for distance calibration, although they are now complemented by other independent techniques [5].

2.2 General equations

Describing the physics of stars rigorously requires adopting a robust mathematical framework. Indeed, stars are complex systems consisting of a self-gravitating gas governed by a wide range of interacting physical processes, but their global behaviour can still be described using a set of basic physical principles. The stellar evolution formulas presented in this section are derived from Refs. [6–8].

2.2.1 Eulerian vs Lagrangian description

Before describing the equations used to model the star behaviour, it is necessary to recall the two ways in which the fluid can be described within the star: the Eulerian and the Lagrangian

descriptions.

The first approach is the Eulerian description. It focuses on observing the fluid at fixed positions in space and describing how physical quantities evolve at these points over time. In this framework, the reference frame is fixed in space and does not move with the fluid. For any quantity q , its Eulerian time variation is given by the partial derivative with respect to time at a fixed position:

$$\frac{\partial q}{\partial t}, \quad (2.1)$$

where the operator $\frac{\partial}{\partial t}$ is thus called the Eulerian time derivative.

The second approach is the Lagrangian description. It focuses on describing the fluid by following the motion of individual fluid particles. Each particle is tracked as it moves through space and time, and its position and properties are described along its trajectory. In this formulation the evolution of the fluid is described from the point of view of the moving particles rather than from a fixed point in space. In this description, the time variation of a quantity q is given by

$$\frac{Dq}{Dt} = \frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q, \quad (2.2)$$

with $\mathbf{v}$ the velocity vector field. The operator $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$ is thus called the Lagrangian (or material) derivative [9].

This second description will be particularly convenient in this work, as it will be necessary to express changes within the star while taking pulsations into account and while remaining at the same relative position inside the star. This will be discussed in more detail later.

2.2.2 Continuity equation

The first main equation used to model stars is the well-known continuity equation from continuum mechanics. It expresses the conservation of mass in any arbitrary control volume of a continuous medium. It can be expressed in both Eulerian and Lagrangian descriptions as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0, \quad (2.3)$$

where ρ is the density of the fluid.

Consider now a simplified model of a star, in which the star is assumed to be non-rotating and perfectly spherically symmetric, so that every quantity can only depend on the radial coordinate r . Hydrostatic equilibrium is also assumed, meaning that the net force acting on each fluid element vanishes. In this framework, the radial structure is time-independent so that the position of each stellar layer does not change in time. Any variation of the stellar radius would modify the internal structure and therefore break the equilibrium condition. This naturally excludes pulsations from the present description.

Under these assumptions, one can define the mass function m as

$$m = \int_0^r 4\pi r'^2 \rho dr'. \quad (2.4)$$

This function thus represents the mass enclosed within a sphere of radius r and the total mass M of the star is therefore linked to the total radius R by

$$M = \int_0^R 4\pi r'^2 \rho dr'. \quad (2.5)$$

Then, differentiating Eq. 2.4 with respect to r directly yields:

$$\frac{dm}{dr} = 4\pi r^2 \rho, \quad (2.6)$$

which expresses mass conservation in this simplified model.

2.2.3 Momentum equation and hydrostatic equilibrium

The second equation that describes the physics of the gas in the star is the momentum equation. This equation, derived directly from Newton's second law, expresses how the fluid accelerates under the action of external forces. In stellar physics, the following form is generally adopted:

$$\frac{D\mathbf{v}}{Dt} = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla P - \nabla \psi, \quad (2.7)$$

where P is the pressure and ψ the gravitational potential, which satisfies the Poisson equation

$$\nabla^2 \psi = 4\pi G \rho, \quad (2.8)$$

with G denoting the Newton's gravitational constant.

According to Eq. 2.7, the forces that drive the motion of the fluid are the pressure-gradient force and gravity. Here, magnetohydrodynamic effects are neglected, so no magnetic field is taken into account. For a hydrostatic equilibrium configuration, this is equivalent to assuming that thermal pressure dominates magnetic pressure, which is fully justified given the very high temperatures in stellar interiors. Furthermore, compared to the classical momentum equation of fluid mechanics, viscosity is also neglected since the Reynolds number (Re) at these scales is very large and inertial effects dominate the dynamics.

Now, returning to the simplified model from Sec. 2.2.2, which assumes spherical symmetry and hydrostatic equilibrium, the left-hand side of Eq. 2.7 vanishes. The equation simplifies to

$$\frac{dP}{dr} = -\rho \frac{d\psi}{dr}, \quad (2.9)$$

and Eq. 2.8 becomes in a spherically symmetric system:

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) = 4\pi G \rho, \quad (2.10)$$

$$\iff r^2 \frac{d\psi}{dr} = G \int_0^r 4\pi r'^2 \rho dr', \quad (2.11)$$

$$\iff \frac{d\psi}{dr} = \frac{Gm}{r^2}. \quad (2.12)$$

Then, combining Eqs. 2.9 and 2.12 yields the expression of the momentum equation for the spherically symmetric model:

$$\frac{dP}{dr} = -\frac{\rho Gm}{r^2} = -\rho g, \quad (2.13)$$

where $g = \frac{Gm}{r^2}$ is the gravity. Finally, integrating this equation and assuming $P(R) = 0$ provides:

$$P = \int_r^R \rho g dr' = \int_r^R \frac{\rho Gm}{r'^2} dr'. \quad (2.14)$$

This expression shows that, in hydrostatic equilibrium, the pressure at a given point is such that it exactly balances the weight of the gas column above this point.

The validity of the hydrostatic equilibrium assumption can be discussed by defining what is called the dynamical time:

$$\tau_{\text{dyn}} \sim \sqrt{\frac{R^3}{GM}}. \quad (2.15)$$

This time gives an order of magnitude of the time taken for the star to collapse under its own gravity and thus to change significantly its radius. For the Sun, it is of the order of:

$$\tau_{\text{dyn},\odot} \sim 26 [\text{min}]. \quad (2.16)$$

Consequently, any breakdown of hydrostatic equilibrium in the Sun would lead to a change in its radius on timescales of the order of tens of minutes. Since no such rapid variations are observed, hydrostatic equilibrium is justified for the Sun and, in fact, for most stars. As said earlier, it is not true for pulsating stars such as Cepheids, where the radius varies periodically with a period of the order of their dynamical time due to hydrostatic disequilibrium. Nevertheless, such a hydrostatic equilibrium structure provides a good starting point for describing the theory of stellar pulsations, which will be tackled in Sec. 2.4.

2.2.4 Matter state

The hydrostatic equilibrium also provides a useful basis for estimating the order of magnitude of the central pressure and temperature. Starting from Eq. 2.13 and using $\rho_c \sim M/R^3$ and $\frac{dP}{dr} \sim P_c/R$, where $P_c = P(r=0)$ is the central pressure and $\rho_c = \rho(r=0)$ the central density, one obtains

$$P_c \sim \frac{GM^2}{R^4} \sim 10^{11} [\text{Pa}], \quad (2.17)$$

for a classical Cepheid.

For an ideal gas, this allows an estimate of the central temperature T_c using

$$T_c \sim \frac{P_c \mu m_u}{k_B \rho_c} \sim 10^7 [\text{K}], \quad (2.18)$$

where μ is the mean molecular weight, m_u is the atomic mass unit, and k_B is the Boltzmann constant.

Furthermore, stars are mainly composed of hydrogen (H), about 70% in mass, and helium (He), about 28%, while the remaining fraction consists of heavier elements referred to as metals. The estimated central temperature is in fact much higher than the ionisation temperature of hydrogen, as well as the first and second ionisation temperatures of helium. The corresponding ionisation processes are:



where e^- denotes an electron. This directly implies that the matter inside stars is in a fully ionised plasma state. In practice, the plasma is fully ionised in the stellar core and becomes partially ionised in the outer layers. More precisely, the ionisation of each species takes place mainly within a given zone called an ionisation zone. These zones are located in the outer layers of the star: the second helium ionisation zone lies deeper in the star, followed by the first helium ionisation zone, while the hydrogen ionisation zone is the outermost one since it requires a lower temperature to ionise.

Furthermore, the central temperature is sufficiently high to ignite hydrogen nuclear fusion in the stellar core. At such temperatures, hydrogen nuclei have enough kinetic energy to overcome the Coulomb barrier and undergo fusion. This process releases a large amount of energy, which acts as the main energy source of the star. Additionally, the rate of nuclear reactions is highly sensitive to temperature, making the stellar core particularly sensitive to any changes in its structure.

2.2.5 Energy equation

The third equation describing stellar hydrodynamics is naturally the energy balance equation. As mentioned above, the main source of energy in stars is nuclear reactions, characterised by the nuclear energy generation rate per unit mass ϵ_n . The second process that can change the internal energy of the gas is, of course, compression or expansion. Finally, the third contribution is the energy flux $\mathbf{F}$, which accounts for the transport of energy through the stellar medium. Gathering these three contributions gives the following equation:

$$\rho \frac{Du}{Dt} = -P \nabla \cdot \mathbf{v} + \rho \epsilon_n - \nabla \cdot \mathbf{F}, \quad (2.22)$$

where u is the specific internal energy of the gas. Now, it is useful to recall the following well-known identity from thermodynamics:

$$T ds = du + P dv, \quad (2.23)$$

with s the specific entropy and $v = 1/\rho$ the specific volume. This relationship allows the rewriting of Eq. 2.22 as

$$\rho T \frac{Ds}{Dt} = \rho \epsilon_n - \nabla \cdot \mathbf{F}. \quad (2.24)$$

Subsequently, the luminosity L is defined for a spherical model by the following equation:

$$L = 4\pi r^2 F, \quad (2.25)$$

where F is the radial component of the energy flux vector. Hence, the divergence of the flux can be rewritten for a purely radial flux as

$$\begin{aligned} \nabla \cdot \mathbf{F} &= \frac{1}{4\pi r^2} \frac{dL}{dr} \\ &= \rho \frac{dL}{dm}, \end{aligned} \quad (2.26)$$

since $dm = 4\pi r^2 \rho dr$ (Eq. 2.6). Inserting Eq. 2.26 into Eq. 2.24 leads to

$$T \frac{Ds}{Dt} = \epsilon_n - \frac{dL}{dm}. \quad (2.27)$$

For a star in thermal equilibrium, so when energy generation balances energy loss, the left-hand side vanishes and the relation becomes the following:

$$\frac{dL}{dm} = \epsilon_n. \quad (2.28)$$

This assumption of thermal equilibrium is actually not valid for Cepheids, as thermal disequilibrium is at the origin of the departure from hydrostatic equilibrium, as will be shown later. Often, it is convenient to rewrite the equation in a similar form, even out of thermal equilibrium. This can be done by defining

$$\epsilon_g = -T \frac{Ds}{Dt}, \quad (2.29)$$

and inserting it into Eq. 2.27, which gives:

$$\frac{dL}{dm} = \epsilon_n + \epsilon_g. \quad (2.30)$$

The term ϵ_g accounts for thermal exchanges.

In the following, the spherical symmetry will always be assumed so that the energy fluxes remain purely radial and can be described by a scalar.

2.2.6 Transport of energy

The previous section addressed the issue of energy balance, in particular by introducing the concept of energy flux. However, the physical nature of this flux has not yet been discussed. In fact, energy within a star can be transported by two distinct physical mechanisms: radiation and convection. The energy flux can thus be decomposed into a radiative part F_{rad} and a convective one F_{conv} :

$$F = F_{\text{rad}} + F_{\text{conv}}. \quad (2.31)$$

These two modes of energy transport occur under different conditions and in different regions, and understanding them is essential for describing the star's behaviour.

Radiation

Radiation is probably the most intuitive way to picture energy transport in stars, since the central temperatures are very high, as discussed in Sec. 2.2.4. Indeed, radiative emission is strongly dependent on temperature. For instance, in the case of a black body, an idealised body that absorbs and re-emits all incident radiation, the radiative flux takes the following form:

$$F_{\text{rad},bb} = \sigma_B T^4, \quad (2.32)$$

where σ_B is the Stefan-Boltzmann constant. This relationship can be used to define the effective temperature of a star (or surface temperature). Considering the flux emitted by the star at the surface $F_{\text{rad},r=R}$ and using Eq. 2.32 makes it possible to define this temperature T_{eff} :

$$T_{\text{eff}} = \left(\frac{F_{\text{rad},r=R}}{\sigma_B} \right)^{1/4}. \quad (2.33)$$

In other words, the effective temperature of a star is the temperature of a black body that would emit the same radiative flux. The surface can then be defined by the layer where the temperature value is the effective temperature. Note that the term "surface" is not rigorously defined in this context and that it is more appropriate to refer to the "photosphere" instead. For Cepheids, the effective temperature is typically of the order of 5×10^3 K, while the central temperature is of the order of 10^7 K, as mentioned earlier. This highlights that very large temperature gradients must develop within the star, implying a huge transport of energy.

From a physical point of view, radiation corresponds to the transport of energy by photons emitted and absorbed by matter. However, in stellar interiors, photons have difficulty propagating through the medium due to frequent interactions. Indeed, these interactions can be classified into four main processes. First, Thomson scattering, which corresponds to the elastic scattering of photons by free electrons, leading to a change in direction without significant energy loss. Second, free-free absorption (inverse bremsstrahlung), where photons are absorbed during interactions between free electrons and ions. Third, bound-free transitions, corresponding to the ionisation of atoms or ions by photon absorption. Finally, bound-bound transitions, in which photons are absorbed or emitted during transitions between different energy levels of atoms [10]. These four interactions are schematised in Fig. 2.3.

These interactions strongly limit the propagation of photons, resulting in a very short mean free path ℓ (the average distance travelled between two interactions), typically

$$\ell \sim 2 \text{ cm}, \quad (2.34)$$

which is extremely small compared to stellar scales. As a consequence of this short mean free path and the resulting random walk process, a photon may take up to several hundred thousand years to travel from the centre of the star to its surface.

In practice, rather than talking about the mean free path, one can define the opacity κ_λ , which measures the ability of a medium to let photons of wavelength λ pass through it. It is thus convenient to define the Rosseland mean opacity κ , which takes all wavelengths into account:

$$\frac{1}{\kappa} = \frac{\pi}{4acT^3} \int_0^\infty \frac{1}{\kappa_\lambda} \frac{\partial B_\lambda}{\partial T} d\lambda, \quad (2.35)$$

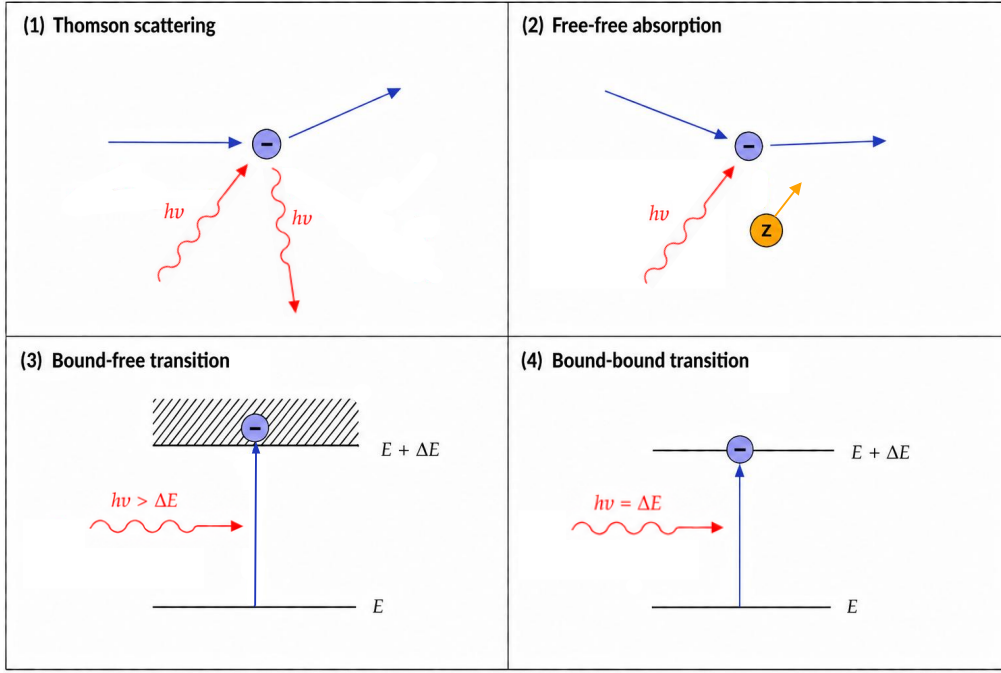


Figure 2.3: Schematic representation of the four main photon-matter interaction processes in stellar interiors. The blue circle containing a minus sign represents a free electron, the yellow circle labelled Z an ion, and $h\nu$ a photon of energy $h\nu$. (1) Thomson scattering: elastic scattering of a photon by a free electron. (2) Free-free absorption: absorption of a photon by a free electron in the presence of an ion. (3) Bound-free transition: ionisation of an atom or ion through the absorption of a photon, promoting an electron from a bound energy level E to the continuum. (4) Bound-bound transition: transition between two bound energy levels, E and $E + \Delta E$, induced by the absorption of a photon.

where $a = 4\sigma_B/c$ is the radiation constant, c is the speed of light, and B_λ is the Planck function describing the spectral distribution of radiation at thermodynamic equilibrium. This mean opacity is in fact directly related to the mean free path through

$$\ell = \frac{1}{\kappa\rho}. \quad (2.36)$$

One can also define the optical depth τ , which measures the attenuation of radiation through a medium. It is given by:

$$d\tau = \kappa\rho dl, \quad (2.37)$$

where dl is the differential path length. The optical depth thus depends on the considered direction. The intensity I of the electromagnetic radiation in that direction then satisfies the radiative transfer equation:

$$\frac{dI}{d\tau} = -I + S_I, \quad (2.38)$$

where S_I is the source function.

Ionisation zones, already introduced in Sec. 2.2.4, are regions where ionisation mainly occurs. They are thus characterised by a large number of bound–free transitions, which make the propa-

gation of photons more difficult, and this leads to an increase in opacity in these regions. These processes produce distinct opacity bumps in those layers. These bumps will play a crucial role in this work, as they are believed to be at the origin of the pulsation mechanism of Cepheids. This will be discussed later when addressing stellar pulsations in Sec. 2.4.

Now that all the relevant quantities have been introduced, an expression for the radiative flux can be written. Note that, in a very general way, the radiative flux is the intensity integrated over all directions:

$$F_{\text{rad}} = \int I \cos \theta d\Omega, \quad (2.39)$$

where θ is the angle between the direction of propagation of the radiation and the chosen reference axis (typically the vertical direction), and $d\Omega$ is the differential solid angle. From there, another expression for the radiative flux can be obtained. Since the derivation is somewhat involved, it is not presented here but can be found in the literature [11]. The resulting expression for the radiative flux is then

$$F_{\text{rad}} = -\frac{4acT^3}{3\kappa\rho} \frac{dT}{dr}. \quad (2.40)$$

One can note the similarity with Fourier's law of heat conduction. Note that this expression is derived under the radiative diffusion approximation, which assumes that the photon mean free path is much smaller than the characteristic dynamical length scales of the system.

Then, recalling Eq. 2.25 and inserting it into 2.40, while considering only the radiative part of the flux, enables the definition of the radiative luminosity L_r :

$$\begin{aligned} L_r &= 4\pi r^2 F_{\text{rad}} \\ &= -\frac{16\pi a c r^2 T^3}{3\kappa\rho} \frac{dT}{dr}. \end{aligned} \quad (2.41)$$

This represents the part of the luminosity due to radiation. Alternatively, using Eq. 2.6, this can be written

$$\begin{aligned} L_r &= 4\pi r^2 F_{\text{rad}} \\ &= -\frac{64\pi a c r^4 T^3}{3\kappa} \frac{dT}{dm}. \end{aligned} \quad (2.42)$$

For purely radiative zones (where only radiation takes place), the luminosity L is equal to the radiative luminosity so that Eq. 2.41 can be rewritten as

$$\frac{dT}{dr} = -\frac{3\kappa\rho L}{16\pi a c r^2 T^3}, \quad (2.43)$$

giving an expression for the temperature gradient in radiative zones.

It is important to emphasise that radiative transport occurs at all layers of a star, since a temperature gradient is always present. However, it may be complemented (and even dominated) by convection in the so-called convective zones. A region of a star is therefore considered radiative if energy is transported purely by radiation, and convective if convection contributes to the energy transport.

Convection

The second way of transporting energy in a star is convection, which arises from hydrodynamical instabilities within the gas. In contrast to radiation, convection is much more complex and constitutes a major aspect of the simulation that will be analysed in this work. A full section is therefore dedicated to its description.

2.3 Stellar convection

This section is essential to the present work, as the study of the convective envelope and its interaction with stellar pulsations forms the core of the analysis. At this stage, however, convection is introduced in a general framework, considered independently from any coupling with pulsations.

2.3.1 Physical mechanism

Convection can occur in stars whenever the fluid becomes unstable to vertical displacements. This instability develops when a displaced fluid element becomes lighter than its surroundings, leading to a convective instability analogous to the Rayleigh–Bénard instability.

Consider a fluid element in a stellar layer that is slightly displaced upward. Since the deeper layers of a star are hotter and denser, the element remains relatively warmer and lighter than the surrounding material at its new position. The resulting buoyancy force, as described by Archimedes’ principle, then accelerates it further upward. This is illustrated in Fig. 2.4.

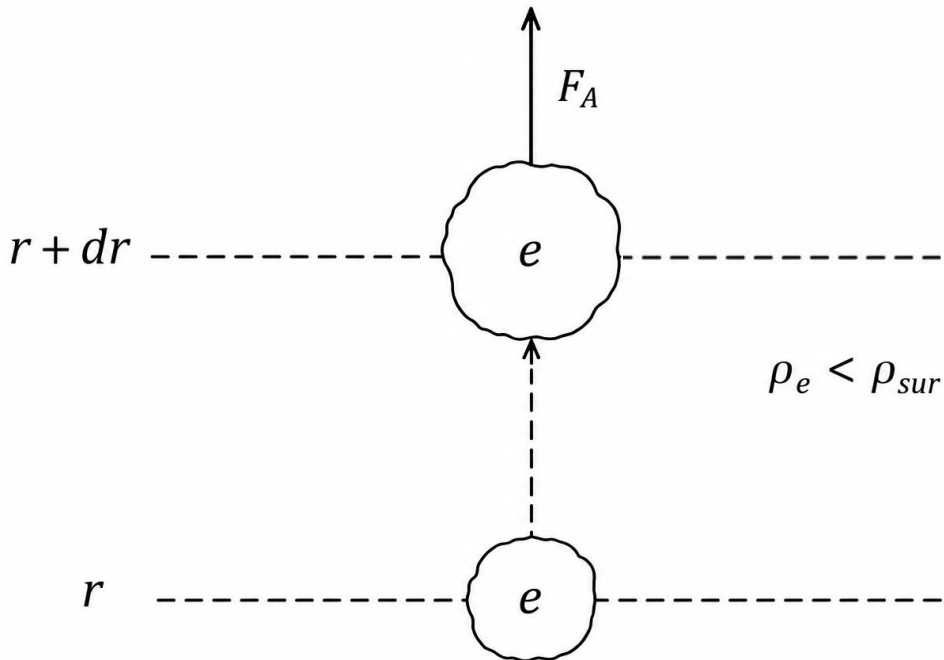


Figure 2.4: Diagram illustrating the convective instability mechanism for a rising fluid element e . The element is displaced from r to $r + dr$ and becomes less dense than its surroundings ($\rho_e < \rho_{sur}$) because of its higher temperature. The resulting Archimedes force, F_A , drives the element further upward.

Conversely, if the element is displaced downward, it becomes cooler and denser than its surroundings and continues to sink. In both cases, the initial perturbation is amplified, which leads to convective motion. Such a mechanism arises only above a certain threshold of the temperature gradient. In fact, if the gradient is not steep enough, any displacement of a fluid element is quickly balanced by radiative energy transport. It is, therefore, convenient to try to determine the critical gradient in order to predict which layer of the star will become convective. This will be done in Sec 2.3.2.

Physically, convection corresponds to large-scale plasma motions, both upward and downward. This gives rise to cellular structures, as can be observed at the solar surface in Fig. 2.5.

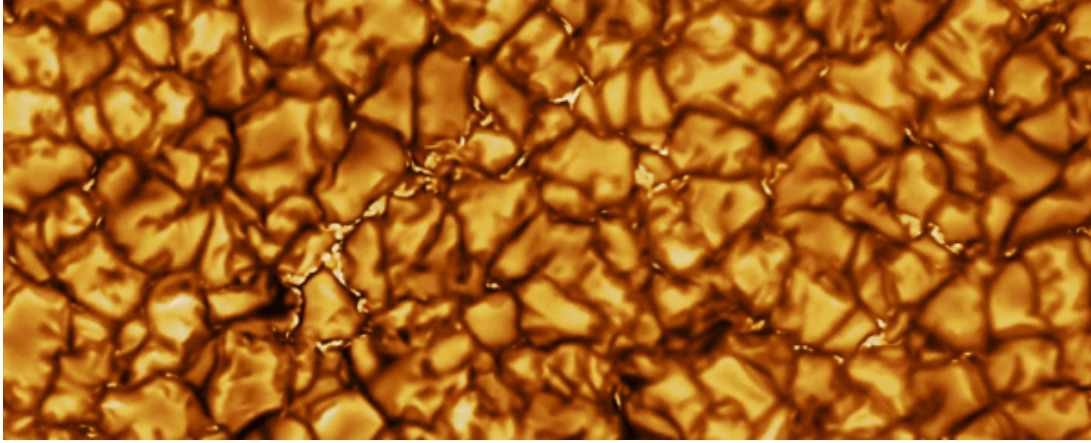


Figure 2.5: Image of convective cells at the surface of the Sun. The upward flows are brighter (hotter), while the downward flows appear darker (cooler). The picture is taken from Ref. [12].

These motions are highly turbulent, three-dimensional and strongly non-linear, which makes them particularly difficult to analyse. The associated Reynolds number Re is typically of the order of

$$Re = \frac{v_{\text{conv}} l_{\text{conv}}}{\nu} \sim 10^{10} - 10^{14}. \quad (2.44)$$

Here, v_{conv} is a characteristic velocity of the bulk motion, l_{conv} is called the "mixing-length" and is a typical length over which a convective element survives before being mixed with its environment, and ν is the kinematic viscosity. This emphasises the dominance of inertial effects over viscous effects.

Other dimensionless numbers are also relevant for describing convective motion, for example the Rayleigh number Ra , which measures the strength of the instability (buoyancy relative to viscosity and thermal diffusion). Here again, it is typically very large in a convective zone:

$$Ra = \frac{g \alpha \Delta T H_P^3}{\nu \chi} \sim 10^{20} - 10^{30}, \quad (2.45)$$

with α the thermal expansion coefficient, $H_P = -\frac{dr}{d \ln P}$ the pressure scale height, which can be defined as the characteristic scale over which the pressure varies significantly, and χ the thermal diffusivity defined as

$$\chi = \frac{16 \sigma_B T^3}{3 \kappa \rho^2 c_p}. \quad (2.46)$$

This quantity can also be compared with momentum diffusivity through the Prandtl number Pr , with typical values of

$$Pr = \frac{\nu}{\chi} \sim 10^{-6} - 10^{-4}. \quad (2.47)$$

This shows that heat diffuses much faster than momentum. Nonetheless, it has been shown in Eq. 2.45 that this thermal diffusivity is not sufficient to counteract the motion of fluid elements, and in practice these elements move so fast that the characteristic timescale of convection, τ_{conv} , is much shorter than the characteristic timescale of thermal diffusion, τ_{diff} :

$$\tau_{\text{conv}} = \frac{l_{\text{conv}}}{v_{\text{conv}}} \ll \tau_{\text{diff}} = \frac{l_{\text{conv}}^2}{\chi}. \quad (2.48)$$

Alternatively, it is also common to define the Péclet number as the ratio between the convective and thermal diffusion timescales [13]:

$$Pe = \frac{v_{\text{conv}} l_{\text{conv}}}{\chi} \sim 10^3 - 10^6. \quad (2.49)$$

For typical Cepheid convective envelopes, it therefore directly quantifies the efficiency of convection [14]. The previous discussion on high convective efficiency is valid in the deeper layers of the convective zone, where convection is highly efficient, whereas it becomes less efficient in the more superficial layers.

Consequently, if one defines the temperature gradient ∇_e as seen by a convective fluid element, one obtains:

$$\nabla_e \equiv \left(\frac{\partial \ln T}{\partial \ln P} \right)_e, \quad (2.50)$$

and the adiabatic gradient, defined for an isentropic process, as

$$\nabla_{\text{ad}} \equiv \left. \frac{\partial \ln T}{\partial \ln P} \right|_s, \quad (2.51)$$

where the vertical bar indicates that the derivative is taken while keeping the variable written after the bar constant. It can thus be assumed that in the deeper layers of convective zones

$$\nabla_e \simeq \nabla_{\text{ad}}. \quad (2.52)$$

Subsequently, other parameters, called respectively the first and the third adiabatic coefficients, can be defined for adiabatic processes and will be relevant later:

$$\Gamma_1 \equiv \left. \frac{\partial \ln P}{\partial \ln \rho} \right|_s, \quad (2.53)$$

$$\Gamma_3 - 1 \equiv \left. \frac{\partial \ln T}{\partial \ln \rho} \right|_s. \quad (2.54)$$

The adiabatic gradient can thus also be expressed as

$$\nabla_{\text{ad}} = \frac{\Gamma_3 - 1}{\Gamma_1}. \quad (2.55)$$

These equations, as well as those in Secs. 2.3.2 and 2.3.3, are taken from [6, 7].

2.3.2 Schwarzschild criterion

It has been said previously that the temperature gradient within a star must be sufficiently steep for convection to occur. It is now time to rigorously derive the corresponding criterion in order to determine in which regions of the star convection takes place.

Consider again the element from Sec. 2.3.1 with density ρ_e , which finds itself pushed upward in surroundings of density ρ_{sur} . As stated earlier, this convective motion occurs if the element is less dense than its surroundings. Mathematically, this translates as:

$$\rho_e < \rho_{\text{sur}}. \quad (2.56)$$

The subscripts "e" and "sur" will be used in the following to denote quantities related to the element and the surroundings, respectively.

Since pressure equilibrates via sound waves, this process is much faster than convection because subsonic flows are here considered so that pressure equilibrium between the element and its surroundings can be assumed. Assuming an ideal gas, this provides:

$$P_e = P_{\text{sur}}, \quad (2.57)$$

$$\Leftrightarrow R_g \rho_e \frac{T_e}{\mu_e} = R_g \rho_{\text{sur}} \frac{T_{\text{sur}}}{\mu_{\text{sur}}}, \quad (2.58)$$

where R_g is the universal gas constant. Combining this with Eq. 2.56 provides the following inequality for convection to occur:

$$\frac{T_e}{\mu_e} > \frac{T_{\text{sur}}}{\mu_{\text{sur}}}, \quad (2.59)$$

and if the chemical composition is assumed to remain the same:

$$T_e > T_{\text{sur}}, \quad (2.60)$$

which shows mathematically that the element must be hotter than its surroundings in order for convection to occur. Note that this directly implies that energy will be transported.

Defining the initial temperature of the element as T_0 , Eq 2.60 can be rewritten:

$$\frac{T_e - T_0}{T_0} > \frac{T_{\text{sur}} - T_0}{T_0}. \quad (2.61)$$

Then, for an infinitesimal displacement and since $\ln P$ decreases outward, one gets:

$$\left(\frac{\partial \ln T}{\partial \ln P} \right)_e < \left(\frac{\partial \ln T}{\partial \ln P} \right)_{\text{sur}}. \quad (2.62)$$

The left-hand side of this expression is, by definition, the gradient seen from the element, as defined in Eq. 2.50. The right-hand side, $\left(\frac{\partial \ln T}{\partial \ln P}\right)_{\text{sur}}$, corresponds to the average stratified medium and is called the real gradient ∇ :

$$\nabla \equiv \left(\frac{\partial \ln T}{\partial \ln P}\right)_{\text{sur}}. \quad (2.63)$$

Moreover, it has been shown previously that, at least in the deep layers of convective zones, the adiabatic gradient and the temperature gradient experienced by a fluid element are very similar, as illustrated by Eq. 2.52. In reality, in convective zones, the gradient of the element is slightly larger than the adiabatic one, since any residual heat exchange requires a steeper temperature gradient in the non-ideal case. Combining this with Eq. 2.62 yields

$$\left.\frac{\partial \ln T}{\partial \ln P}\right|_s < \left(\frac{\partial \ln T}{\partial \ln P}\right)_e < \left(\frac{\partial \ln T}{\partial \ln P}\right)_{\text{sur}}, \quad (2.64)$$

or, in compact form,

$$\nabla_{\text{ad}} < \nabla_e < \nabla. \quad (2.65)$$

In a stable region where convection does not occur, these inequalities are exactly reversed. The necessary and sufficient condition for convection to occur is then

$$\nabla_{\text{ad}} < \nabla. \quad (2.66)$$

However, this criterion is not convenient for practical use. Indeed, the actual gradient already depends on the mode of energy transport, and it is thus required to know in advance which regions are convective in order to compute it properly. This is not desirable, as the goal is to have a criterion that determines which set of energy transport equations, given by Eqs. 2.43 and 2.77, must be solved in each region. To overcome this issue, one introduces the radiative gradient ∇_{rad} , which represents the hypothetical temperature gradient that would be established if energy transport were purely radiative. To derive its expression, it is first convenient to rewrite the actual temperature gradient, for which the subscript is no longer required:

$$\begin{aligned} \nabla &= \frac{\partial \ln T}{\partial \ln P} \\ &= \frac{P}{T} \frac{\partial T / \partial r}{\partial P / \partial r} \\ &= \frac{r^2 P}{G m \rho T} \frac{\partial T}{\partial r}. \end{aligned} \quad (2.67)$$

Substituting Eq. 2.41 into the above expression yields

$$\nabla = \frac{3 \kappa P L_r}{16 \pi a c G m T^4}. \quad (2.68)$$

The radiative gradient, denoted by ∇_{rad} , is then obtained by assuming that the entire flux is transported by radiation. This corresponds to replacing L_r with the total luminosity L in

Eq. 2.68:

$$\nabla_{\text{rad}} = \frac{3\kappa PL}{16\pi acGmT^4}. \quad (2.69)$$

As stated above, ∇_{rad} represents the temperature gradient required for radiation alone to transport the entire energy flux. This gradient is larger than the real gradient since

$$L > L_r. \quad (2.70)$$

As a result, the following inequality holds in convective regions:

$$\nabla_{\text{ad}} < \nabla_e < \nabla < \nabla_{\text{rad}}, \quad (2.71)$$

and since this inequality is reversed in radiative regions where convection does not occur, the criterion

$$\nabla_{\text{ad}} < \nabla_{\text{rad}}, \quad (2.72)$$

represents a necessary and sufficient condition for the onset of convection. This is known as the Schwarzschild criterion. This formulation is now easier to use in computations, since one can assume that the whole star is radiative and then check where the criterion is satisfied in order to identify convective regions. Note that this criterion is only valid for a chemically homogeneous gas, and that more general criteria can be extended to account for chemical composition gradients.

The knowledge of this criterion now makes it possible to identify which regions of a star may become convective. In fact, convection typically occurs in two main regions. First, it can appear in the central regions of stars, especially in massive stars, where the luminosity per unit mass L/m is very large due to strong nuclear energy production. This leads to a steep radiative gradient since $\nabla_{\text{rad}} \propto L/m$, making the core convectively unstable. On the other hand, convection may also occur in the outer envelope of stars, as is the case for the Sun. In these regions, it arises because of the strong increase in opacity, mainly due to partial ionisation. In this case, $\nabla_{\text{rad}} \propto \kappa/T^4$, and the decrease in temperature together with the increase in opacity leads to a large radiative gradient. This second case is the main focus of this work, as convection will be analysed in the convective envelope of Cepheids. The classical structure of a Cepheid, in terms of energy transport layers, is shown in Fig. 2.6.

It should be mentioned, additionally, that being able to precisely predict which regions of a star will become convective is a crucial issue in stellar evolution. Indeed, in addition to energy transport, convection induces a strong mixing of chemical elements within convective zones. This can radically change the evolutionary path of a star, since the chemical composition change is the main driver of its evolution. It is in fact difficult to precisely define the outer boundary of a convective core and the inner boundary of a convective envelope. This difficulty arises because the Schwarzschild criterion is intrinsically limited by its local nature, since it depends only on the thermodynamic variables evaluated at a given point. This is computationally very convenient, but physically incomplete. In reality, convection depends on the global behaviour of fluid elements and on their ability to transport energy over a finite distance. One of the clearest manifestations of the limitations of a local criterion, due to non-local effects, is the following. The Schwarzschild criterion provides information about where the buoyancy force (Archimedes' force) changes sign and where fluid elements start to be accelerated upward or

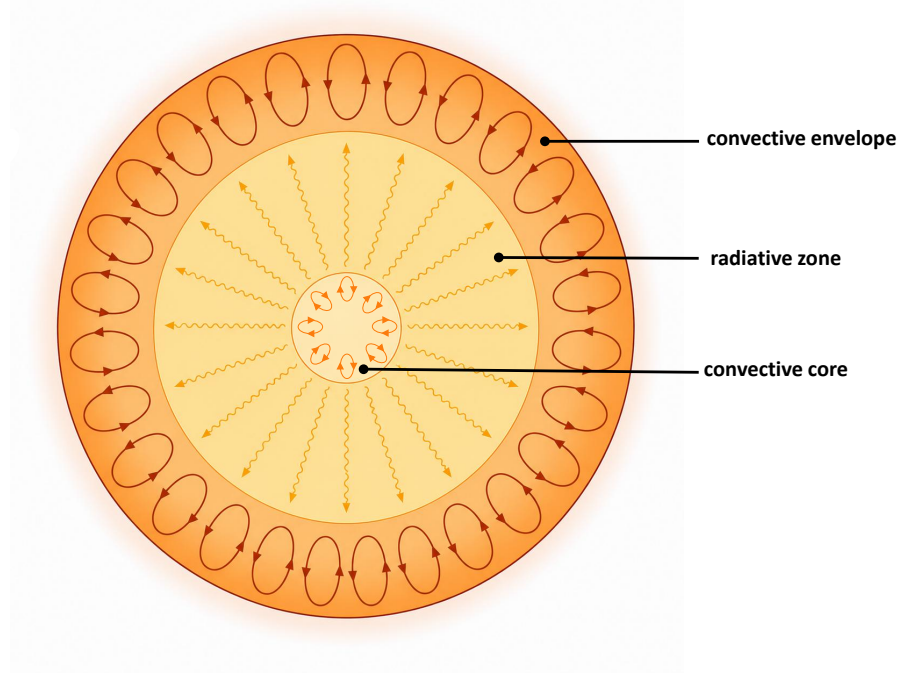


Figure 2.6: Schematic 2D representation of the typical internal structure of a Cepheid in terms of energy transport regions. The star consists of a convective core, surrounded by a radiative layer and an outer convective envelope.

downward. However, forces determine accelerations, not velocities. As a consequence, convective elements that reach the theoretical Schwarzschild boundary of a convective core with a non-zero velocity can penetrate into the surrounding stable region due to their inertia. This phenomenon is known as overshooting. It leads to an extension of the convective region beyond its formal boundary and must therefore be taken into account in stellar models. In practice, this effect is often parameterised through an overshooting parameter. A similar process can occur for downward-moving elements at the base of a convective envelope and is referred to as undershooting.

2.3.3 Convective transport

One can now try to find an expression for the energy flux carried by convection. The general way to formulate this is to express the convective flux as an enthalpy flux:

$$F_{\text{conv}} = \langle \rho v_r \Delta h \rangle_r, \quad (2.73)$$

where Δ denotes the difference of a quantity between the considered point and the mean value at the same depth, and h is the enthalpy. The operator $\langle \cdot \rangle_r$ denotes the spatial average over a sphere of radius r , since a spherically symmetric model is considered. This average thus takes into account all the fluctuations for upward and downward motions. However, the definition of the convective flux can also be extended locally by removing this average. Then, recalling that for a perfect gas of specific heat capacity at constant pressure c_p :

$$\Delta h = c_p \Delta T, \quad (2.74)$$

Eq 2.73 can be written

$$F_{\text{conv}} = \langle \rho v_r c_P \Delta T \rangle_r. \quad (2.75)$$

The value of the convective flux is therefore positive if the upward motions are hotter and the downward motions are colder, which is indeed the case in convective zones. However, this description of this flux remains somewhat limited since the value of the convective flux is given as a function of v_r , which remains still unknown. It is thus necessary to have a more elaborate theory to model the physics of convective zones. It will be addressed in the next section (Sec. 2.3.4).

It is also convenient to derive an expression for the temperature gradient, similar to what has been done for radiative transport in Eq. 2.43. To do that, assuming that Eq. 2.52 is verified, Eqs. 2.50 and 2.51 can be combined to give:

$$\frac{dT}{dP} = \nabla_{\text{ad}} \frac{T}{P}. \quad (2.76)$$

Recalling the hydrostatic equilibrium expression for $\frac{dP}{dr}$ from Eq. 2.13, this leads to the following expression for the temperature gradient in convective zones:

$$\begin{aligned} \frac{dT}{dr} &= \frac{dT}{dP} \frac{dP}{dr} \\ &= -\nabla_{\text{ad}} \frac{T}{P} \frac{Gm\rho}{r^2}. \end{aligned} \quad (2.77)$$

This can also be written:

$$\frac{dT}{dr} = \frac{dT}{d \ln T} \frac{d \ln T}{d \ln P} \frac{d \ln P}{dr} = -T \frac{\nabla}{H_P}. \quad (2.78)$$

2.3.4 Mixing-Length Theory

The most widely used model to close the problem of the convective flux in 1D is the Mixing-Length Theory (MLT). The basic idea of this model is to assume that convective elements travel a characteristic distance l_{conv} , already introduced in Sec. 2.3.1, before releasing their excess energy and dissolving into the surrounding medium. This is illustrated in Fig. 2.7.

In this framework, the mixing length is related to the pressure scale height, also introduced in Sec. 2.3.1, through

$$l_{\text{conv}} = \alpha_{\text{conv}} H_P, \quad (2.79)$$

where α_{conv} is the mixing length parameter, and is typically of the order of unity. This model thus assumes that convective structures have a typical size. In other words, this is equivalent to saying that, in the Fourier domain, the convection would be described by a single wavenumber.

Under this assumption, the convective flux from Eq. 2.75 can be written:

$$F_{\text{conv}} = \rho \overline{v_r} c_P \overline{\Delta T}, \quad (2.80)$$

where the overbar denotes a time average of the quantity over the entire trajectory of an ele-

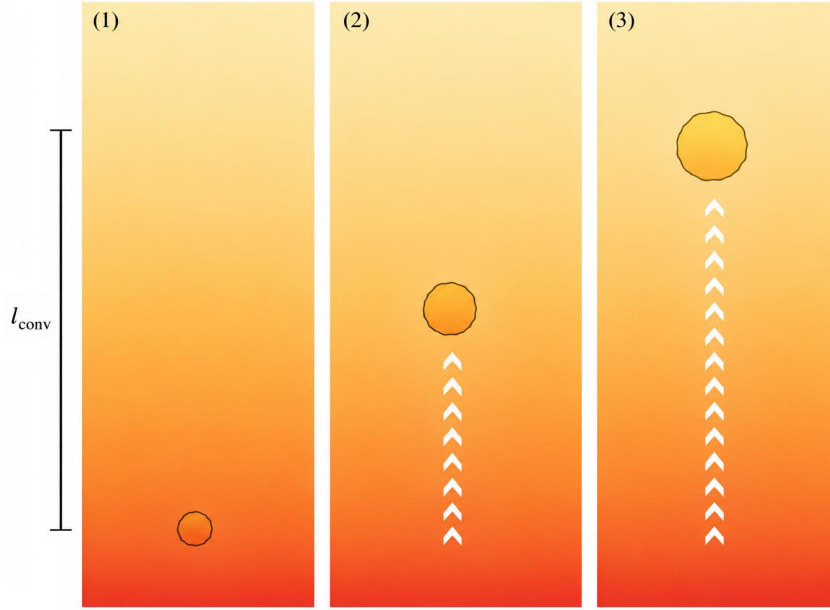


Figure 2.7: Schematic illustration of the motion of a convective element in the framework of the MLT. (1) A convective element is generated at a given depth and rises owing to buoyancy forces. (2) The element reaches a displacement of $l_{\text{conv}}/2$, at which the thermodynamic excesses between the element and its surroundings are evaluated in the MLT formalism. (3) The element continues its ascent until it reaches the characteristic mixing length l_{conv} , where it is assumed to merge with the surrounding medium.

ment. The spatial average over all the elements is not necessary anymore since all elements are assumed to behave the same way.

The principle of the MLT is to approximate path averages by the values at mid-path. In particular, the mean difference between the element temperature considered adiabatic behaviour and its surroundings is given by

$$\overline{\Delta T} \approx \left[\frac{dT_{\text{ad}}}{dr} - \frac{dT}{dr} \right] \frac{l_{\text{conv}}}{2} = (\nabla - \nabla_{\text{ad}}) \frac{T}{H_P} \frac{l_{\text{conv}}}{2}, \quad (2.81)$$

where Eq. 2.78 has been used. To calculate the mean velocity, the density excess must be calculated. It is given by

$$\overline{\Delta \rho} \approx \left[\frac{d\rho_{\text{ad}}}{dr} - \frac{d\rho}{dr} \right] \frac{l_{\text{conv}}}{2} = -\rho \delta \left[\frac{d \ln T_{\text{ad}}}{dr} - \frac{d \ln T}{dr} \right] \frac{l_{\text{conv}}}{2} = \rho \delta (\nabla_{\text{ad}} - \nabla) \frac{l_{\text{conv}}}{2H_P}, \quad (2.82)$$

with $\delta = -\frac{\partial \ln \rho}{\partial \ln T} \Big|_P$ the thermal expansion coefficient and using again Eq. 2.78. The radial buoyancy force per unit volume is written as $f_{\text{buoy}} = -g \Delta \rho$. In MLT, its mean value along the trajectory is approximated by half of its value at mid-path, namely

$$f_{\text{buoy}} \approx \frac{1}{2} f_{\text{buoy}} \left(\frac{l_{\text{conv}}}{2} \right) \approx -\frac{1}{2} g \Delta \rho \left(\frac{l_{\text{conv}}}{2} \right). \quad (2.83)$$

Using the expression of the density excess of Eq. 2.82, this becomes

$$f_{\text{buoy}} \approx \frac{1}{2} \rho g \delta (\nabla - \nabla_{\text{ad}}) \frac{l_{\text{conv}}}{2H_P}. \quad (2.84)$$

Then, a fraction 1/2 of the buoyancy work is assumed to be converted into kinetic energy of the fluid element, this means

$$\frac{1}{2} f_{\text{buoy}} \left(\frac{l_{\text{conv}}}{2} \right) = \frac{1}{2} \rho \bar{v}_r^2, \quad (2.85)$$

with v_r the radial velocity.

The remaining part of the work is assumed to be dissipated along the trajectory. This leads to an estimate of the mean convective velocity:

$$\bar{v}_r^2 = \frac{g \delta}{8H_P} (\nabla - \nabla_{\text{ad}}) l_{\text{conv}}^2. \quad (2.86)$$

Combining this expression with Eqs. 2.80 and 2.81, the convective flux is obtained:

$$F_{\text{conv}} = \rho c_P T (g \delta)^{1/2} (\nabla - \nabla_{\text{ad}})^{3/2} \frac{l_{\text{conv}}^2}{4\sqrt{2}H_P^{3/2}}, \quad (2.87)$$

which is the final expression of the convective flux in the framework of MLT. Note that this expression remains valid regardless of whether the fluid element moves upward or downward, since both the radial velocity and the temperature excess change sign simultaneously, leaving the convective flux unchanged. One can also notice that, for a fixed convective flux, a higher temperature means a smaller difference between the two gradients, as will be illustrated later in this work. The derivation presented here is based on Ref. [15].

Eq 2.87 provides an expression for the convective flux in terms of local variables, although it relies on several strong assumptions, such as the various numerical factors 1/2 introduced throughout the derivation and, more importantly, the assumption that the relevant quantities remain constant along the trajectory of the fluid element. Moreover, the output of the MLT model is highly dependent on the choice of the mixing length parameter. Fig. 2.8 shows different trajectories in the HR diagram computed for various values of this parameter to illustrate that. In addition, similarly to the Schwarzschild criterion, MLT is a local theory, whereas convection is intrinsically non-local. Finally, the theory also assumes a certain symmetry between upward and downward-moving elements. This assumption is not always valid and will constitute a major point of discussion in Ch. 4.

Despite all these assumptions and the apparent oversimplification of the model, the mixing-length theory has long been the reference framework for modelling convection in stellar interiors. In practice, it provides remarkably good predictions for a variety of stellar structure profiles and sometimes yields results that are very close to both observations and more advanced simulations [17–19]. As an example, Fig. 2.9 compares the difference between the actual and adiabatic temperature gradients predicted by MLT with that obtained from a more advanced 3D simulation of the Sun. Since this quantity is directly related to the strength of the convective instability and the associated energy flux, it provides a useful diagnostic of the model performance. The agreement between the two approaches is in fact remarkably good, with the overall shape of the

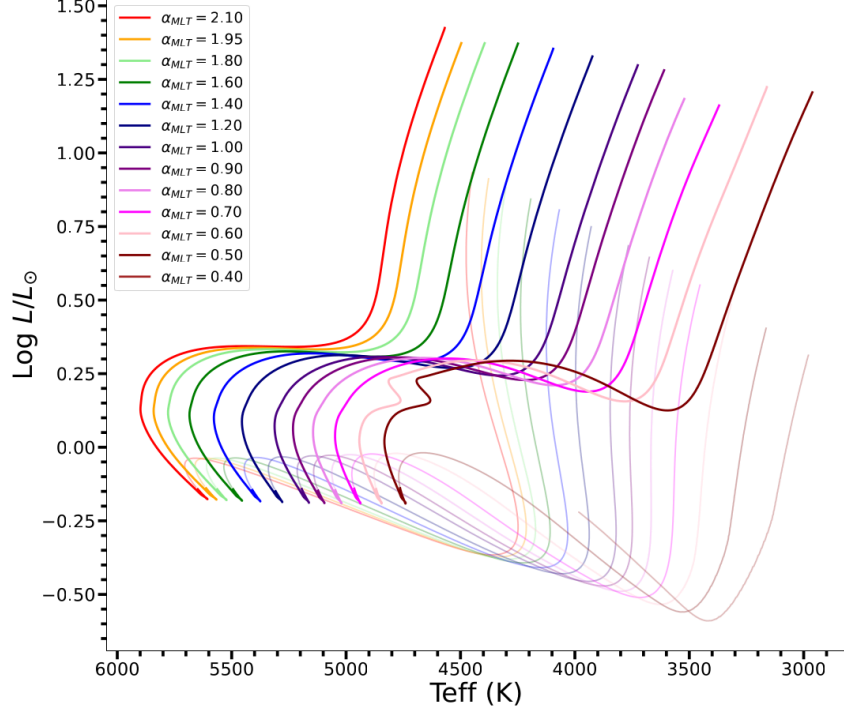


Figure 2.8: Evolutionary tracks in the HR diagram for a $1 M_{\odot}$ star computed with different values of the mixing length parameter, denoted here by α_{MLT} . The pre-main-sequence phase is shown in a lighter colour. The figure is taken from Ref. [16].

profile being well reproduced. This demonstrates that, despite its simplicity, the mixing-length theory is far from useless and has played a major role in advancing our understanding of stellar convection.

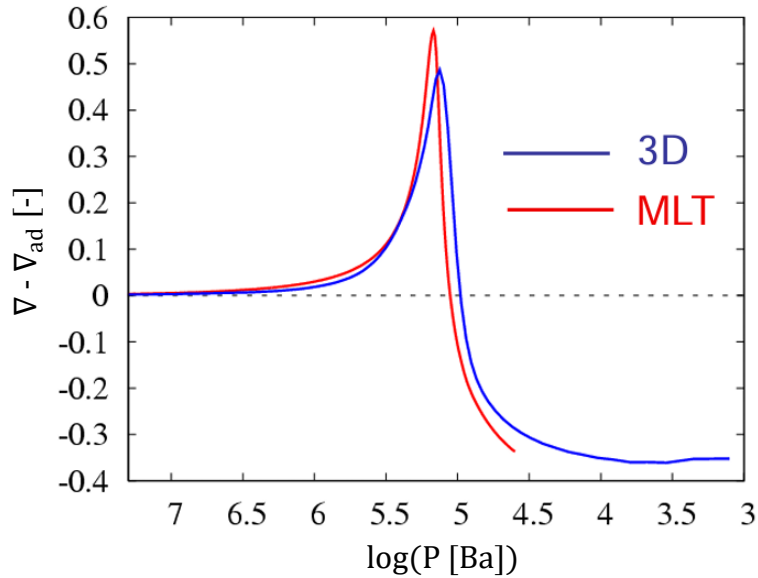


Figure 2.9: Comparison of the difference between the actual and adiabatic temperature gradients obtained from a 3D hydrodynamical simulation of the solar convective envelope and those predicted by MLT. The figure is taken from Ref. [8], where it was originally adapted from Ref. [19].

2.3.5 Hydrodynamical simulations

Although the MLT is a useful model for accounting for convection in a computationally inexpensive way in codes (for example, 1D models where many coupled equations must be solved), it remains highly limited for understanding the detailed mechanisms of convection. Therefore, the most natural approach to studying convection more accurately is to simulate it numerically using hydrodynamical (or magnetohydrodynamic) simulations. This allows one to resolve turbulent structures more precisely, especially in three dimensions, since turbulence is intrinsically a 3D phenomenon. It is such hydrodynamic simulation that constitutes the analysis of this work. Those kinds of simulations enable a broad range of studies beyond the analysis of the flow itself, for instance in terms of spectroscopic data, interferometry, stellar parameter calibration, and many other applications [20]. However, numerical simulations imply other problems to be tackled, especially the problem of turbulence resolution/modelling.

Before discussing that, it is important to recall the mechanism of turbulence as described by the famous Kolmogorov theory [21]. The main idea of this theory is to view turbulence as a hierarchy of eddies spanning a continuous range of scales, as illustrated in Fig. 2.10.

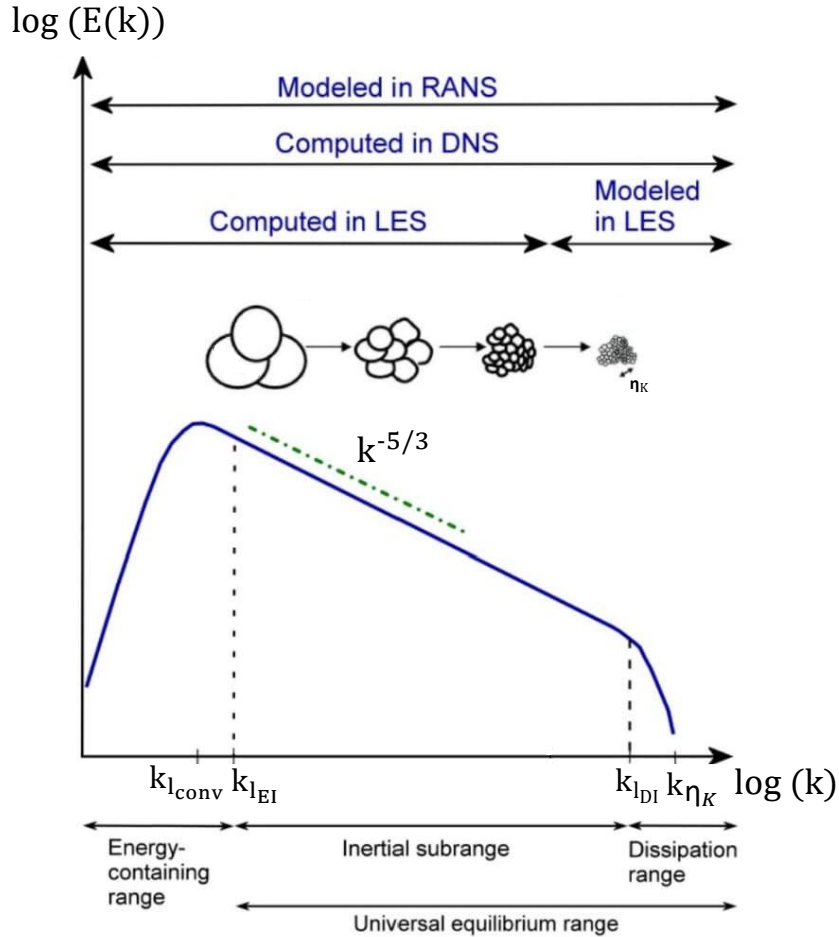


Figure 2.10: Representation of the Kolmogorov energy spectrum in the wavenumber domain. The three main turbulence regimes are highlighted and delimited by the wavenumbers k_{EI} and k_{DI} . The wavenumber k_{η_K} is associated with the Kolmogorov scale. The portions of the spectrum that are either modelled or directly resolved by the different turbulence approaches are also indicated. Adapted from Ref. [22].

At the largest scales (typically the characteristic scales of the flow), the eddies are generated by the mean flow, are strongly anisotropic, and contain most of the kinetic energy of the system. These large eddies are then broken down into progressively smaller and smaller structures through a cascade process until reaching the so-called Kolmogorov scale η_K where viscous effects become comparable to inertial effects and the energy is dissipated. At these smallest scales, the theory assumes that the anisotropy present at large scales has been lost so that eddies can be considered statistically isotropic and homogeneous. Because they depend only on the viscosity and the dissipation rate, these scales characterise the dissipative range of turbulence independently of the large-scale flow dynamics. They are therefore commonly regarded as universal scales of small-scale turbulent motions. Between these two extremes lies the inertial subrange, where energy is transferred from large to small scales without being created or dissipated. Note that, in the case of the MLT approximation, the mixing length is typically associated with the eddy scale corresponding to the maximum of the turbulent energy spectrum. It is therefore related to the wavenumber $k_{l_{\text{conv}}}$ shown in Fig. 2.10.

Once this is known, it is important to recall the three approaches possible when wanting to take into account turbulence in a hydrodynamical simulation. First, the Reynolds-averaged Navier-Stokes (RANS) approach, which consists in decomposing the flow variables into mean and fluctuating components and then averaging the Navier-Stokes equations. This leads to equations for the mean flow but introduces additional unknown terms, called the Reynolds stresses, which represent the effect of turbulent fluctuations on the mean flow. For instance, the Reynolds stress tensor appears under a divergence operator in the averaged momentum equation and quantifies the influence of turbulent fluctuations on the dynamics of the mean flow. These terms are not directly known and must be modelled using closure relations, which makes RANS a fully averaged and strongly model-dependent description of turbulence. In practice, this approach is less commonly used in stellar astrophysics than the following one, and since it will not be used in this work, it will not be further described. The second one is the Large Eddy Simulation (LES) approach, which consists in resolving only the largest eddies while modelling the smaller ones down to the Kolmogorov scales. This approach is in fact the most widely used in astrophysical hydrodynamical simulations and will be described in more detail in the following paragraph. Finally, the third approach is Direct Numerical Simulation (DNS), which consists simply in resolving all scales of turbulence down to the smallest dissipative scales. The main limitation of this method is that it requires the grid size to be of the order of the Kolmogorov scale, which is in practice unfeasible for stellar convection. Indeed, the typical scaling of the number of floating-point operations required grows approximately as Re^3 , making DNS prohibitively expensive at the very high Reynolds numbers characteristic of stellar convection. As a result, even the most powerful computers would require longer than the age of the Universe to compute a single dynamical timescale of stellar convection using DNS [23]. A summary of the ranges modelled by each approach is also shown in Fig. 2.10.

To return to the LES description, which, as just mentioned, resolves only the largest eddies while modelling the smaller ones. This approach is in fact far more computationally efficient than DNS, as the grid only needs to be of the order of the largest resolved eddies. Moreover, this approach is particularly well-suited to stellar convection, since the main goal is to compute the energy transport and, as discussed earlier, most of the kinetic energy is contained in the largest eddies. A brief description of how LES works is given below.

The LES implementation consists of four main steps. The following description of these steps is based on information from Ref. [24] and inspired by Ref. [25]. The four steps are:

1. **Separation by filtering.** This first step consists in defining precisely which scales are resolved and which are modelled. To do that, a low-pass filter is applied to the velocity field $\mathbf{v}$ so that it is divided into two components:

$$\mathbf{v} = \bar{\mathbf{v}} + \mathbf{v}', \quad (2.88)$$

where $\bar{\mathbf{v}}$ denotes the filtered (resolved) component and $\mathbf{v}'$ the unresolved subgrid-scale contribution. The filtered field can then be resolved on the computational grid, while the effects of the subgrid scales must be modelled.

As a matter of fact, the required grid resolution depends directly on the filter size. If the filter width becomes larger than the characteristic turbulent scales of the flow, the approach tends towards a RANS description. On the contrary, reducing the filter width allows a larger portion of the turbulent spectrum to be explicitly resolved, approaching the DNS limit.

2. **Formulation of the equations.** It is then necessary to rewrite the Navier-Stokes equations to describe the evolution of the filtered variables. The resulting equations have a form similar to the original Navier-Stokes equations, except for the appearance of an additional residual stress tensor, usually referred to as the subgrid-scale stress tensor. This tensor arises from the interaction between the resolved (filtered) scales and the unresolved subgrid scales, and accounts for the effect of the latter on the dynamics of the former.
3. **Closure model.** The model must then be closed by providing a suitable expression for this tensor. In practice, the most commonly used approach is an eddy-viscosity model based on the Boussinesq hypothesis.
4. **Numerical computation.** The resulting set of filtered equations is solved using numerical methods in order to obtain the resolved flow field.

This description is rather qualitative than mathematical, as the main part of this thesis is the physical analysis of the simulation rather than the numerical implementation that has been done upstream. A more precise description of the LES implementation in the case of the analysed simulation will be given in Sec. 3.1.3.

2.4 Stellar pulsations

Nearly all the main elements required for this thesis have now been introduced, in particular the equations of stellar structure and the description of energy transport. However, stellar pulsations have not yet been addressed, as most of the equations derived so far describe only equilibrium configurations based on hydrostatic and thermal equilibrium, which is in fact not valid at all for Cepheids.

Cepheids pulsations arise from the cyclic storage and release of energy within specific stellar layers. They are characterised by large, strongly non-linear radial oscillations, in which the stellar radius and other thermodynamic quantities undergo significant variations over each cycle. These oscillations are inherently non-adiabatic, meaning that energy is exchanged between the pulsating layers and their surroundings during the cycle. This leads to phase shifts between thermodynamic quantities such as pressure, density, and temperature. So, to describe Cepheid variables, stellar pulsations will now be carefully introduced based on Ref. [8].

2.4.1 Non-adiabatic radial stellar oscillations

The theory of non-adiabatic radial stellar oscillations is based on linear perturbation theory. It consists in describing stellar pulsations as small deviations from a reference equilibrium state. In this framework, the physical quantities characterising the star are expressed as the sum of their equilibrium value and a small perturbation. One may introduce the current radial position $\mathbf{r}$ and the equilibrium (Lagrangian) position $\mathbf{r}_0$. These are related through the radial displacement $\delta\mathbf{r}$ as

$$\mathbf{r} = \mathbf{r}_0 + \delta\mathbf{r}(\mathbf{r}_0, t). \quad (2.89)$$

The symbol δ denotes the Lagrangian perturbation. For any quantity q , the Lagrangian perturbation is defined as

$$\delta q(\mathbf{r}_0, t) = q(\mathbf{r}_0, t) - q_0(\mathbf{r}_0), \quad (2.90)$$

where the subscript "0" labels the equilibrium state. This thus represents the discrepancy from equilibrium following a fluid element. On the other hand, the Eulerian perturbation, denoted by q' , is defined at a fixed position $\mathbf{r}$ as

$$q'(\mathbf{r}, t) = q(\mathbf{r}, t) - q_0(\mathbf{r}). \quad (2.91)$$

It represents the variation of the quantity measured with respect to the equilibrium state at a fixed spatial position. Assuming small perturbations and using a first-order Taylor expansion, it is possible to show that these quantities are related by:

$$\delta q = q' + \nabla q_0 \cdot \mathbf{r}. \quad (2.92)$$

In this case of the study, it is more convenient to use a description based on Lagrangian perturbations. Indeed, the goal here is to describe pulsation dynamics, and since every layer of the star is in motion, it is natural to follow the evolution of physical quantities associated with each fluid element with respect to its equilibrium position.

A natural choice for the equilibrium configuration in this problem is the stationary, spherically symmetric model presented in Sec. 2.2. It is described by four equations: the simplified continuity equation (Eq. 2.6), hydrostatic equilibrium (Eq. 2.13), which is the simplified form of the momentum equation, the simplified energy equation (Eq. 2.28) in thermal equilibrium, as well as the energy transport equation for radiation (Eq. 2.43). Convective motions are not taken into account here for the sake of simplicity.

From there, the general equations of continuity, momentum, and energy can be perturbed. The perturbation of the continuity equation (Eq. 2.3) can be obtained since the velocity vector is given by:

$$\mathbf{v} = \frac{D(\mathbf{r}_0 + \delta\mathbf{r})}{Dt} = \frac{D\delta\mathbf{r}}{Dt} = \frac{\partial\delta\mathbf{r}}{\partial t}, \quad (2.93)$$

at first order. Introducing this in the general continuity equation (Eq. 2.3) yields:

$$\frac{\delta\rho}{\rho} = -\nabla \cdot \delta\mathbf{r}. \quad (2.94)$$

In practice, Cepheid oscillations are known to be radial, typically occurring in the fundamental

radial mode, where the whole envelope expands and contracts with a period of the order of the dynamical timescale introduced in Eq. 2.15. This allows Eq. 2.94 to be rewritten as

$$\frac{\delta \rho}{\rho} = -\frac{1}{r^2} \frac{d(r^2 \delta r)}{dr}. \quad (2.95)$$

Similarly, for the momentum equation (Eq. 2.7), the general perturbed form is

$$\frac{\partial^2 \delta \mathbf{r}}{\partial t^2} = -\nabla \psi' - \frac{\nabla P'}{\rho} + \frac{\rho'}{\rho^2} \nabla P, \quad (2.96)$$

with

$$\nabla^2 \psi' = 4\pi G \rho'. \quad (2.97)$$

For perfectly radial oscillations, this becomes

$$\frac{\partial^2 \delta \mathbf{r}}{\partial t^2} = -\delta \left(\frac{Gm}{r^2} + 4\pi r^2 \frac{\partial P}{\partial m} \right), \quad (2.98)$$

where once again Eq. 2.6 has been used. The perturbed momentum equation can finally be rewritten

$$\begin{aligned} \frac{\partial^2 \delta \mathbf{r}}{\partial t^2} &= -\delta \left(\frac{Gm}{r^2} + 4\pi r^2 \frac{\partial P}{\partial m} \right) = -\delta \left(g + 4\pi r^2 \frac{\partial P}{\partial m} \right) \\ &= -\delta g - 8\pi r^2 \frac{\partial P}{\partial m} \frac{\delta r}{r} - 4\pi r^2 \frac{\partial \delta P}{\partial m} \\ &= 2g \frac{\delta r}{r} + 2g \frac{\delta r}{r} - \frac{1}{\rho} \frac{\partial \delta P}{\partial r} \\ &= 4g \frac{\delta r}{r} - \frac{1}{\rho} \frac{\partial \delta P}{\partial r}. \end{aligned} \quad (2.99)$$

Then, the energy equation (Eq. 2.27) can be perturbed around the thermal equilibrium model. This gives, again for purely radial oscillations, the following:

$$T \frac{\partial \delta s}{\partial t} = \delta \epsilon - \frac{d\delta L}{dm}. \quad (2.100)$$

The last equation that must be perturbed is the energy transport equation. Here, one assumes a purely radiative zone so that Eq. 2.42 can be perturbed as

$$\frac{\delta L}{L} = -\frac{\delta \kappa}{\kappa} + 4 \frac{\delta r}{r} + 3 \frac{\delta T}{T} + \frac{d(\delta T)/dm}{dT/dm}. \quad (2.101)$$

These four equations contain a total of 8 unknowns ($\delta \rho$, δr , δP , δs , $\delta \epsilon$, δL , δT , $\delta \kappa$), and additional equations are therefore required to close the system. These are thermodynamic state

equations, assuming the following dependencies:

$$\rho = \rho(P, s) \Rightarrow \frac{\delta \rho}{\rho} = \left. \frac{\partial \ln \rho}{\partial \ln P} \right|_s \frac{\delta P}{P} + \left. \frac{\partial \ln \rho}{\partial \ln s} \right|_P \frac{\delta s}{s} = \frac{1}{\Gamma_1} \frac{\delta P}{P} - \frac{\nabla_{\text{ad}} \rho T}{P} \frac{\delta s}{s}, \quad (2.102)$$

$$T = T(P, s) \Rightarrow \frac{\delta T}{T} = \left. \frac{\partial \ln T}{\partial \ln P} \right|_s \frac{\delta P}{P} + \left. \frac{\partial \ln T}{\partial \ln s} \right|_P \frac{\delta s}{s} = \nabla_{\text{ad}} \frac{\delta P}{P} + \frac{\delta s}{c_P}, \quad (2.103)$$

$$\kappa = \kappa(\rho, T) \Rightarrow \frac{\delta \kappa}{\kappa} = \left. \frac{\partial \ln \kappa}{\partial \ln \rho} \right|_T \frac{\delta \rho}{\rho} + \left. \frac{\partial \ln \kappa}{\partial \ln T} \right|_\rho \frac{\delta T}{T} = \kappa_\rho \frac{\delta \rho}{\rho} + \kappa_T \frac{\delta T}{T}. \quad (2.104)$$

The new coefficients κ_ρ and κ_T are sensitivity coefficients of the opacity.

The system is now closed, and one can seek a solution in the complex domain:

$$\begin{aligned} \delta q(r, t) &= \Re(\delta q(r) e^{i\sigma t}) \\ &= |\delta q(r)| \cos(\omega t + \phi_q(r)) e^{\eta t}, \end{aligned} \quad (2.105)$$

where ϕ_q is the phase shift of the considered quantity. σ represents the complex frequency and ω (the real frequency) and η are respectively its real and minus its imaginary parts:

$$\sigma = \omega - i\eta. \quad (2.106)$$

η is often called the growth rate of the mode, as its sign determines whether the mode is stable or unstable. Indeed, if $\eta < 0$, the exponential factor in Eq. 2.105 tends to zero and the perturbation is damped, the mode is thus stable. Conversely, if $\eta > 0$, the exponential term causes the perturbation to grow exponentially and the mode is unstable. Since this is a linear theory of small perturbations, the subsequent evolution cannot be predicted, as nonlinear effects will quickly become important. It is thus expected that observable modes are unstable modes for which the amplitude is then limited by nonlinear effects, the stable modes being damped before being even observable. It is also important to clarify the term instability, since it is rather broad when stated without further specification. Here, the discussion concerns vibrational instability, which must be distinguished from dynamical instability. The latter occurs, for instance, when pressure can no longer balance gravity. This is not the case here, and Cepheids are therefore vibrationally unstable but dynamically stable. In the following, the term instability will refer to vibrational instability.

Subsequently, the momentum and energy equations must be rewritten in the complex domain since they contain time derivatives, with $\frac{\partial}{\partial t} = i\sigma$. Eqs. 2.99 and 2.100 respectively become:

$$-\sigma^2 \delta r = -\frac{1}{\rho} \frac{\partial \delta P}{\partial r} + 4g \frac{\delta r}{r}, \quad (2.107)$$

$$i\sigma T \delta s = \delta \varepsilon - \frac{d\delta L}{dm}. \quad (2.108)$$

It is worth mentioning that the validity of this linear theory can indeed be questioned for Cepheids due to their intrinsic non-linear pulsations. It nevertheless has the advantage of being simple and will enable the identification of basic aspects such as the energy and work associated with the pulsation cycle.

2.4.2 Energy and work

The most important quantity in the study of stellar oscillations is the work done during one pulsation cycle and, more generally, the study of the thermodynamic cycle of the gas. The general form of the work by unit of mass dW is

$$dW = \oint dP dv, \quad (2.109)$$

with v the specific volume and $\oint$ denoting the integral over one pulsation cycle. As in every thermodynamic cycle, a positive work means that the system provides mechanical energy to its surroundings, while a negative work means that energy is extracted from the surroundings. For the motion to be amplified, the gas must provide energy to it, so the global work W must be positive:

$$W > 0. \quad (2.110)$$

The work by unit of mass can be calculated by using again the general form of the solution for the perturbation, given by Eq. 2.105, for the pressure and the specific volume:

$$P = P_0 + |\delta P| \cos(\omega t + \phi_P), \quad (2.111)$$

$$v = v_0 + |\delta v| \cos(\omega t + \phi_v). \quad (2.112)$$

Note that the growth rate term has been removed in these expressions. This can be justified by the fact that any eventual growth of the mode is assumed to occur on a timescale much longer than a single oscillation cycle, mathematically:

$$\omega \gg \eta. \quad (2.113)$$

The work can thus be calculated as follow:

$$\begin{aligned} dW &= \int_0^{2\pi/\omega} P \frac{dv}{dt} dt \\ &= \int_0^{2\pi/\omega} (P_0 + |\delta P| \cos(\omega t + \phi_P)) (-\omega |\delta v| \sin(\omega t + \phi_v)) dt. \end{aligned} \quad (2.114)$$

Since the contribution of the equilibrium pressure vanishes over a closed cycle, the term in P_0 drops out. Using basic trigonometric identities, the expression can thus be written:

$$\begin{aligned} dW &= \int_0^{2\pi/\omega} (P_0 + |\delta P| \cos(\omega t + \phi_P)) (-\omega |\delta v| \sin(\omega t + \phi_v)) dt \\ &= -\omega |\delta P| |\delta v| \int_0^{2\pi/\omega} \cos(\omega t + \phi_P) \sin(\omega t + \phi_v) dt \\ &= -\frac{\omega}{2} |\delta P| |\delta v| \int_0^{2\pi/\omega} [\sin(\phi_v - \phi_P) + \sin(2\omega t + \phi_v + \phi_P)] dt \\ &= -\frac{\omega}{2} |\delta P| |\delta v| \sin(\phi_v - \phi_P) \int_0^{2\pi/\omega} dt \\ &= -\pi |\delta P| |\delta v| \sin(\phi_v - \phi_P) \end{aligned} \quad (2.115)$$

$$= -\pi \Im(\delta P \delta v^*),$$

where the symbol $*$ denotes the complex conjugate. The global work is thus directly given by

$$W = \int_0^M dW dm = - \int_0^M \pi \Im(\delta P \delta v^*) dm, \quad (2.116)$$

and the mean power is obtained by dividing it by the period:

$$\frac{dW}{dt} = -\frac{\omega}{2} \int_0^M \Im(\delta P \delta v^*) dm. \quad (2.117)$$

After that, the growth rate can be expressed as a function of the work. To do that, the perturbed momentum equation (Eq. 2.107) can be multiplied by δr^* and integrated over the whole star to give

$$-\sigma^2 \int_0^M |\delta r|^2 dm = - \int_0^M \frac{1}{\rho} \delta r^* \frac{\partial \delta P}{\partial r} dm + \int_0^M 4g \frac{|\delta r|^2}{r} dm. \quad (2.118)$$

Then, inserting Eq. 2.6 into the first term on the right-hand side and integrating by parts gives:

$$\begin{aligned} - \int_0^M \frac{1}{\rho} |\delta r| \frac{\partial \delta P}{\partial r} dm &= -4\pi \int_0^R r^2 \delta r^* \frac{\partial \delta P}{\partial r} dr \\ &= -4\pi [r^2 \delta r^* \delta P]_0^R + 4\pi \int_0^R \delta P \frac{d(r^2 \delta r^*)}{dr} dr \\ &= 4\pi \int_0^R \delta P \frac{d(r^2 \delta r^*)}{dr} dr. \end{aligned} \quad (2.119)$$

The boundary term arising from the integration by parts vanishes for the following reasons. At the centre, $r = 0$ implies $r^2 \delta r^* = 0$ by definition. At the surface, the pressure is zero. Writing $P = P_0 + \delta P$, and since $P_0 = 0$ at the surface of the equilibrium configuration, it follows that $\delta P = 0$.

This form has the advantage of making the conjugate of the term $\frac{d(r^2 \delta r)}{dr}$ appear, which also arises in the perturbed continuity equation (Eq. 2.95). This makes it possible to use this equation in the expression and return to a mass integral. This allows Eq. 2.118 to be rewritten as

$$-\sigma^2 \int_0^M |\delta r|^2 dm = - \int_0^M \frac{\delta P \delta \rho^*}{\rho^2} dm + \int_0^M 4g \frac{|\delta r|^2}{r} dm. \quad (2.120)$$

Taking the imaginary part of this and recalling $\frac{\delta P \delta \rho^*}{\rho^2} = \delta P \delta v^*$ yields

$$2\omega \eta \int_0^M |\delta r|^2 dm = - \int_0^M \Im(\delta P \delta v^*) dm. \quad (2.121)$$

In this expression, the growth rate can be isolated:

$$\eta = -\frac{1}{2\omega} \frac{\int_0^M \Im(\delta P \delta v^*) dm}{\int_0^M |\delta r|^2 dm} = \frac{dW/dt}{2E_m}. \quad (2.122)$$

The last expression has been obtained using Eqs. 2.117 and by defining E_m as the energy of the mode according to

$$E_m = \frac{\omega^2}{2} \int_0^M |\delta r|^2 e^{2\eta t} dm. \quad (2.123)$$

The justification of why that represents the energy of the mode can be obtained by taking the derivative of Eq. 2.123 which provides:

$$\frac{dE_m}{dt} = \eta \omega^2 \int_0^M |\delta r|^2 e^{2\eta t} dm = 2\eta E_m, \quad (2.124)$$

so that this expression is exactly identical to the one obtained for dW/dt in Eq. 2.122. Since the mean power is, by definition, the rate of change of the energy with time, E_m is therefore identified as the mode energy.

Subsequently, one can show that, using a similar decomposition as the state equations introduced in Sec. 2.4.1, the following identity holds:

$$\frac{\delta P}{\rho} = c^2 \frac{\delta \rho}{\rho} + (\Gamma_3 - 1) T \delta s, \quad (2.125)$$

$$\frac{\delta T}{T} = (\Gamma_3 - 1) \frac{\delta \rho}{\rho} + \frac{\delta s}{c_p}. \quad (2.126)$$

Gathering successfully these equations in the numerator allows to show that

$$\eta = -\frac{1}{2\omega} \frac{\int_0^M \Im \left(T \delta s \frac{\delta T^*}{T} \right) dm}{\int_0^M |\delta r|^2 dm}. \quad (2.127)$$

This is in fact a very important result. The appearance of entropy in this term shows that the vibrational stability of the mode is directly linked to the non-adiabatic nature of the pulsations. This entropy term can also be replaced by its expression given in the perturbed energy equation (Eq. 2.108) to give the final expression of the growth rate:

$$\eta = -\frac{1}{2\omega} \frac{\int_0^M \Re \left(\frac{1}{\sigma} \left(\frac{d\delta L}{dm} - \delta \varepsilon \right) \frac{\delta T^*}{T} \right) dm}{\int_0^M |\delta r|^2 dm}. \quad (2.128)$$

This expression is even more important, as it shows that the condition for an unstable mode is that, during the hot phase (when $\delta T^*/T > 0$), the gas must receive energy from its surroundings, meaning $\left(\frac{d\delta L}{dm} - \delta\epsilon\right) < 0$. Conversely, during the cold phase (when $\delta T^*/T < 0$), the gas must release energy to its surroundings, meaning $\left(\frac{d\delta L}{dm} - \delta\epsilon\right) > 0$.

2.4.3 Carnot cycle

This conclusion is in fact very similar to what occurs in a car engine, and an analogy can be drawn between the two phenomena. To illustrate this, one may consider the idealised case of a Carnot cycle, whose pressure–volume diagram (P - V) is shown in Fig. 2.11.

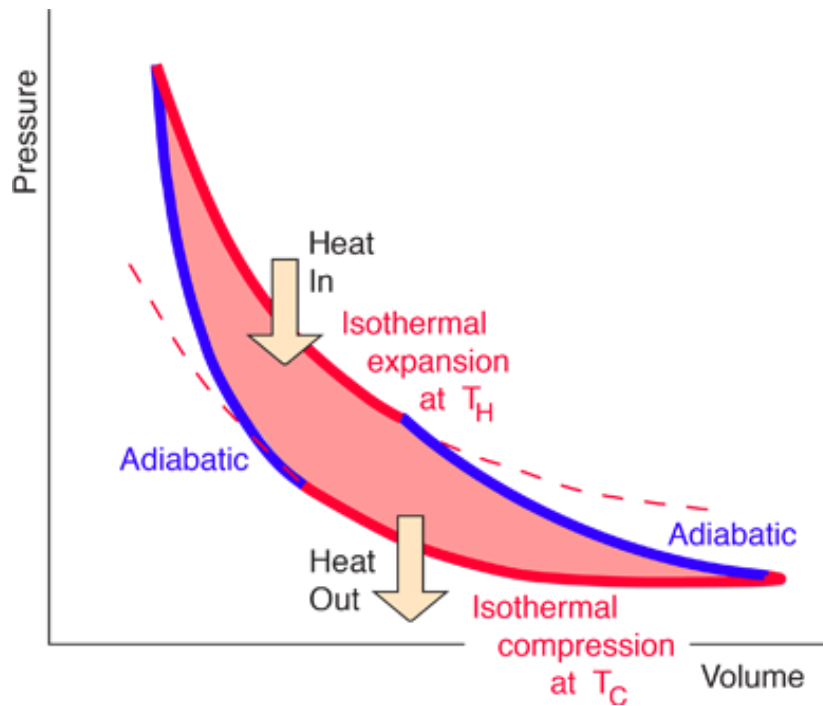


Figure 2.11: P - V diagram of the Carnot cycle. The four stages of the cycle are clearly visible. The area enclosed by the cycle, highlighted in pinkish-red, corresponds to the work produced during the cycle. This diagram is taken from Ref. [8].

As a reminder, the Carnot cycle consists of four phases. The first is an isothermal expansion at the hot temperature, during which the gas receives heat from its surroundings. The second is an adiabatic expansion, during which the gas continues to expand without heat exchange and its temperature decreases. The third phase is an isothermal compression at the cold temperature, during which the gas releases heat to its surroundings. Finally, the fourth phase is an adiabatic compression, during which the gas is compressed without heat exchange and its temperature increases, returning the system to its initial state. In addition, the area enclosed by the cycle in Fig. 2.11 represents the total work of the cycle, which is therefore converted into mechanical energy.

For pulsations, the thermodynamic cycle is quite similar. However, it is not possible to directly associate each phase with one of the four phases of the Carnot cycle. Nevertheless, the main principle remains the same: the gas must absorb heat during the hot phase and release heat

during the cold phase. Here as well, the total area enclosed by the cycle in the P - V diagram represents the total work transferred by the gas to the pulsational motion.

2.4.4 κ mechanism

It has been shown in Sec. 2.4.2 that the condition for a thermodynamic driving cycle is that the system receives energy during the hot phase and loses energy during the cold phase. However, the physical mechanism responsible for this behaviour has not yet been discussed. Focusing on the envelope where no nuclear reaction takes place, the condition in the hot phase for an unstable mode is simply:

$$\frac{d\delta L}{dm} < 0. \quad (2.129)$$

Several quantities can in fact be at the origin of luminosity variations within the star. These are clearly described by Eq. 2.101 and correspond to changes in opacity, radius, and temperature. Generally, the opacity term is considered to be the main driver of the pulsations through a mechanism known as the κ -mechanism. Other processes can also excite stellar pulsations, although the κ -mechanism is widely believed to be the dominant driving process in Cepheids [26].

To understand this mechanism, it is important to recall from Sec. 2.2.4 the existence of the ionisation layers, where the ionisation of helium (He I and He II) and hydrogen mainly takes place. Moreover, it has also been shown in Sec. 2.2.6 that, due to ionisation, photon-matter interactions were more numerous in those regions, creating opacity bumps. Consider such a bump in a given ionisation zone, illustrated in Fig. 2.12.

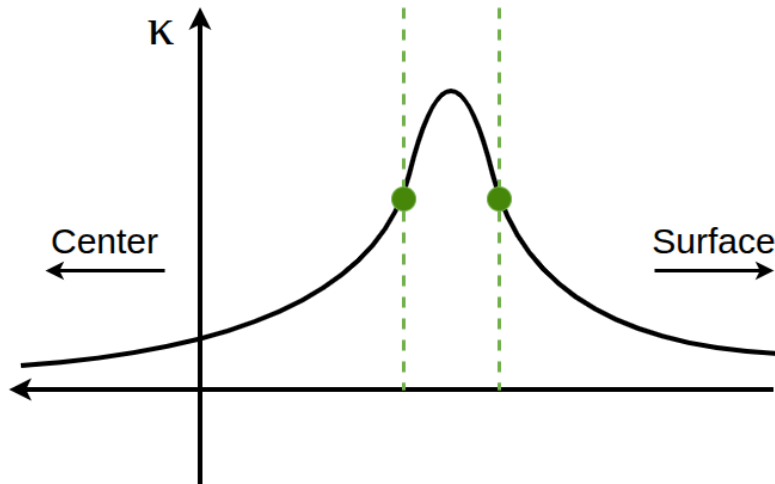


Figure 2.12: Simplified diagram of an opacity-bump ionisation zone. The layer under consideration, delimited by the green dots and the green dashed lines, is initially symmetric with respect to the opacity bump.

The green dots in that figure indicate the boundaries of the considered layer. Now consider the layer undergoing compression. Such compression induces a rise in temperature within the layer. This corresponds to the hot phase. On the opacity-temperature diagram, this temperature increase shifts the two boundaries of the layer towards higher temperatures. However, since the location of the opacity peak is primarily determined by temperature, it remains unchanged. This behaviour is illustrated in Fig. 2.13.

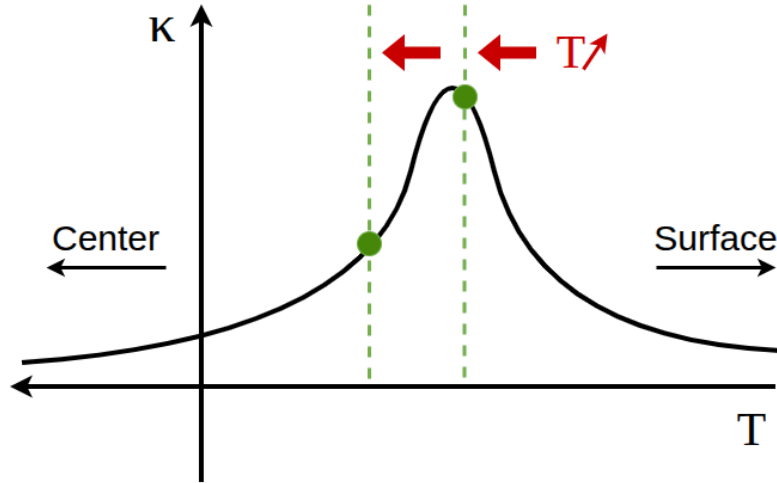


Figure 2.13: Simplified diagram of an opacity-bump ionisation zone during the hot phase. The layer under consideration, delimited by the green dots and the green dashed lines, is shifted toward higher temperatures, while the opacity bump remains at the same temperature. Heat can therefore easily enter the layer but cannot escape as efficiently, resulting in a temporary trapping of energy.

The result is that, during the hot phase, the initial equilibrium between the two boundaries of the layer is disrupted. On the one hand the heat coming from the centre can more easily enter the layer, since the opacity at the inner boundary is lower. On the other hand, it cannot escape as efficiently through the outer boundary, where the opacity is higher.

The expansion of the layer has the opposite effect, as the gas temperature decreases. The two boundaries are therefore shifted towards lower temperatures, while the opacity peak remains once again unchanged. This behaviour is shown in Fig. 2.14. In this phase, the layer releases much more energy than it receives, due to the difference in opacity between its two boundaries.

The behaviour of each layer must be taken into account when characterising the global response of the star, as other layers tend to damp this mechanism. A key quantity is the thermal relaxation time, defined as

$$\tau_{\text{th}} \sim \frac{\int u dm}{L}, \quad (2.130)$$

which represents the characteristic time required for a layer to radiate away its internal energy content. The most relevant layer for the dynamics is then the one for which this thermal timescale is of the same order as the pulsation period, and this defines the so-called transition region. Consequently, a star will pulsate when this region coincides with an opacity peak.

For Cepheids, this pulsational behaviour is driven by the second helium ionisation zone. This condition in fact defines the instability strip: the region of the Hertzsprung–Russell diagram where the pulsation transition region coincides with the opacity peak associated with the second helium ionisation zone. The position of a star with respect to the instability strip is thus determined by the location of the transition region relative to the opacity bump, as illustrated in Fig. 2.15.

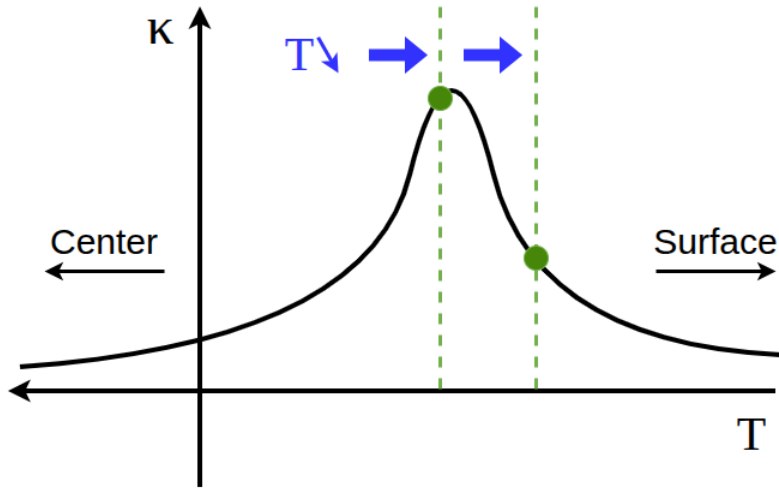


Figure 2.14: Simplified diagram of an opacity-bump ionisation zone during the cold phase. The layer under consideration, delimited by the green dots and the green dashed lines, is shifted toward lower temperatures, while the opacity bump remains at the same temperature. Heat can therefore escape the layer more easily than it can enter it. As a result, more energy is released than absorbed.

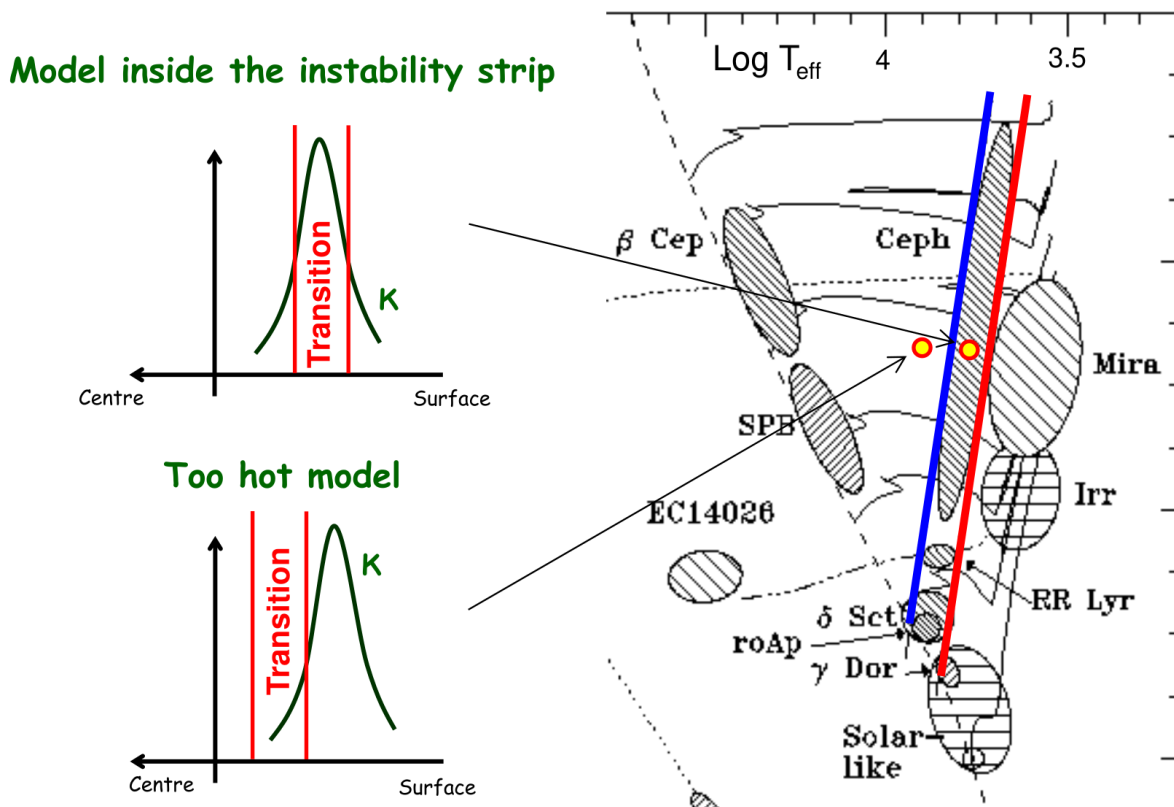


Figure 2.15: Illustration of the position of the transition region relative to the second helium ionisation zone for stellar models located inside and outside the instability strip. Efficient mode excitation occurs when the transition region is located in the vicinity of the He II opacity bump, whereas the two regions are separated outside the instability strip. The figure is adapted from Ref. [8].

2.4.5 Interactions with convection

As convection has been addressed without taking stellar pulsations into account, and stellar pulsations have now been introduced under the assumption of a purely radiative energy transport, no theory for the coupling between convection and pulsation has been presented so far. Moreover, the κ -mechanism responsible for driving Cepheid pulsations is intrinsically radiative in nature.

Although several theoretical frameworks have been proposed to describe the interaction between convection and pulsation, including modified mixing-length theories that attempt to account for pulsational effects [27], these coupled approaches remain significantly more complex than decoupled treatments and still inherit the intrinsic limitations of standard MLT formulations. In particular, the convection-pulsation coupling remains only partially understood and is difficult to model in a consistent and general way, due to the strong non-linearity, time dependence, and non-local nature of convective transport in a pulsating medium. As a result, no fully satisfactory and universally accepted description of convection–pulsation coupling currently exists.

Two limiting cases are, however, interesting to mention when comparing the characteristic timescales of convection and pulsations. The first is the case where the convective timescale is much larger than the pulsation timescale, as observed in stars known as γ Doradus stars. In this case, the radiative flux coming from below the convective envelope cannot be accommodated by convection, which does not have enough time to adapt. As a result, the flux is partially blocked, creating a trapping mechanism that acts as the main driver of the oscillations. This case is known as frozen convection, and several models have been developed to describe it [28, 29].

The other limiting case occurs when the convective timescale is much shorter than the pulsation timescale, as in white dwarfs. This also leads to simpler models [30].

The simulation analysed in this work is not expected to belong to either of these two limiting cases. Instead, the two timescales are believed to be comparable, or at least neither of them is negligible. It is precisely this similarity in timescales that makes the problem particularly difficult to analyse.

Chapter 3

Numerical framework

This chapter presents the numerical framework necessary for the analysis of this work.

After an introduction to CO5BOLD, the code used for the analysed 3D simulation, the simulation setup is described. Finally, CLÉS, the 1D stellar evolution code used for comparison with the 3D results, is introduced.

3.1 CO5BOLD

3.1.1 Generalities

CO5BOLD (COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions, with $L = 2, 3$) is an astrophysical hydrodynamics code designed to simulate realistic compressible convection, winds, and shocks in stellar environments in two or three dimensions. It is important to emphasise that this code is not primarily designed to model stellar pulsations, although such mechanisms can arise from hydrodynamic processes, as will be shown later in this work. The code can also take into account magnetohydrodynamic effects, but it will not be used here.

This code operates mainly in two different configurations. The first is the "box-in-a-star" (local) setup, and the second is the "star-in-a-box" (global) setup. In the box-in-a-star approach, only a small portion of the stellar radius is modelled using a Cartesian computational domain. This typically includes the upper convective layers and extends into the stellar atmosphere. In contrast, the star-in-a-box configuration models the whole star within a single Cartesian grid. It is used for global simulations of stellar structure. In this thesis, only a box-in-a-star simulation is analysed, and the star-in-a-box configuration is not considered.

3.1.2 Numerics

From a numerical and practical point of view, CO5BOLD solves the non-linear equations of compressible hydrodynamics with non-local radiative transport. This corresponds to the conservation equations of mass, momentum, and energy. In this framework, the chosen independent variables in 3D are:

$$\rho, v_x, v_y, v_z, e_{\text{tot}},$$

where v_x , v_y , and v_z denote the components of the velocity field along the Cartesian axes x , y , and z , respectively. The same notation convention applies to all vector quantities throughout this work. The variable e_{tot} represents the total specific energy of the gas. It can be decomposed as follows:

$$\rho e_{\text{tot}} = \rho u + \rho \frac{v_x^2 + v_y^2 + v_z^2}{2} + \rho \psi, \quad (3.1)$$

and is thus the sum of the internal, kinetic, and gravitational potential energies.

Therefore, in Cartesian notation, the mass conservation law of Eq. 2.3 can be rewritten as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} + \frac{\partial(\rho v_z)}{\partial z} = 0. \quad (3.2)$$

The momentum equation (Eq. 2.7) is then written

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho v_x \\ \rho v_y \\ \rho v_z \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho v_x^2 + P \\ \rho v_x v_y \\ \rho v_x v_z \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v_y v_x \\ \rho v_y^2 + P \\ \rho v_y v_z \end{pmatrix} + \frac{\partial}{\partial z} \begin{pmatrix} \rho v_z v_x \\ \rho v_z v_y \\ \rho v_z^2 + P \end{pmatrix} = \begin{pmatrix} \rho g_x \\ \rho g_y \\ \rho g_z \end{pmatrix}, \quad (3.3)$$

with g_x , g_y , and g_z the components of the gravitational field $\mathbf{g}$.

Finally, the energy equation (Eq. 2.22) becomes

$$\frac{\partial(\rho e_{\text{tot}})}{\partial t} + \frac{\partial[(\rho e_{\text{tot}} + P)v_x]}{\partial x} + \frac{\partial[(\rho e_{\text{tot}} + P)v_y]}{\partial y} + \frac{\partial[(\rho e_{\text{tot}} + P)v_z]}{\partial z} + \frac{\partial F_{\text{rad},x}}{\partial x} + \frac{\partial F_{\text{rad},y}}{\partial y} + \frac{\partial F_{\text{rad},z}}{\partial z} = 0. \quad (3.4)$$

The pressure is obtained from the density and internal energy using a tabulated equation of state. The equation of state also provides, from the same input variables, additional thermodynamic quantities. In total, it provides:

$$s; \quad P; \quad T; \quad \left. \frac{\partial P}{\partial u} \right|_{\rho}; \quad \left. \frac{\partial P}{\partial \rho} \right|_u; \quad \left. \frac{\partial T}{\partial u} \right|_{\rho}.$$

The equation of state also accounts for the ionisation balance of hydrogen and helium, as well as representative metal species. From there, all thermodynamic coefficients can be computed using standard thermodynamic relations. For example, for the first and third adiabatic coefficients:

$$\Gamma_1 \equiv \left. \frac{\partial \ln P}{\partial \ln \rho} \right|_s = \frac{\rho}{P} \left. \frac{\partial P}{\partial \rho} \right|_u + \frac{1}{P} \left. \frac{\partial P}{\partial u} \right|_{\rho}, \quad (3.5)$$

$$\Gamma_3 - 1 \equiv \left. \frac{\partial \ln T}{\partial \ln \rho} \right|_s = \frac{1}{\rho} \left. \frac{\partial P}{\partial u} \right|_{\rho}. \quad (3.6)$$

The full list is given in the user guide [31].

Furthermore, some equations are solved for non-local radiative transport, which accounts for the frequency dependence of the opacities. In practice, this is achieved by defining a set of discrete frequency groups. For each group, the opacity is provided by tables as a function of pressure and temperature. From these quantities, the optical depth is computed, which is then

used to determine the specific intensity and, finally, the radiative flux (see Eqs. 2.37, 2.38, and 2.39).

To solve all the governing equations, the code uses a finite-volume approach on a Cartesian grid. Using operator splitting, the multidimensional hydrodynamical equations are reduced to a sequence of one-dimensional problems along each spatial direction. The fluxes at cell interfaces are then computed using a Roe approximate Riemann solver [32]. Concerning the time integration schemes, the code supports several explicit methods, including first-order Euler schemes, the Hancock predictor-corrector scheme, as well as second- and third-order Runge-Kutta schemes (RK2 and RK3). All other specifications may be found in the original presentation article [33].

3.1.3 Turbulence modelling

As already discussed in Sec. 2.3.5, turbulent modelling plays a crucial role in hydrodynamical simulations. In this code, a LES-like approach is adopted in the sense that only the largest eddies are explicitly resolved, since resolving all turbulent scales is not practically feasible.

In practice, the smallest scales are not represented using a classical subgrid-scale turbulence model. Instead, their effect is implicitly accounted for through additional artificial diffusion and artificial viscosity terms. The term "viscosity" is somewhat misleading in this context, as it does not correspond to any physical viscosity but rather acts as a numerical smoothing mechanism applied to velocity gradients. This approach is motivated primarily by the stringent requirements on numerical stability inherent to such simulations. The main challenge is therefore to maintain numerical stability, which is achieved by damping steep gradients through these additional dissipative terms. Furthermore, it is important to emphasise that a significant portion of the numerical dissipation is already provided by the Roe Riemann solver. This intrinsic dissipation is generally sufficient to obtain stable simulations of solar-like stars. However, under the more extreme conditions encountered in Cepheid simulations, additional artificial diffusivity becomes necessary.

3.2 3D simulation setup

3.2.1 General presentation and computational domain

The simulation analysed in this work were performed by Vasiliev et al. This simulation originates from earlier two-dimensional numerical simulations carried out using CO5BOLD by the same group [34, 35]. These 2D simulations, with initial conditions corresponding to a static parallel plane configuration with added perturbations, revealed unexpected self-excited pulsation modes with a period of approximately 2.8 days. These simulations were then extended to a three-dimensional simulation with similar characteristics, leading to the present high-resolution 3D simulation.

The computational domain of the simulation is, as already stated, a fixed Cartesian box with axes x , y , and z . Sphericity and rotation are therefore neglected. Indeed, the Coriolis and centrifugal forces are expected to play a negligible role compared to the gravity and pressure gradients. The z -axis corresponds to the radial direction (neglecting sphericity). The computational box is static and therefore fully Eulerian. Moreover, the origins of the x - and y -axes are located at the sides of the computational box, such that their coordinates are always positive.

In contrast, the origin of the z -axis is defined at the photospheric (surface) level of the star at the initial time, with negative values corresponding to the stellar interior and positive values corresponding to the atmosphere above the surface.

The computational domain contains $n_x \times n_y \times n_z = 600 \times 600 \times 580$ grid points, corresponding to a total of more than 2×10^8 cells. This illustrates the high-resolution and computationally demanding nature of the simulation. The physical dimensions of the domain are given by $L_x \times L_y \times L_z = 1.12 \cdot 10^{12} [\text{cm}] \times 1.12 \cdot 10^{12} [\text{cm}] \times 5.4 \cdot 10^{11} [\text{cm}]$. The grid points are equidistant and thus have spacings $\Delta x = \Delta y = 1.88 \cdot 10^9 [\text{cm}]$ and $\Delta z = 9.38 \cdot 10^8 [\text{cm}]$. This will be shown in Ch.4, but one can already anticipate that this simulation covers approximately 1/6 of the total size (in terms of radius) of the star and is thus not negligible at all compared to the stellar radius. This estimate does not take into account the region beyond the photosphere (the stellar surface), since the simulation extends further.

The size of the computational domain is, as will be shown later, sufficient to encompass the entire convective envelope as well as the extended region beyond the Schwarzschild boundary resulting from overshooting. The latter is relatively small compared to the solar case, making such a setup possible. It is therefore possible to analyse the convection-pulsation coupling as a whole. It also contains a part of the atmosphere and the simulation also encompasses the entire transition region presented in Sec. 2.4.4, where the thermal timescale and the pulsation period are of the same order. This makes it possible to directly analyse the full thermodynamic cycle of the pulsations. Finally, in terms of horizontal extent, it will again be shown later that the computational domain is much larger than the characteristic size of the downflow regions, thereby enabling a proper description of the large convective structures while maintaining a high spatial resolution.

In terms of time, the present simulation covers approximately 5.2 days of stellar evolution, corresponding to slightly less than two full pulsation periods. The duration of the simulation is, both in terms of simulated time and computational cost, significantly larger than that of most simulations of the same kind. This is because it is necessary to follow the entire pulsation cycle, which has a relatively long period and, as will be shown later, involves large variations in several physical quantities. This differs substantially from many other applications of CO5BOLD that do not involve long-period pulsations. In such cases, a much shorter simulation interval is sufficient to obtain realistic temperature and radial velocity profiles.

3.2.2 Model specifications

Concerning the model specifications, the chemical composition is imposed in terms of the mass fractions X , Y , and Z , corresponding respectively to hydrogen, helium, and heavier elements (metals). Their values are given by:

$$X \simeq 0.703, \quad Y \simeq 0.279, \quad Z \simeq 0.018. \quad (3.7)$$

Additionally, the gravity field is assumed to be uniform on the box and thus takes the form:

$$\mathbf{g} = \begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -g \end{pmatrix}, \quad (3.8)$$

where $\log(g [\text{cm/s}^2]) = 2$ for the simulation. This assumption is common to all star-in-a-box simulations performed with CO5BOLD. Furthermore, the nominal effective temperature $T_{\text{eff},n}$ of the model is :

$$T_{\text{eff},n} = 5600 [\text{K}]. \quad (3.9)$$

This value serves as a reference temperature and can be interpreted as a target effective temperature of the model. Since pulsations develop in the simulation, the real effective temperature varies significantly, as will be shown in Ch. 4. In practice, this nominal effective temperature appears in the boundary conditions of the problem.

3.2.3 Boundary and initial conditions

At this point, the kinematic boundary conditions of the problem are first discussed. Lateral boundary conditions are periodic, while the upper and lower boundaries are imposed such that the mass flux vanishes. These conditions therefore act as rigid walls. This represents a first important limitation of the present study. Indeed, the physical system under consideration involves stellar pulsations, which are, by definition, characterised by significant matter displacements, whereas the present numerical setup constrains such motions at the boundaries. This choice is motivated by several practical considerations. It is in fact not straightforward to design more physically adapted boundary conditions while simultaneously ensuring mass, energy, and momentum conservation at the boundaries, as well as maintaining numerical stability. A major advantage of the present approach is therefore its simplicity and robustness. It is worth stressing once again that ensuring the stability of this simulation was particularly challenging. This largely explains why the focus was placed on introducing sufficient dissipation to maintain the stability of the numerical scheme rather than on achieving an exact modelling of turbulence.

Although these boundary conditions are not strictly realistic, they do not compromise the main objective of the study, which is to investigate the underlying driving physics of the pulsations. However, these rigid boundaries may introduce numerical artefacts, in particular in the upper layers of the atmosphere where shock waves can develop. To mitigate these effects, an additional damping layer of 10 grid points is introduced below the upper boundary. Such boundary conditions may also influence the global pulsation properties, for instance, leading to deviations in the pulsation period compared to the actual stellar value, due to the finite size of the computational domain and partial wave reflection at the boundaries. This aspect will be further discussed in the analysis of the results in Ch. 4.

Regarding the thermal boundary conditions, the lower boundary provides an imposed radiative flux directly determined by the nominal effective temperature given in Eq. 3.9. At the upper boundary, the radiative flux is allowed to pass freely through the boundary.

3.2.4 Output files

Several types of output files are produced by CO5BOLD. Among them, the two most relevant for the present work are the "full" and "mean" files.

The first file type simply corresponds to the full output box, providing the complete three-dimensional state of the simulation at a given time step. As stated earlier, this represents more than 2×10^8 grid points for which only the five independent quantities presented in Sec. 3.1.2 are

stored. The remaining physical quantities can then be recovered from the equation of state by the user, for instance, using dedicated IDL routines. Due to the extremely large amount of data involved, these files are particularly heavy and correspond to binary outputs of approximately 4.2GB for each time step in the present simulation. It is therefore not practical to analyse every full 3D box at every time step, making it necessary to select a limited number of carefully chosen snapshots. This selection process will be discussed in Ch. 4.

The second type of file, referred to as the "mean" file, is much easier to manipulate since the data are averaged over each xy plane. As a consequence, the different quantities are only provided as functions of z . In addition, many derived quantities are directly computed by the code and included in these files. This average considerably reduces the amount of data, and for the simulation analysed here, such files only represent about 180MB for 20 time steps. These files can therefore be analysed over the entire duration of the simulation, allowing the study of the temporal evolution of the different vertical profiles. The total number of time steps in the analysed simulation for which the averaged data are available is 1800.

3.3 CLÉS

3.3.1 Generalities

During the analysis, it will be useful to compare the 3D results with those obtained from other models. In particular, comparisons between one-dimensional stellar models and the quantities averaged over each xy plane (mean files) will be of special interest. For this purpose, the selected 1D model is CLÉS (Code Liégeois d'Évolution Stellaire), literally translated as "Liège Stellar Evolution Code" in English, developed by Scuflaire et al. [36]. CLÉS is a stellar evolution code designed to compute stellar evolutionary tracks and the associated internal structures.

The structure equations that are solved by this code are globally the structure equations presented in Ch. 2 for the spherically symmetric model. This is thus described by Eqs. 2.6, 2.13 and 2.30. Note that ϵ_g in the code is slightly modified since it also takes into account chemical differences. For the radiative zones, the gradient is described using Eq. 2.43. The convective zones are found using the Ledoux criterion, which is similar to the Schwarzschild criterion presented in Sec. 2.3.2, but once again taking into account the differences in chemical composition. Finally, these convective zones are described using the mixing-length theory presented in Sec. 2.3.4, with a mixing length parameter α_{conv} that can of course be chosen by the user. The overshooting and undershooting effects are also controlled by the choice of parameters. These models thus have the limitations of local models such as MLT and the Schwarzschild criterion, and comparing them with the 3D hydrodynamical simulation will be particularly interesting, while highlighting these limitations.

Regarding the boundary conditions, the mass and luminosity must vanish as r^3 at the centre. At the outer layers, the simulation is matched to a pre-calculated atmospheric model, which provides the external boundary conditions for the interior structure.

The stellar tracks are calculated starting from an initial model. Then, at each time step, the chemical composition is updated. The equations are not detailed here, as they are not directly relevant to this work. Once this is done, the updated stellar structure equations are solved again until convergence using the Newton–Raphson algorithm.

3.3.2 MAD

The models provided by CLÉS are useful for comparing the profiles of the different quantities. However, they do not capture the temporal variability that will be present in the 3D simulation. As a result, meaningful comparisons will only be possible using time-averaged quantities or at specific phases of the pulsation cycle. It would therefore be particularly interesting to compare them with models that explicitly account for stellar pulsations. To do that, MAD, an extension of CLÉS, was used.

This code, developed by Dupret et al. [37], solves the linear, non-adiabatic perturbation equations for stellar pulsations, as presented in Sec. 2.4.1, starting from a model output by CLÉS. This can also handle non-radial oscillations, but it will not be used here. The result is the computation of the eigenmodes, including their shapes and stability properties, which can be compared with the temporal evolution of quantities in the 3D simulation. These eigenmodes are, however, limited by the linear approximation, and it will be interesting to compare them with "real" pulsations, which are strongly non-linear. MAD also contains a 1D convection-pulsation coupling model [27], so that this study will also be able to highlight its limitations.

Chapter 4

Simulation analysis

This chapter is the most important of this thesis, as it presents the complete analysis of the simulation. It begins with a preliminary study in which relevant coordinates and comparison models are constructed and the simulation is introduced through a global overview. The second part then analyses the main thermodynamical quantities together with quantities related to energy transport. Next, a distinction is made between downflows and upflows in order to gain a deeper understanding of the underlying physical mechanisms of the convective flow. Finally, the chapter concludes by addressing the important question of the thermodynamical cycle, with the aim of identifying the true physical origin of the pulsations.

4.1 Preliminaries

4.1.1 Coordinate system and data representation

Before proceeding to the analysis of the simulation results, it is important to emphasise again that the analysed Cartesian domain is purely Eulerian. This is in fact not well suited for the analysis of pulsational motions. By definition, pulsations naturally cause the star to expand and contract in the radial direction. As will be seen shortly, this results in significant displacements of the photosphere within the Eulerian box. In other words, each stellar layer, corresponding to a given position relative to the stellar radius, moves during the pulsation cycle. Consequently, remaining at a fixed Eulerian position amounts to analysing different regions of the star at different time steps. This therefore makes a detailed analysis of the results impossible. For example, studying the κ -mechanism requires following a given stellar layer, while a complete analysis of the thermodynamic cycle requires tracking the motion of fluid elements.

To remedy this, it is necessary to switch to a Lagrangian description. However, a fully Lagrangian approach, as described in Sec. 2.2.1, which follows individual fluid particles, would be both impractical and difficult to interpret. Indeed, due to the highly turbulent motion and associated mixing, a given particle follows a chaotic trajectory and does not remain associated with a well-defined stellar layer when referenced to the global stellar radius.

A third description is therefore adopted, referred to as a pseudo-Lagrangian description. This approach consists of constructing new coordinates in the z direction that follows the motion of the stellar layers. In other words, it is equivalent to following the mean motion of the fluid rather than individual particles. Instead of using the radius to define the notion of a layer, it is more

convenient to use the integrated mass. The notion of a layer is then redefined as a shell bounded by fixed mass coordinates, which move in radius as the star pulsates. In this framework, the mass contained above and below a given pseudo-Lagrangian coordinate remains constant in time. Note that this is only valid because mass is conserved within the computational box due to the imposed no-flux and periodic boundary conditions. In practice, a function analogous to the mass function presented in Eq. 2.4 is defined, here denoted m_b . This function is equivalent to the standard mass function, except that the integration is restricted to the computational box and is performed between the considered point and the top boundary of the simulation domain. It is given by:

$$m_b(t, z) = S \int_z^{z_{\text{top}}} \rho(t, z) dz, \quad (4.1)$$

where S is the constant surface area of the xy -plane, and the subscripts "top" refers to quantities evaluated at the top of the simulation domain. Numerically, defining the indices n as the time index and i as the spatial quasi-radial index, the function m_b is represented as a 2D array ($n_t \times n_x$), where $m_b[n, i]$ represents the mass present above the point of the box at the z position corresponding to index i at time n . Told like this, it is not very intuitive, but representing graphically the evolution of the quantities with respect to these varying coordinates enables one to visualise the evolution at fixed values of that mass function, and thus at fixed layers.

From this, a second pseudo-Lagrangian coordinate z_0 can be defined, representing the position of a given layer at $t = 0$, which is probably more intuitive than the mass present above the layer for tracking layers, where $t = 0$ is taken as the beginning of the simulation. At each time step, the corresponding z_0 is thus constructed from the Cartesian Eulerian coordinates z , by evaluating m_b at each of these coordinates and interpolating the initial layer positions using the initial mass distribution $m_b[0, i]$. It is thus completely equivalent to m_b but converts that mass into a difference in initial radius. $z_0[n, i]$ therefore represents the initial position of a layer that is now at index i of the box at time n . The resulting z_0 is stored as a 2D array of size ($n_t \times n_z$). The interpolation is represented schematically in Fig. 4.1. Note that since $z = 0$ at $t = 0$ corresponded to the photosphere, this implies that $z_0 = 0$ is the pseudo-Lagrangian coordinate following the photosphere at any time.

The description presented previously is in fact sufficient when one wants to show graphically the evolution of a given quantity q . However, two issues arise. First, it is more convenient numerically to work with time-independent coordinates so that only 1D arrays are considered. Additionally, it will be necessary in the following, especially for the analysis of the thermodynamic cycle, to track at each time step the value of the quantity q for a given layer. This is not yet possible since the quantities are still expressed in Eulerian form, and only the coordinates are updated to account for the motion.

To solve this, one may in fact apply the same interpolation that has been applied to z to construct z_0 , but this time to the quantity q . One thus again computes $m_b(t = 0)$ on the Eulerian grid and then interpolates the value of q at each time step. Doing so, $q_{\text{lag}}[n, i]$ represents the value of q at time n which was initially located at position i at $t = 0$. One can now follow the evolution of the quantity for a layer initially at $i = i^*$ simply by looking at the 1D array $q_{\text{lag}}[n, i^*]$. Graphically, plotting this new q_{lag} in terms of $z(t = 0)$ is thus equivalent to plotting q in terms of z_0 , but now with a 1D coordinate representation. To avoid any confusion in the following graph labels, the quantities will still be denoted without the "lag" subscript, while the z_0 abscissa label will be indicated to denote pseudo-Lagrangian coordinates.

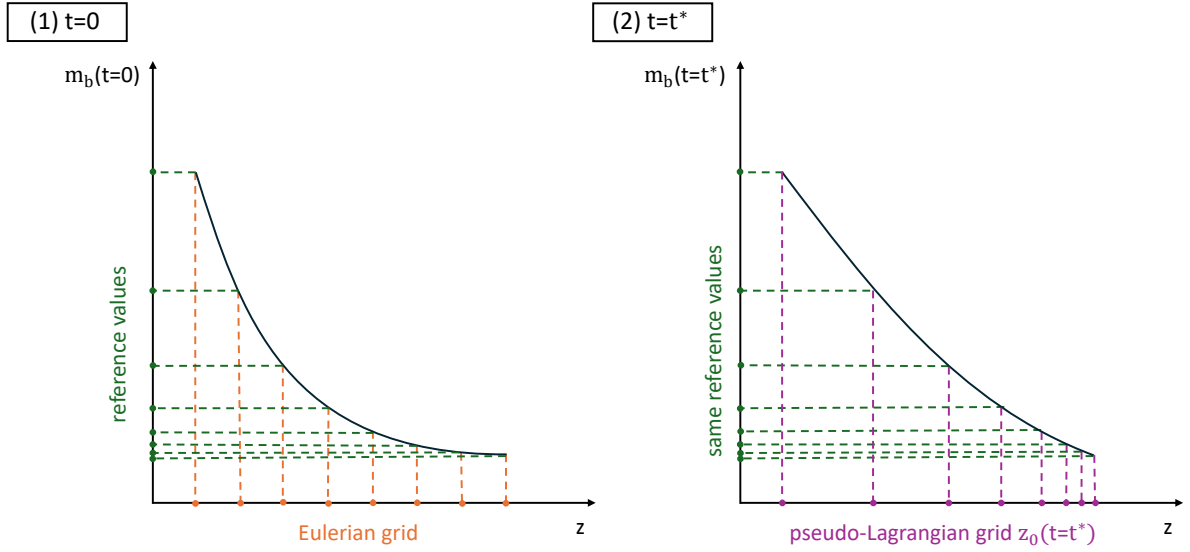


Figure 4.1: Illustration of the procedure used to construct the pseudo-Lagrangian coordinate z_0 at a given time t^* . (1) The initial mass distribution associated with the Eulerian grid is computed. (2) The same mass values are then identified in the mass distribution at time $t = t^*$, allowing the corresponding pseudo-Lagrangian coordinate $z_0(t = t^*)$ to be determined. The initial mass distribution only needs to be computed once, whereas this second step is repeated at each time step. The mass function is equal to zero at the maximum value of z by definition. Its value has been shifted slightly upward in the figure for visibility.

4.1.2 Overview of the simulation

In those preliminaries, it is also interesting to look at the simulation in a more global way before going into a more detailed analysis. The first step is to visualise temporarily the simulation and observe the oscillations. To do that, one good reference is to look at the temporal evolution of the effective temperature of the star, defined through the surface radiative flux as presented by Eq. 2.33. This temporal evolution is displayed in Fig. 4.2.

Fig. 4.2 clearly displays nearly two complete pulsation periods during a total duration of more than 5 days. During these oscillations, the effective temperature of the star varies significantly, from slightly below 5350 [K] to above 5700 [K]. Such a variation is substantial, since stellar properties may differ markedly for stars spanning this range of effective temperatures. Furthermore, the oscillations are clearly not perfectly sinusoidal, as they are intrinsically non-linear. The respective positions and amplitudes of the two maxima and the two minima also differ noticeably, and the simulation seems to be still converging towards its equilibrium oscillatory state, although two periods are, of course, far too few to draw such a conclusion.

For the remainder of the analysis, it is necessary to define a pulsation cycle precisely, since several quantities related to the thermodynamic cycle, for instance the work performed during one oscillation, will be evaluated using a single cycle. Owing to the noticeable differences between the two pulsation shapes, defining such a cycle is not entirely straightforward. In the present study, the pulsation cycle is therefore defined as the interval between the two maxima of the effective temperature. All analyses requiring a single pulsation cycle are performed over this interval, which is illustrated between the dashed lines in Fig. 4.2. This cycle will be referred to as the main cycle.

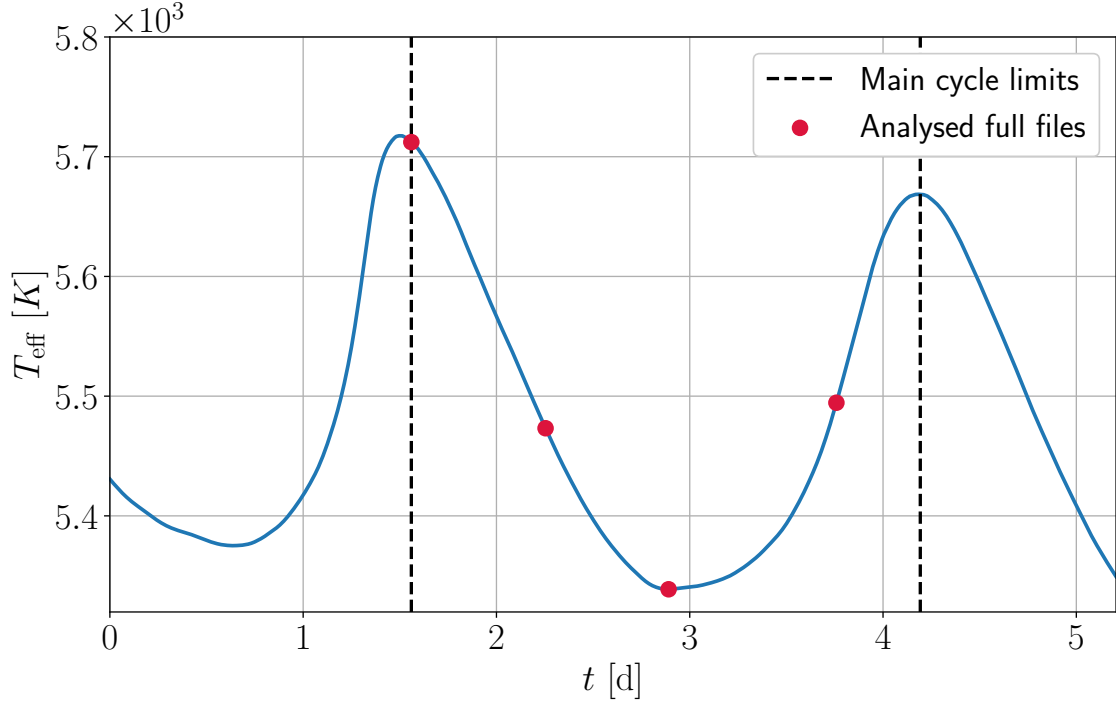


Figure 4.2: Temporal evolution of the effective temperature T_{eff} derived from the radiative flux at the photosphere. The limits of the main cycle are indicated, together with the four time steps selected for detailed analysis.

The cycle is described by four distinct phases. The first one, corresponding to the maximum effective temperature, is called the hot phase. This is the phase where the star is fully contracted and therefore at its hottest. The second phase is the dilatation phase, during which the effective temperature decreases significantly while the star expands. This is followed by the so-called cold phase, where the star is fully expanded and its surface temperature reaches a minimum. The last phase is the contraction phase, during which the star contracts. After this phase, a new hot phase begins, completing the cycle. This definition of the cold and hot phases deserves particular attention, as it is, to some extent, arbitrary. Indeed, due to the strongly non-adiabatic nature of the pulsations, all physical quantities are phase-shifted with respect to one another. The maximum in temperature does not perfectly coincide with the minimum in radius, and similarly for the minimum temperature and maximum radius. It is therefore important, throughout this study, to recall that the different phases are strictly defined with respect to the effective surface temperature. In addition, phase shifts may also occur between different layers of the star, such that the location of maximum surface temperature does not necessarily correspond to the maximum temperature in all other regions. These effects are unavoidable but must be kept in mind when interpreting the results.

Subsequently, it has previously been emphasised in Sec. 3.2.4 that the files describing the full 3D domain are very large, making it impractical to analyse all time steps from the full datasets, in contrast to the mean files, which are used throughout the entire simulation. The selection of which full files to analyse is therefore an important consideration. In this study, the choice has been made to focus on the four phases introduced in the previous paragraph, which are highlighted by red dots in Fig. 4.2. The hot and cold phases correspond thus respectively to the time steps of maximum and minimum effective temperature. For the contraction and expansion phases, the selected times correspond to the instances when the effective temperature reaches

its mean value over the main cycle. It should however be noted that, due to the lower temporal sampling rate of the full files compared to the mean files, these selected snapshots do not coincide exactly with the true extrema or exact mean-crossing times, but represent the closest available time steps.

The computation of time derivatives is also required in this study. To evaluate them, the full files immediately before and after each of the red dots have been analysed too, so that each quantity can be used to compute its time derivative using centred finite differences. This results in a total of 12 different full-box time steps being considered.

4.1.3 Construction of comparison models

The last step before heading to the real analysis is to construct the 1D model that will serve as a point of comparison with the averaged 3D data (mean files).

The goal here is to find a model computed using CLÉS that can be compared to the 3D simulation. Finding a model that is directly comparable is not straightforward either, as the exact evolutionary state of the star is unknown, especially when considering a star crossing the Hertzsprung–Russell diagram in a post-main-sequence phase.

The main parameter that drives the stellar evolution of the star is its mass, which is considered to remain constant during the evolution. The mass that must be considered here is also unknown, although it is expected to correspond to that of a typical Cepheid, thus in the range of 4–20 solar masses. However, the main quantities that must be matched and that are known in this model are, first, the gravity, which is constant and equal to $\log(g [\text{cm/s}^2]) = 2$. Secondly, the range of effective temperatures over which the star oscillates is known in the 3D simulation, and this also allows the surface temperature profile to be constrained. The chosen effective temperature for the model will be taken as the mean effective temperature over the main cycle $\overline{T_{\text{eff}}}^m$, which is equal to

$$\overline{T_{\text{eff}}}^m = 5474.68 [\text{K}]. \quad (4.2)$$

The process to find good models is the following: starting from an arbitrary mass, the evolution track of the star in the $T_{\text{eff}}/\log g$ diagram (called the Kiel diagram, analogous to the HR diagram but using gravity instead of luminosity) is computed. The post-main-sequence phase of the model is then compared to the target point, and the mass is adjusted accordingly. If the model's $\log g$ is too high, the mass is increased and if it is too low, the mass is decreased. This is motivated by the relation $g \propto \frac{M}{R^2}$, where the radius increases significantly for massive stars, and this effect dominates over the increase in g due to mass. This procedure is repeated for several masses until a satisfactory match is obtained. A good match has been found for a stellar mass of $5.475 M_{\odot}$, with a corresponding $\log(g [\text{cm/s}^2]) = 1.99$ and $T_{\text{eff}} = 5472.68 [\text{K}]$. The successful track is displayed in Fig. 4.3.

This has not yet been mentioned, but the results presented here were obtained using a mixing-length parameter for convection $\alpha_{\text{conv}} = 2$. This parameter can significantly affect the evolutionary behaviour of the star and has a strong influence on the temperature, pressure, density, and related profiles. It is known to typically lie in the range $1 \lesssim \alpha_{\text{conv}} \lesssim 3$. Such variations can lead to noticeable differences in stellar structure, and it is therefore interesting to investigate the sensitivity of the models to this parameter. To account for this, additional evolutionary tracks were computed using the same stellar mass but with $\alpha_{\text{conv}} = 1.5$ and $\alpha_{\text{conv}} = 2.5$. These values were chosen because CLÉS is not able to compute models for significantly lower or higher

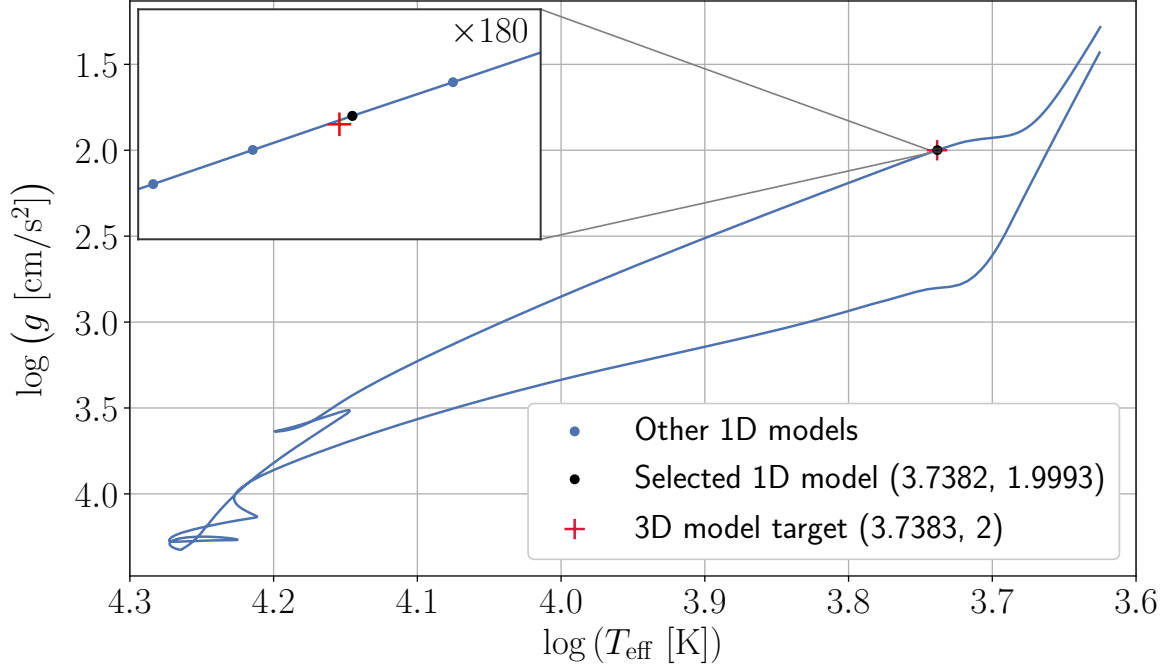


Figure 4.3: Evolutionary track in the Kiel diagram computed with CLÉS for a $5.475 M_{\odot}$ star, from which a model matching the target parameters of the 3D simulation was identified.

values. Keeping the same mass is in fact a simplification intended to avoid the procedure of re-identifying the best-matching mass. This assumption does not guarantee that both T_{eff} and $\log g$ can be matched simultaneously. In practice, for the $\alpha_{\text{conv}} = 1.5$ case, the model that best matched the target in T_{eff} also corresponded to the model that best matched $\log g$, and both criteria selected essentially the same model. In contrast, for the $\alpha_{\text{conv}} = 2.5$ case, the models that best matched T_{eff} and $\log g$ were different, and both differed significantly from the reference solution. In reality, neither of these two models for $\alpha_{\text{conv}} = 2.5$ was used. Instead, a model along the same evolutionary track was selected, which provides the best match to the temperature profile at the base of the simulation. This choice is somewhat abstract at this stage and is intentionally not yet illustrated here for clarity.

Before that, constructing these models provides a useful overview of the simulation setup and complements Sec. 4.1.2. By examining a given radial profile, here the temperature profile, it is possible to estimate how the computational box compares to the stellar model in the 1D description and thus to assess the approximate extent of the domain relative to the stellar structure. This temperature profile is shown in Fig. 4.4 for the three 1D models and the 3D simulation in the cold and hot phases. As a reminder, the coordinate z_0 is negative inside the star and equal to zero at the photosphere. Note that z_0 is directly compatible with the 1D models since those models are static and thus z_0 remains constant. These models are correctly aligned in the plot by taking the stellar surface as a reference.

Fig. 4.4 shows, as already mentioned earlier, that the computational box covers approximately one sixth of the stellar radius predicted by the 1D models. The goal here is not to analyse in detail what is visible in this figure but only to give a spatial overview of the different models. Moreover, in the following sections, the focus will be placed on the computational box so that only the part of the star described by the 3D model is considered, and the deeper interior struc-

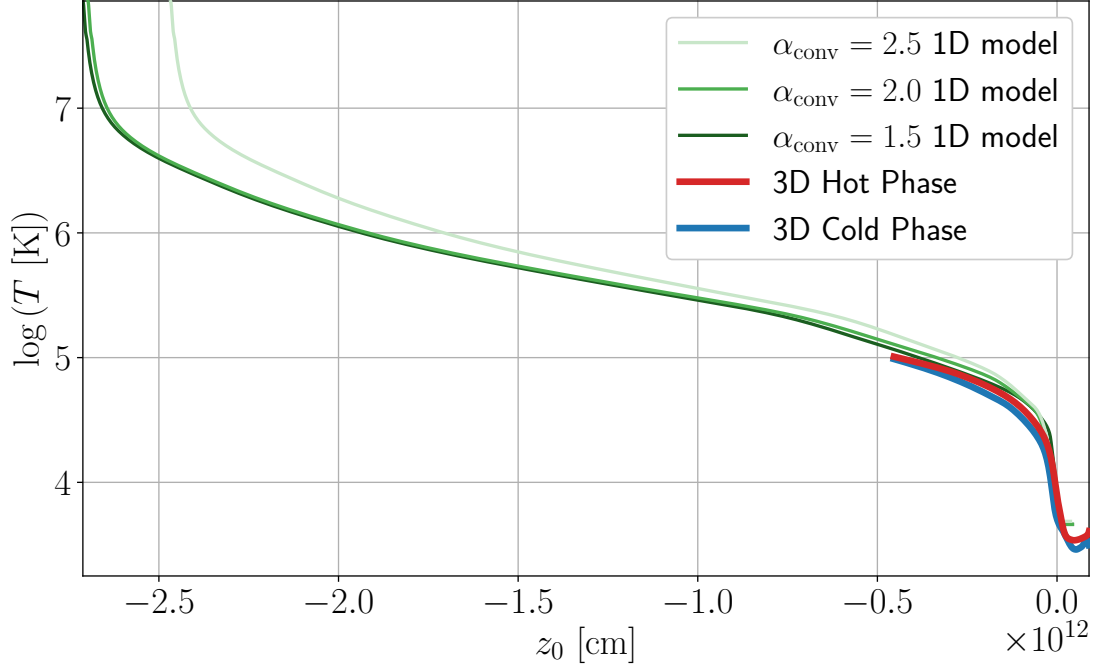


Figure 4.4: Overview of the full logarithmic temperature profiles predicted by three 1D models with $\alpha_{\text{conv}} = 1.5, 2$, and 2.5 , compared with the hot and cold phases of the 3D simulation.

ture is not discussed further. It should thus be kept in mind that the figures presented in the following only represent the outer, superficial part of the star. However, while still considering the full stellar model, it can be noted from Fig. 4.4 that the strong temperature gradients discussed in Ch. 2 are well visible.

For now, three 1D models have been constructed, but pulsational motions are not taken into account in those models. In the comparison with the 1D model, a comparison with eigenmodes predicted by the linear theory of Sec. 2.4.1 will be performed. To obtain those eigenmodes, MAD was used (presented in Sec. 3.3.2). This code enables one first to compute the different eigenmodes of the model. However, a crucial question arises from there: which eigenmodes should be compared with the 3D simulations? This question is not easy at all. In real life, about half of Cepheids are observed to pulsate in the fundamental radial mode, corresponding to the lowest-order global oscillation of the star, in which the entire stellar structure expands and contracts coherently. About 42% pulsate in the first overtone, which is a higher-order radial mode characterised by the presence of one internal radial node, and about 7% pulsate in the second overtone, which contains two radial nodes [38]. These modes are numbered according to their number of nodes, starting from $n = 0$ for the fundamental mode, followed by $n = 1$ for the first overtone and $n = 2$ for the second overtone. In the simulations, it is quite delicate to define a meaningful comparison mode, since the geometry differs significantly between the 1D and 3D cases (spherical versus Cartesian), and the boundary conditions are also fundamentally different. An analogy can be drawn with the eigenmodes of a string between two fixed walls. In this case, the modes correspond to those of the complete star in the 1D representation. On the other hand, the 3D simulation can be seen as taking a subdomain between the two walls and introducing an additional boundary. The eigenmodes are therefore not the same, since a node is imposed at this new boundary.

This situation is analogous for the two simulations, so equivalence cannot be guaranteed. However, the best choice to minimise the differences is still to match the characteristic pulsation period. One should therefore select the eigenmode whose period is closest to that of the 3D simulation (approximately 2.8 days).

Since the frequencies obtained for the three 1D models are very similar, only the case $\alpha_{\text{conv}} = 2$ is considered to present the results computed with MAD. Table 4.1 summarises the properties of the five first modes. It shows that the mode with the closest period is the first overtone ($n = 1$),

Mode n	Period T [d]	Stability
$n = 0$	4.32	Unstable
$n = 1$	2.92	Unstable
$n = 2$	2.24	Unstable
$n = 3$	1.78	Unstable
$n = 4$	1.48	Unstable

Table 4.1: Summary of the first five modes of the 1D model with $\alpha_{\text{conv}} = 2$, showing their mode number, period, and stability.

which is notably quite close. This mode (and the others) appear to be vibrationally unstable (see Sec. 2.4.1). This is expected, since a mode must be unstable in order to be observed in the system. It should be noted that the period of the 3D simulation is not perfectly well-defined, as the signal is not strictly periodic. As a result, the estimated period may vary depending on the method or time interval used for its computation. Despite this uncertainty, the first overtone has been selected for comparison.

With this, the preliminary analysis is concluded, and the main results can now be addressed.

4.2 Basic quantities' analysis

4.2.1 Temperature

1D profile

The first step in analysing the results is to examine the different thermodynamical quantities produced by the simulation. To begin with, it is natural to start with the temperature profile, illustrated in Fig. 4.5 where it is compared with the 1D models. This is simply Fig. 4.4 zoomed into the computational domain, this time using a linear scale on the ordinate instead of a logarithmic one.

In this figure, the first point to notice is the temperature difference between the hot and cold phases. Of course, all layers are expected to warm and cool during the pulsation, but the amplitude of this variation is not uniform throughout the star. In particular, there is almost no variation in the stellar atmosphere ($z_0 > 0$). In the 1D models, this behaviour results from the adopted atmospheric treatment, namely the Eddington atmosphere model, which is known to produce a profile that becomes asymptotically isothermal. For the 3D simulation, the origin of this behaviour is less clear. However, the additional damping layer implemented at the upper boundary to absorb shocks may contribute to it. Furthermore, the surface temperature is similar in both the 1D and 3D models. This is expected, since the effective temperature was matched when constructing these models, but it is more surprising to observe that the interior profiles

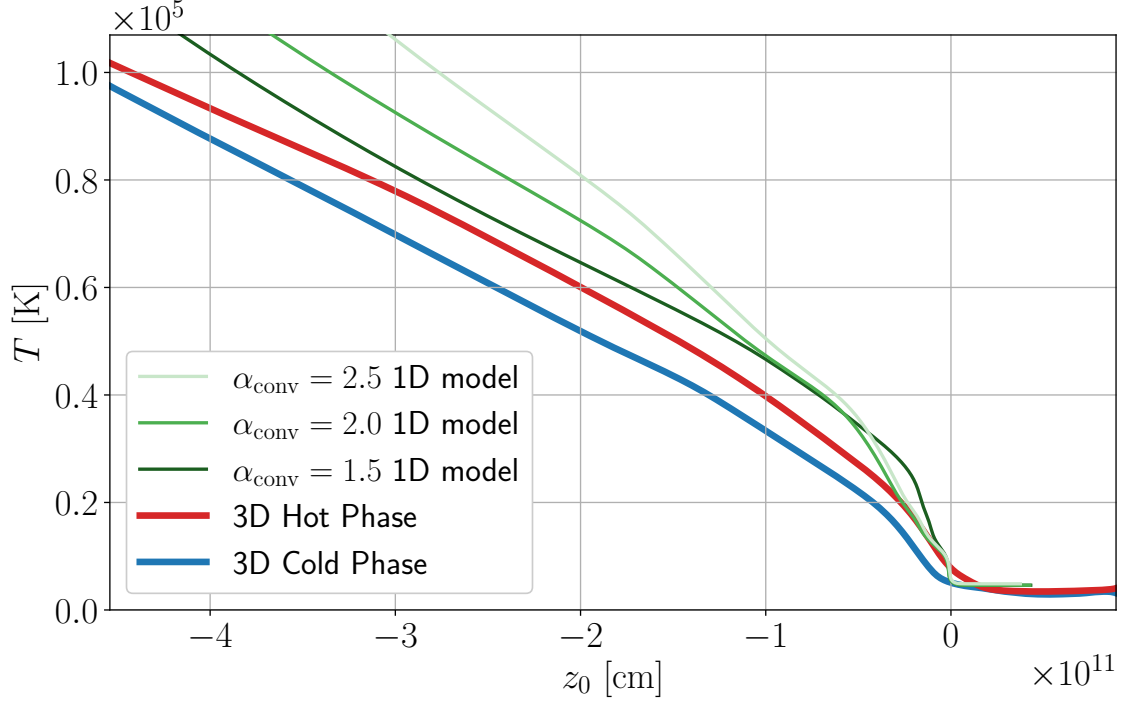


Figure 4.5: Temperature T as a function of the pseudo-Lagrangian radius z_0 for the 3D simulation during the hot and cold phases, compared with those predicted by the three 1D models with $\alpha_{\text{conv}} = 1.5, 2$, and 2.5 .

do not match as closely even if a lower mixing-length parameter seems to improve the match. Note also the big differences between the 1D models due only to the mixing length parameter. In fact, the difference between the 1D and 3D models is larger than the difference between the two phases of the 3D simulation, which already differ significantly from each other and represent two very different behaviours. This may call into question the construction of the models, but before drawing any conclusions, it is good to examine the same profiles using a different coordinate. Instead of using z_0 , the initial pressure P_0 is used as the horizontal axis, together with a logarithmic scale for the ordinate. This coordinate is equivalent to z_0 but follows each layer according to its initial pressure. This is illustrated in Fig. 4.6.

Fig. 4.6 provides a different perspective, where the atmospheric regions are more visible, since they span a larger range of pressure orders of magnitude. This representation is also somewhat surprising, as the behaviour observed for the temperature profiles as a function of radius appears to be reversed. The profiles now seem to converge towards similar values in the stellar interior. This is in fact good news, as it suggests that the considered models are not as far apart as initially thought. This also indicates that the pressure profiles are significantly different and emphasises that the conclusions must be drawn carefully, as the observed behaviour may vary depending on the coordinate system used for the analysis.

In passing, as already stated in Sec. 4.1.3, the model with $\alpha_{\text{conv}} = 2.5$ was not chosen to match either the effective temperature or $\log g$, but was instead matched at the base of the simulation. It is worth revisiting this point, as this choice was made because the model matched in T_{eff} and $\log g$ did not reproduce the same convergence at the base of the simulation in Fig. 4.6. Consequently, a model from the same evolutionary track that better satisfies this condition was selected. It is therefore expected that this model matches more closely, since it was specifi-

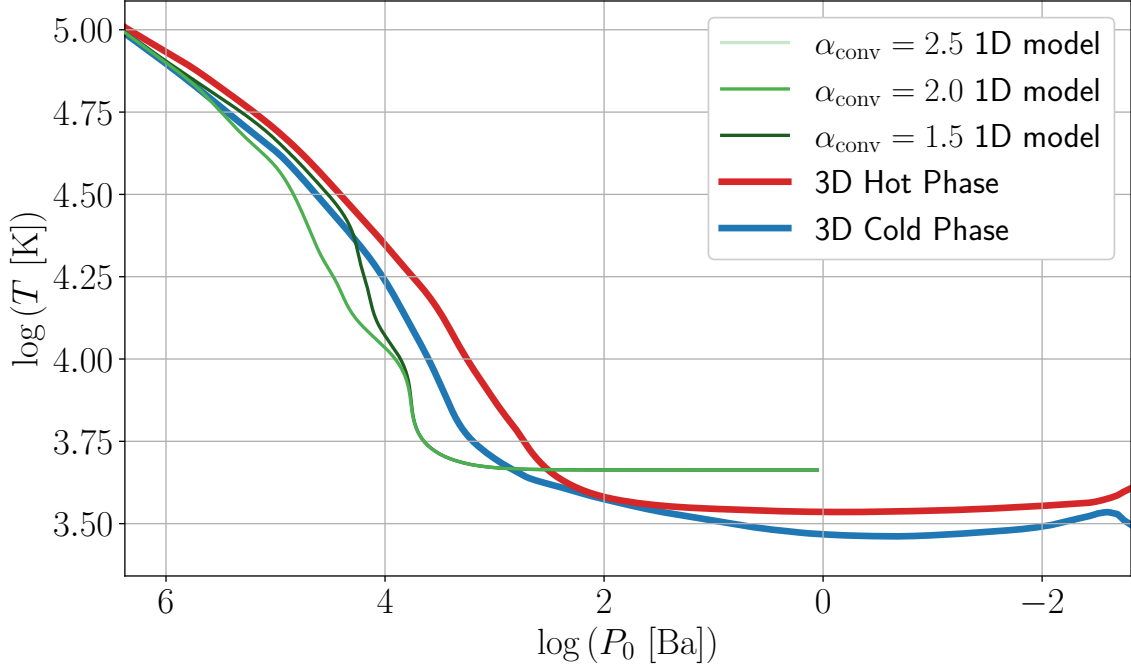


Figure 4.6: Logarithmic temperature $\log(T)$ as a function of the logarithmic pseudo-Lagrangian pressure $\log(P_0)$ for the 3D simulation during the hot and cold phases, compared with those predicted by the three 1D models with $\alpha_{\text{conv}} = 1.5, 2, \text{ and } 2.5$.

cally chosen for this purpose, whereas the other models already matched without requiring any adjustment, based on the standard matching procedure previously presented.

To conclude the discussion about Fig. 4.6, one may already notice a strong temperature gradient near $\log(P_0 [\text{Ba}]) \approx 3.75$, which is not present in the 3D simulations. It can also be noted that the slope of this figure is, by definition, the real gradient ∇ , introduced in Eq. 2.63.

After that, it is useful to visualise the time evolution of the profile in the 3D case. To do that, the relative variation of the temperature with respect to the mean temporal value of each layer can be analysed. Mathematically, and generalising to a given quantity q , it is defined as:

$$\delta q_{\text{rel}}(t, z_0) = \frac{q(z_0, t) - \bar{q}(z_0)}{\bar{q}(z_0)}. \quad (4.3)$$

The evolution of the relative temperature variations, obtained by comparing successive profiles in time during the main cycle, is displayed in Fig. 4.7. For clarity, the evolution of the profiles is separated into phases of expansion and compression. As a reminder, dilatation corresponds to the transition from the hot phase to the cold phase, while compression corresponds to the transition from the cold phase to the hot phase.

Several points can be highlighted from these results. First, the temperature variations are clearly much more significant in the superficial layers, whereas they remain very small at the base of the simulation. A peak is visible just below the photosphere. Furthermore, as already mentioned, the hot and cold phases defined here do not necessarily correspond to the actual temperature maxima and minima at every location in the simulation. Nevertheless, it remains the case throughout the stellar interior, unlike in the atmospheric layers.

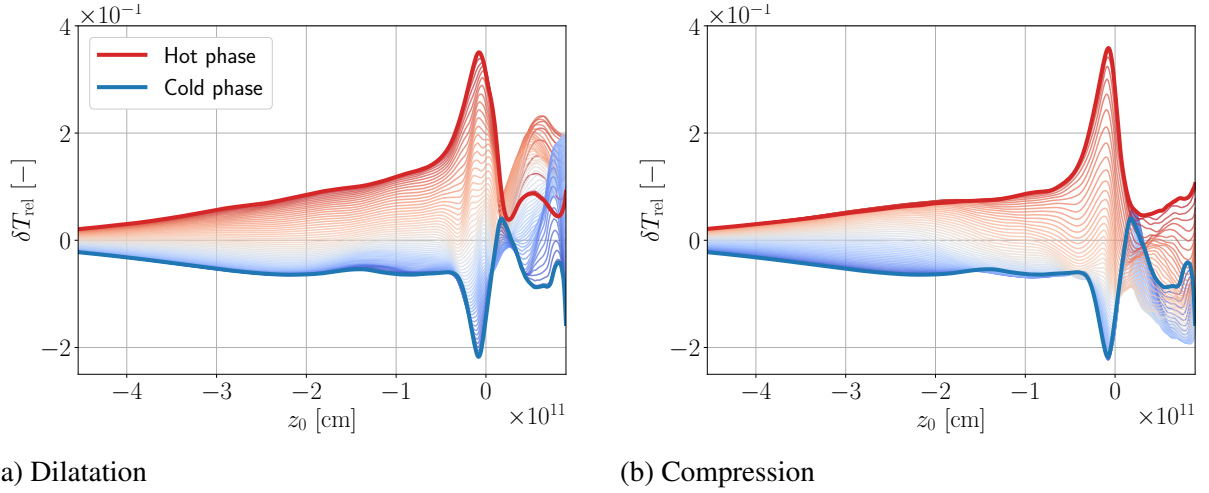


Figure 4.7: Temporal evolution of the relative temperature variation δT_{rel} during the main pulsation cycle. The expansion and compression phases are shown separately.

2D snapshots

The 1D profiles are useful since they provide a global view of the evolution of the layer, but they do not give a clear insight into the convective flow. A more complete understanding can be obtained by analysing the other dimensions of the simulation. In particular, the snapshots correspond to views of the flow in the xy plane at a given z_0 . By examining several such planes at different z_0 , a more comprehensive picture of the flow structure can be obtained.

Starting by looking at a given phase of the pulsation (here arbitrarily chosen as the hot phase), the different snapshots at successive depths can be visualised. This is shown for the spatial relative variations of temperature with respect to the average of the considered layer for six depths in Fig. 4.8. Mathematically, this average is defined for q as

$$\Delta q_{\text{rel}}(t, z_0) = \frac{q(z_0, t) - \langle q \rangle(t)}{\langle q \rangle(t)}. \quad (4.4)$$

The six selected depths were chosen arbitrarily to illustrate the various behaviours encountered in the star and range from relatively deep layers to regions close to the photosphere. Note that the colour bar scales differ from one snapshot to another. This is because the amplitude of the relative variations strongly depends on the layer considered, and although this representation is not the most convenient one, it provides the clearest view of the flow.

Fig. 4.8 shows some radically different behaviours depending on the layer location. At the centre, the temperature appears nearly uniform, suggesting that the region is still part of the radiative zone rather than the convective one. This will of course be checked later. As one moves upwards, convective cells begin to appear. However, rather than classical convective cells, this manifests as small, thin cold regions which correspond to the downward motions since colder elements are denser and sink. As one progresses towards the outer layers, these structures also start to connect and form convective patterns that differ significantly from those shown in Fig. 2.5 for the Sun. Here, the hot upward-moving cells appear particularly large, with a relatively moderate temperature excess. In contrast, the downward structures are very thin but exhibit much larger temperature deviations with respect to the mean. Once the atmospheric layers are reached, these structures disappear, but this region is not of interest in the present

study.

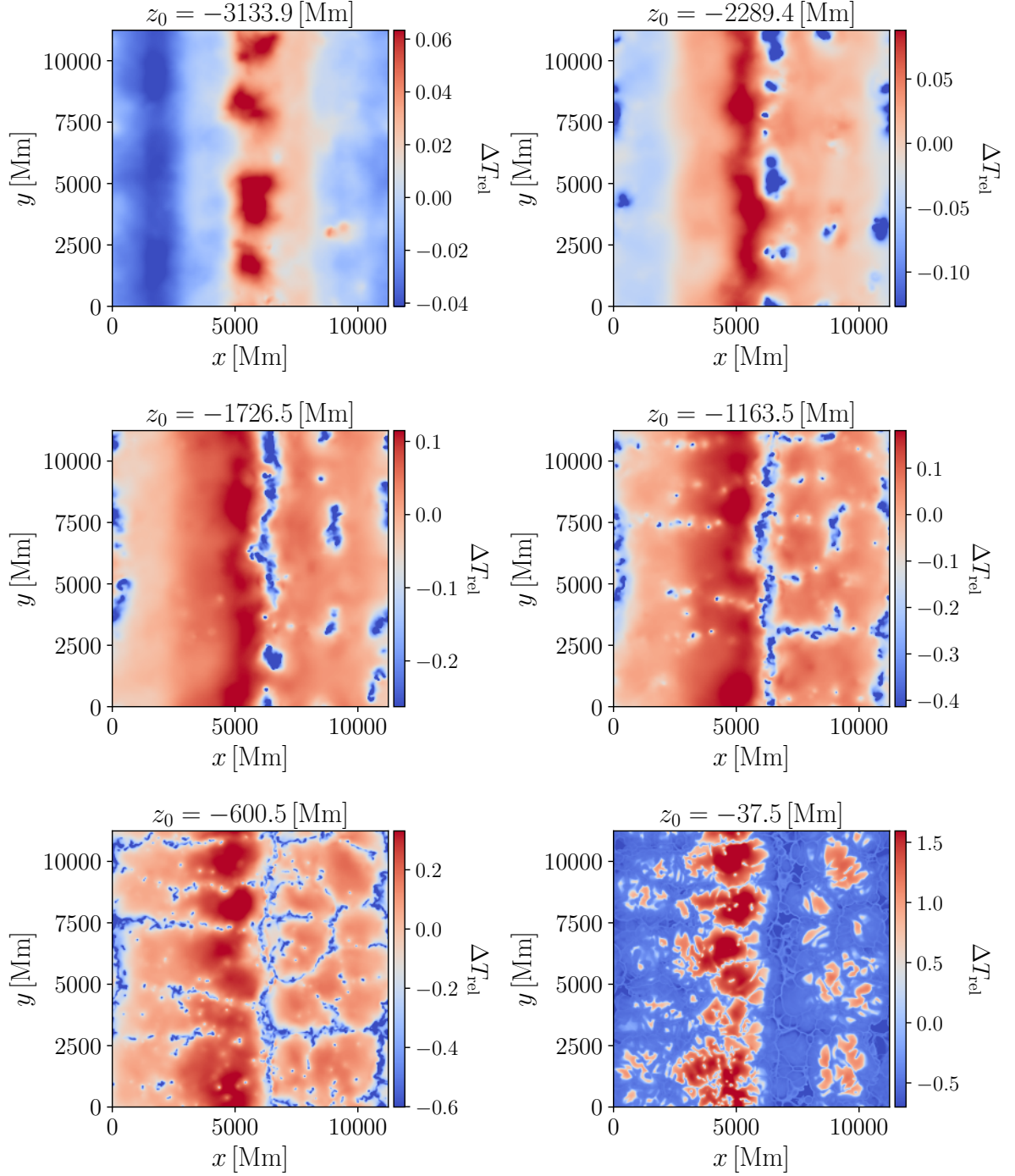


Figure 4.8: Snapshots of the spatial relative temperature variation ΔT_{rel} with respect to the mean value of the considered layer at six different depths during the hot phase. The limits of the colour bar scale are set to the 2nd and 98th percentiles of the data in each snapshot.

In the following, the analysis will therefore focus on the regions where convective motions are present. Note that the colour scale in Fig. 4.8 was truncated to the 2nd and 98th percentiles of each layer to preserve visibility, although the actual values of the downflows extend beyond this range.

Another point of interest is that, in the deeper snapshots, some structures parallel to the y direction are visible. This can be due to two things. The most probable explanation is artefacts from the 2D simulations that were used as initial conditions, suggesting that the simulations may not have fully converged. In fact, the thermal relaxation time is much longer in the deeper layers. As a result, the model has not yet fully relaxed in these regions, and the horizontal structures inherited from the initial conditions are still present. One may also suspect the effect of non-radial modes, which is contrary to the hypothesis made so far (radial mode). This will be checked carefully when addressing the pressure in Sec. 4.2.3.

After that, the snapshots can also be compared temporally at some given layer for the different phases. This is shown in Fig. 4.9 for $z_0 \simeq -1.163 \cdot 10^{11}$ [cm] which corresponds to the location where convective structures are clearly visible in Fig. 4.7. These snapshots were obtained by interpolation between the available depth levels in order to compare all phases at the same depth.

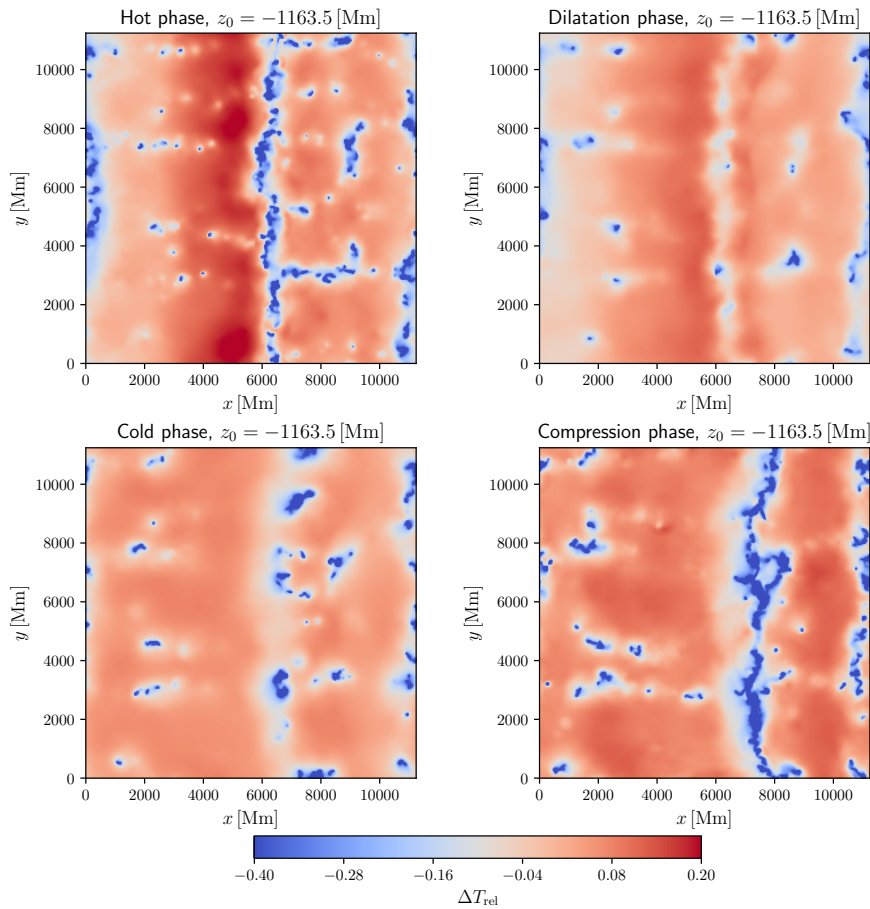


Figure 4.9: Snapshots of the spatial relative temperature variation ΔT_{rel} with respect to the mean value of the considered layer during the four main phases of the pulsation cycle at $z_0 \simeq -1.163 \cdot 10^{11}$ [cm]. The colour scale is here fixed arbitrarily.

In Fig. 4.9, the difference between each phase is visible, with the proportion of upward and downward motions varying significantly depending on the phase, while the temperature variations remain similar. The downward motions appear to occur more in the hot phase than in the cold one. To check how these proportions evolve, the temperature distribution in this layer at each phase is shown in Fig. 4.10.

This shows that the distribution of the different flows varies significantly depending on the

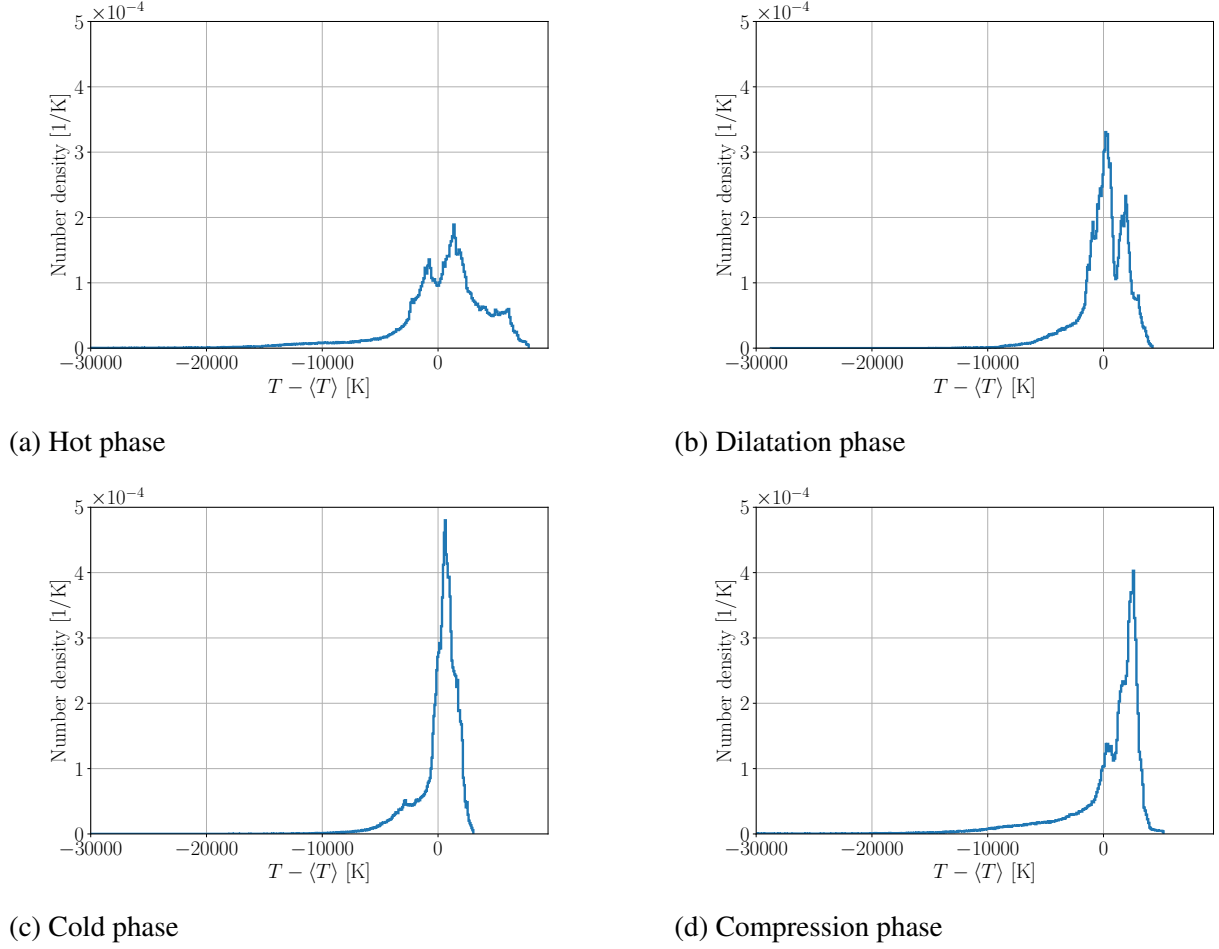


Figure 4.10: Distribution of the absolute temperature fluctuations, $T - \langle T \rangle$, for the four main phases of the pulsation cycle at $z_0 \simeq -1.163 \times 10^{11}$ [cm].

phase, which corroborates what is seen on the snapshots. It also illustrates what has already been seen in the snapshots, namely that temperatures in downflows deviate much more from the mean value. This has an additional implication: downflows span a wide range of temperature values and therefore exhibit a large diversity of properties, whereas upflows are roughly all at the same temperature and are thus nearly identical. Moreover, this figure confirms that the proportion of downflows ($T - \langle T \rangle < 0$) varies significantly from one phase to another, with a higher proportion occurring during the hot phase.

4.2.2 Density

1D profile

One can now move to the second quantity of interest: the density. Its 1D profile as a function of the initial pressure is displayed in Fig. 4.11.

In this figure, the main discrepancy occurs around $\log(P_0 [\text{Ba}]) = 4$, where, while the density profile continues decreasing in the 3D simulations, its derivative changes sign and the density starts to increase. This can be understood easily by starting from the ideal gas law $P = \frac{k_B \rho T}{\mu m_u}$.

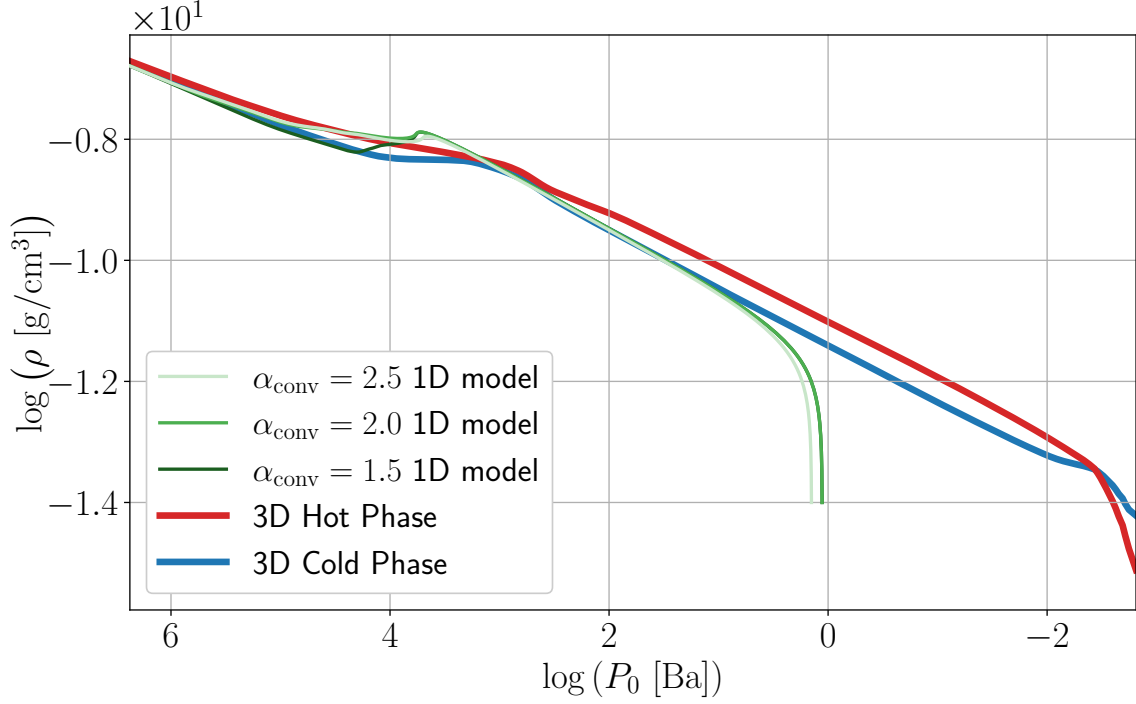


Figure 4.11: Logarithmic density $\log(\rho)$ as a function of the logarithmic pseudo-Lagrangian pressure $\log(P_0)$ for the 3D simulation during the hot and cold phases, compared with those predicted by the three 1D models with $\alpha_{\text{conv}} = 1.5, 2, \text{ and } 2.5$.

Taking the logarithm, assuming a constant molecular weight, and differentiating yields:

$$\frac{d \log \rho}{d \log P} = 1 - \frac{d \log T}{d \log P}. \quad (4.5)$$

The left-hand side is the slope of Fig. 4.11 and can thus change sign if the temperature gradient becomes sufficiently large and exceeds 1 (since $\frac{d \log T}{d \log P}$ is positive as temperature and pressure decrease toward the surface). In fact, this is due to the strong temperature gradient predicted by the 1D model and already mentioned in Fig. 4.11. This clearly highlights how a priori small and seemingly benign differences between two profiles can lead to completely different behaviour of other quantities and emphasises how all profiles are closely related. The same figure also shows that the atmosphere is more extended in the 3D model.

The analysis now turns to the temporal evolution of the profiles as done with the temperature, and it is displayed in Fig 4.12 for the relative variations. Here, large variations are observed at the top of the box. These large relative variations are expected, as the density decreases sharply in these layers. In terms of Eulerian perturbations, this would lead to extremely large perturbation amplitudes. The use of pseudo-Lagrangian coordinates does not completely remove this effect, since these coordinates are not strictly Lagrangian. As for the temperature, the variations are not significant at the base of the simulation but become increasingly important towards the surface. One can notice that the relative variations are much higher here than for the temperature. It is also worth emphasising the strong asymmetry of the profile with respect to zero between the two phases, which highlights the strong non-linearity of these oscillations.

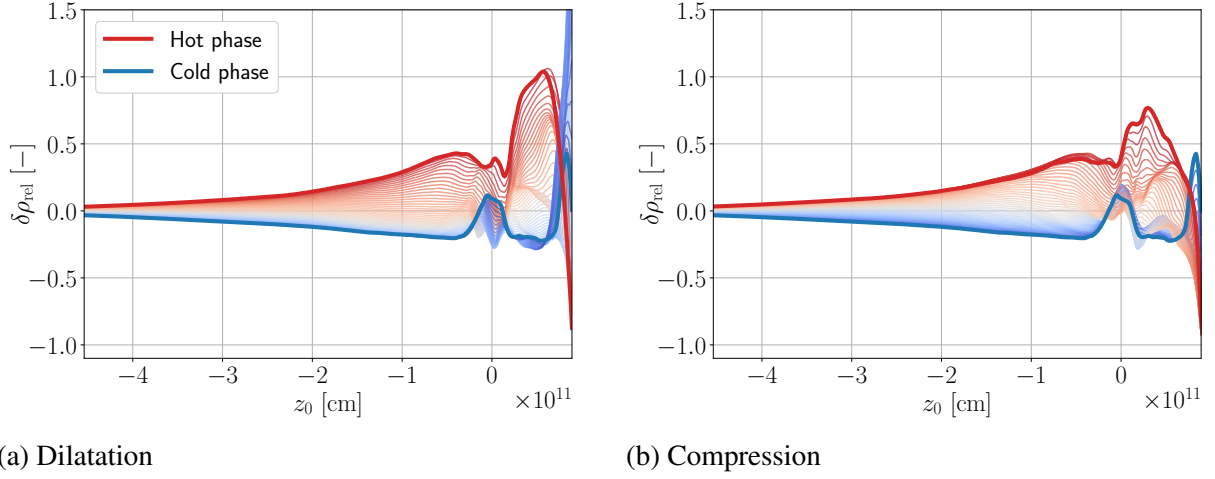


Figure 4.12: Temporal evolution of the relative density variation $\delta\rho_{\text{rel}}$ during the main pulsation cycle. The expansion and compression phases are shown separately.

2D snapshots

The 2D snapshots can also be analysed for the density. These snapshots are shown in Fig. 4.13 for the four phases, this time at a depth closer to the photosphere.

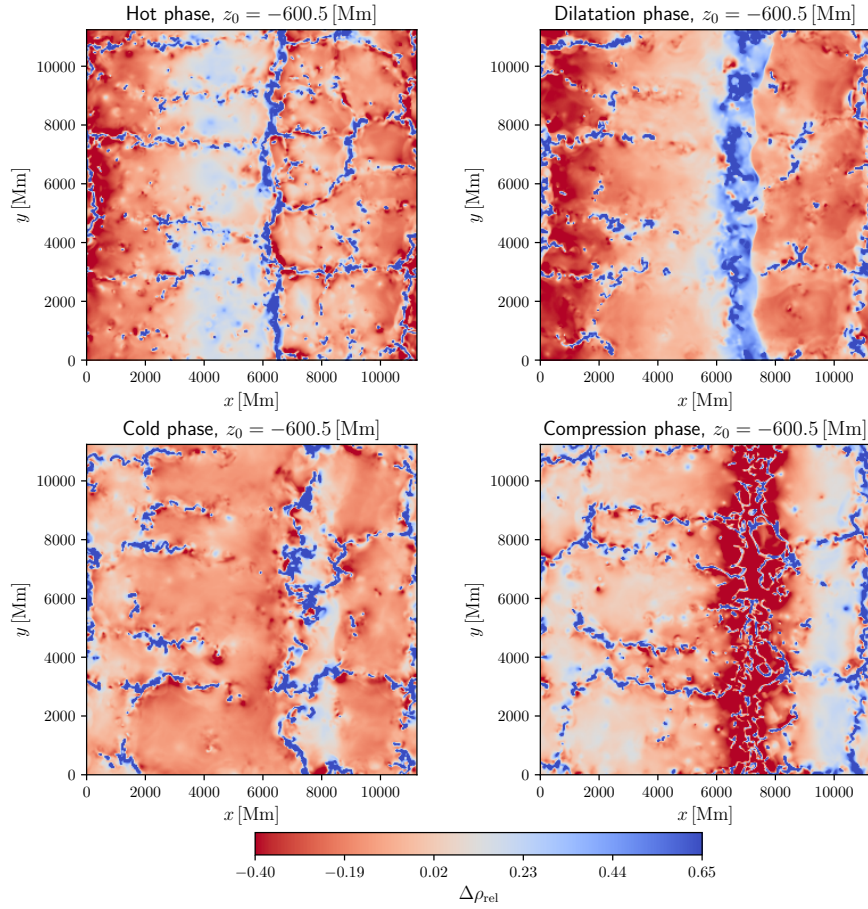


Figure 4.13: Snapshots of the spatial relative density variation $\Delta\rho_{\text{rel}}$ with respect to the mean value of the considered layer during the four main phases of the pulsation cycle at $z_0 \simeq -0.6 \cdot 10^{11}$ [cm]. The colour scale is here fixed arbitrarily.

The conclusion are same than for the temperature, as the same structures are visible with thin downflows and wide upflows. The cold downflows are also denser, and the temperature contrast is stronger in the downflows, while the temperature excess remains moderate in the upflows.

4.2.3 Pressure

1D profiles

The last classical thermodynamical quantity to analyse is the pressure. The 1D profile can be analysed, but this time with respect to the radius. It is presented in Fig. 4.19. The pressure considered here is the gas pressure. There is, of course, also a contribution from the turbulent pressure. However, its analysis is misleading, as it is difficult to separate the velocity component associated with the pulsation from that arising from turbulent motions, the latter being responsible for the turbulent pressure.

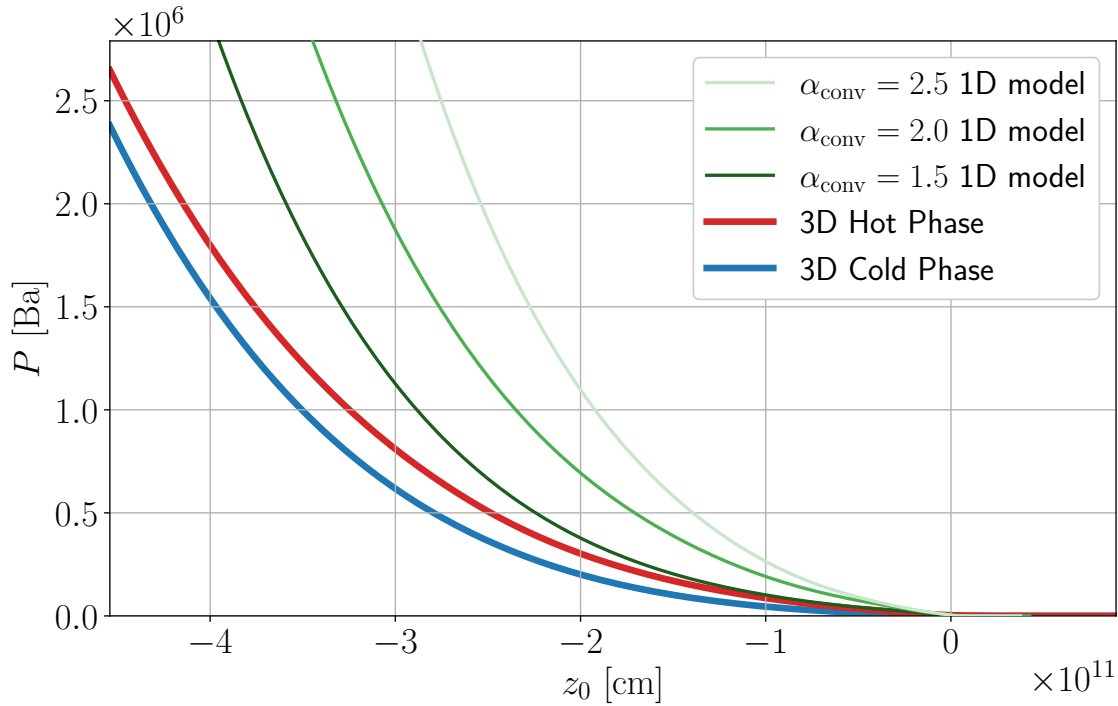


Figure 4.14: Pressure P as a function of the pseudo-Lagrangian radius z_0 for the 3D simulation during the hot and cold phases, compared with those predicted by the three 1D models with $\alpha_{\text{conv}} = 1.5, 2$, and 2.5 .

The profile shown in this figure differs significantly between the 3D simulation and the 1D models. This was somewhat expected, since the temperature profile shown earlier demonstrated that comparing quantities as a function of radius or pressure leads to very different behaviours, already suggesting that the pressure profile would be significantly different.

As previously, one can also show the evolution of the pressure in time. This is displayed in Fig. 4.15. Nothing more to say about that figure, the conclusions are the same as for the temperature and the density. Note, however, the similarity of the curves compared to the curves of the density.

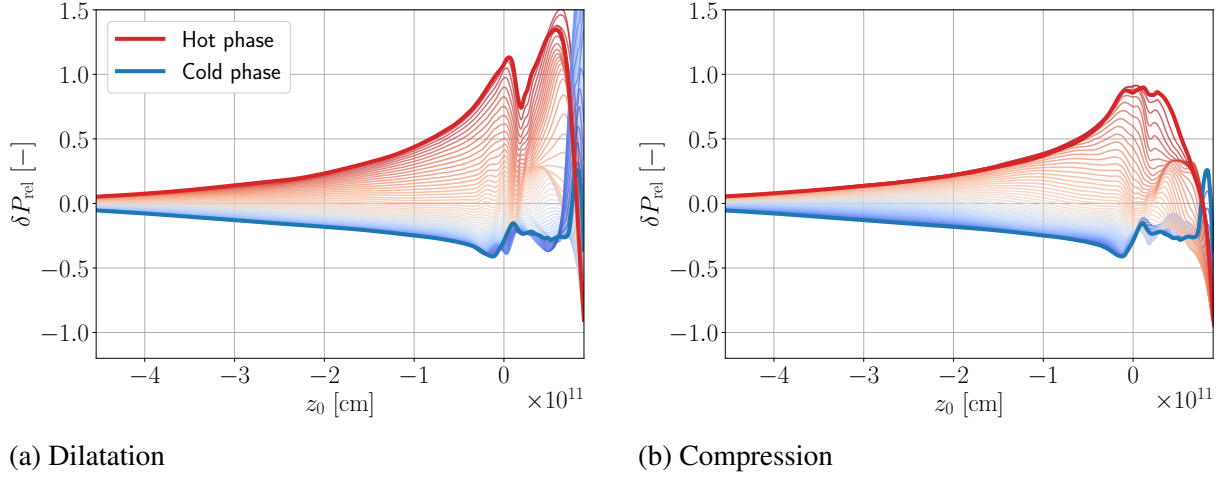


Figure 4.15: Temporal evolution of the relative pressure variation δP_{rel} during the main pulsation cycle. The expansion and compression phases are shown separately.

After that, and for the first time, it becomes possible to compare the 3D model with the eigenmodes obtained using MAD since it provides directly δP_{rel} . For the 3D model, these variations were shown to be non-symmetric in Fig. 4.15. Therefore, the most convenient way to compare the 3D model with the 1D eigenmode is to superimpose the 3D profiles, this time over the whole simulation time, and compare their envelope with the eigenmode shape and its symmetric counterpart, obtained by reversing its sign, it is done in Fig. 4.16. Moreover, note that the eigenmodes are defined up to a multiplicative factor, so a normalisation has been applied. The main point of comparison here is therefore the shape.

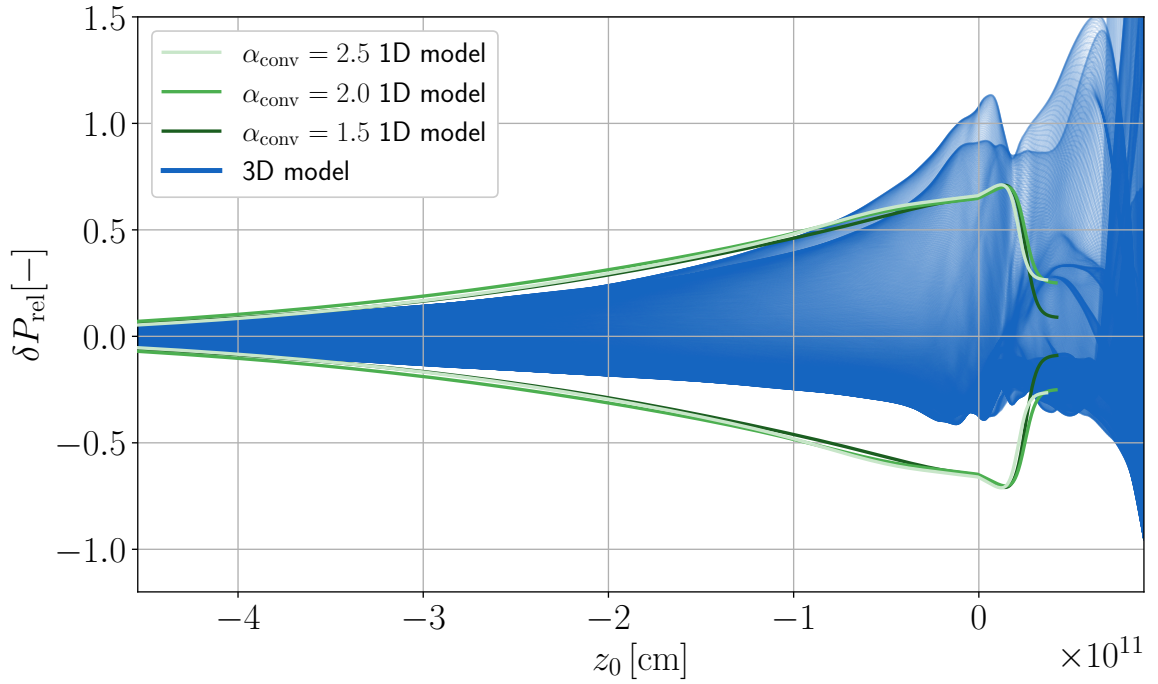


Figure 4.16: Comparison between the envelope of the relative pressure variations δP_{rel} during the whole simulation and the eigenmode shapes of the 1D models with $\alpha_{\text{conv}} = 1.5, 2.0$, and 2.5 . Both signs of each eigenmode are shown.

First, Fig. 4.16 again shows a strong asymmetry of the solution. Secondly, the eigenmodes do not appear to match the 3D simulation closely. This may suggest that the first overtone is not the appropriate mode. However, this analysis has also been performed for both the fundamental mode and the second overtone, and neither appears to provide a satisfactory match. As a consequence, the comparison with the eigenmodes remains difficult, likely due to the significantly different boundary conditions that have already been discussed. An additional effect may in fact play a significant role and help explain such a discrepancy. This time, however, it arises from the assumptions underlying the 3D simulation, namely the use of a constant gravity. One can understand this starting from the perturbed momentum equation in the spherical case, Eq. 2.99:

$$\begin{aligned}\frac{\partial^2 \delta \mathbf{r}}{\partial t^2} &= -\delta \left(\frac{Gm}{r^2} + 4\pi r^2 \frac{\partial P}{\partial m} \right) = -\delta \left(g + 4\pi r^2 \frac{\partial P}{\partial m} \right) \\ &= 4g \frac{\delta r}{r} - \frac{1}{\rho} \frac{\partial \delta P}{\partial r}.\end{aligned}\tag{4.6}$$

Therefore, if gravity is assumed to be constant, its perturbation δg vanishes and the corresponding terms disappear. The perturbed momentum equation then reduces to

$$\frac{\partial^2 \delta r}{\partial t^2} = -\frac{1}{\rho} \frac{\partial \delta P}{\partial r}.\tag{4.7}$$

This form differs significantly from the case where gravity varies with radius. Such a difference in the fundamental equations governing the modes may therefore contribute significantly to the discrepancies observed in the eigenmode comparison. Of course, the 3D simulation does not strictly obey this linear theory, but this already provides a glimpse of the impact of neglecting variations in the gravitational potential. Moreover, strictly speaking, the derivation should be carried out in Cartesian coordinates to match the geometry of the 3D simulation. Nevertheless, the underlying argument remains unchanged.

2D snapshots

The 2D snapshots of the relative pressure variations do not provide much additional information and will therefore not be shown here. However, other pressure snapshots can be analysed to test an important assumption made so far, namely that the oscillations are purely radial. Although Cepheids are generally believed to pulsate in radial modes, it cannot yet be confirmed that this is the case in the present simulation. Moreover, as seen in the snapshots presented in Sec. 4.2.1, some vertical structures appear, which may indicate the presence of a non-radial mode. In fact, observing such non-radial behaviour would be problematic given all the developments presented so far about the radial modes theory and would directly render the MAD models obsolete.

To investigate this possibility, it is useful to examine snapshots of the pressure difference between each phase and an arbitrary reference phase, chosen here as the hot phase. Indeed, in the case of a purely radial mode, the pressure difference with respect to the reference phase should remain nearly uniform across each xy plane. Conversely, the presence of non-radial modes would lead to some regions exhibiting a pressure increase while others exhibit a pressure decrease relative to the reference phase. The snapshots are shown in Fig. 4.17 for 3 different layers, ranging from the deepest layers to the superficial layer, and compared to the pressure at the hot phase P_{hot} .

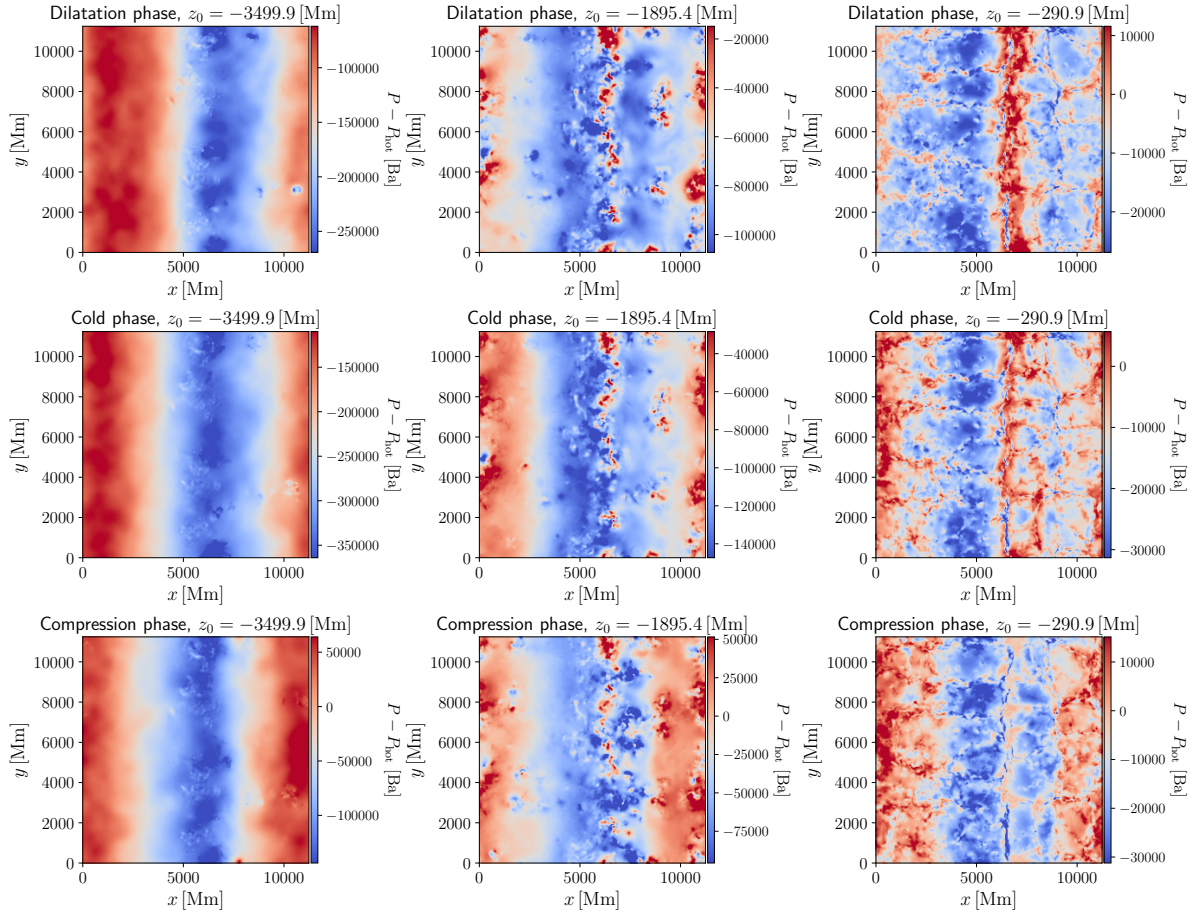


Figure 4.17: Pressure difference $P - P_{\text{hot}}$ relative to the hot phase for three representative layers (deep, intermediate, and superficial) during the three remaining phases of the pulsation cycle.

What is observed is that, in the deeper layers, despite the presence of clear vertical patterns, the pressure perturbations remain of the same sign. At higher altitudes, sign changes begin to appear. However, the radial relative pressure variations shown in Fig. 4.15 are in practice significantly larger than the horizontal relative variations in the layers where these patterns are observed. This suggests that the oscillations remain predominantly radial despite the presence of these vertical patterns, and the assumption of radial pulsations can therefore be considered valid. Note that non-radial modes may still be present, but the point here is to assess whether they are significant compared to the radial modes. Consequently, these discrepancies are instead believed to arise from artefacts related to the 2D initial conditions and the incomplete thermal relaxation of some layers.

4.2.4 Radial velocity

Another relevant quantity for understanding the simulation is the radial velocity, as it allows the layers undergoing the largest expansion and contraction during the pulsation cycle to be identified. Rather than using the classical velocity, it is more convenient to introduce a mass-weighted velocity defined as:

$$v_{z,\rho} = \frac{v_z \rho}{\langle \rho \rangle}, \quad (4.8)$$

with the numerator that represents the mass flux.

Here, the analysis of this quantity is restricted to 1D profiles, as the snapshots are, once again, very similar to the others. The variations in each layer are displayed in Fig. 4.18. Note that these are not relative variations but real values.

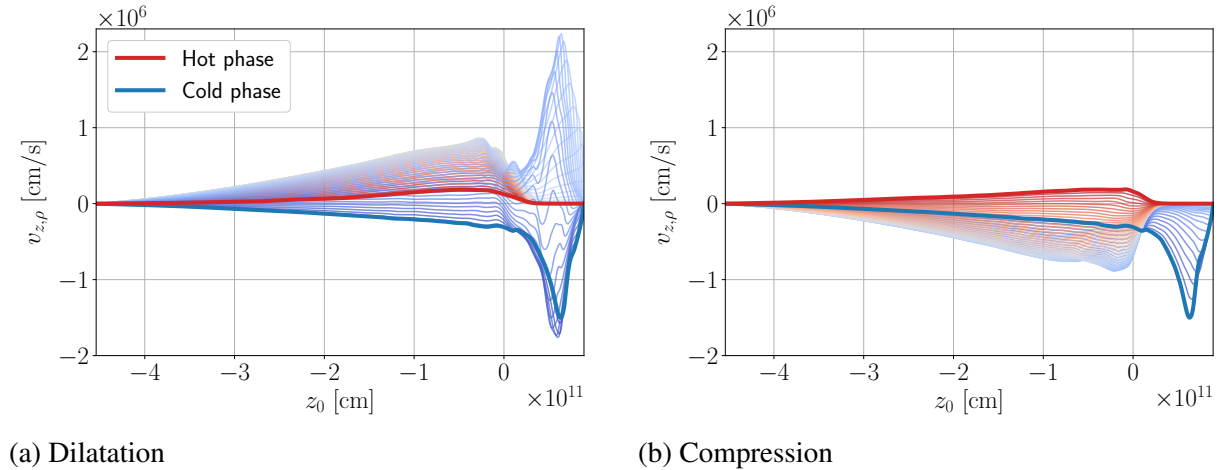


Figure 4.18: Temporal evolution of the mass-weighted radial velocity $v_{z,\rho}$ during the main pulsation cycle. The expansion and compression phases are shown separately.

The phase shift and the complex nature of the pulsations are clearly visible here. In the absence of a phase shift between radius and temperature, one would expect nearly zero velocities during both the hot and cold phases, since these phases would coincide with the reversal of the motion. This is clearly not the case here and highlights the significant difference between the defined hot phase and the phase of minimum radius. The figure also shows which layers undergo the largest radial displacements. As expected, the outer layers exhibit the largest velocities, whereas the inner layers experience only weak pulsations. Note that the boundary conditions are clearly visible in this figure, since both the mass flux and, consequently, the mass-weighted velocity vanish at the domain boundaries. In fact, in the absence of these boundaries, even larger variations could be expected in the outermost layers. This highlights a clear limitation of the zero-mass-flux boundary conditions.

4.2.5 Opacity

For now, all the relevant thermodynamical quantities have been shown to provide a global view of the flow. It is now time to switch to quantities related to energy transport within the star in order to start understanding the energy exchanges in the system. As already stated several times, the κ mechanism is believed to be the driver of these oscillations, and it is thus natural to start with the analysis of its profile. The 1D profile of the opacity is presented in Fig. 4.19.

For the 1D models, Fig. 4.19 clearly shows two opacity peaks corresponding to the different ionisation zones presented in Sec. 2.2.4. The innermost opacity peak corresponds to the second ionisation zone of helium, which is expected to be the driver of Cepheids' pulsations. The second peak corresponds to the first ionisation zone of helium and hydrogen, since these two are in practice indistinguishable as they occur very close to each other.

This shape is once again radically different from the results of the 3D simulations. For these

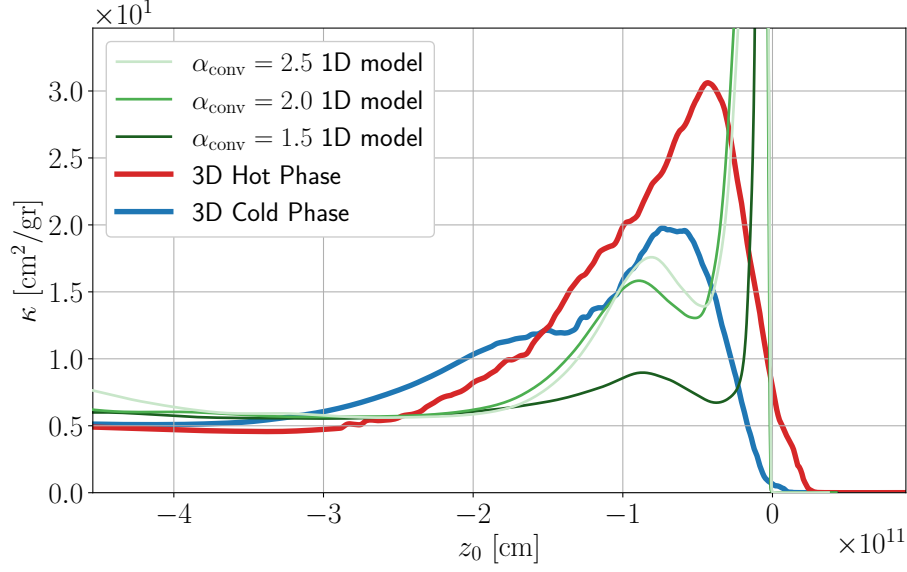


Figure 4.19: Opacity κ as a function of the pseudo-Lagrangian radius z_0 for the 3D simulation during the hot and cold phases, compared with those predicted by the three 1D models with $\alpha_{\text{conv}} = 1.5, 2$, and 2.5 .

simulations, the first noticeable feature is the strong difference in opacity between hot and cold phases, where the opacity varies significantly with phase, since it depends strongly on temperature. The peak seems to slide during the cycle, this is in fact expected since ionisation mainly depends on temperature, and a fixed layer obviously does not have a constant temperature. The ionisations are thus closer to the surface in the hot phase. The two peaks of ionisation are, however, not clearly visible, which may be surprising at first. Nevertheless, the averaged profile corresponds to an average over all flows within each layer, and, as seen earlier, the flow is composed of very strong and thin downflows with very low temperature, high density, and high velocity, while the large upflows remain more moderate in these quantities. Since the opacity in the ionisation zones depends strongly on the local thermodynamic quantities, and since the distributions of temperature and density are already highly heterogeneous, the opacity distribution is expected to be also heterogeneous. This can be checked by showing the distribution of opacities, just as has been done for temperature in Fig. 4.10. It is done in Fig. 4.20 for the exact same layer.

The distribution has similarities but is somewhat different from the temperature distribution. First, most of the values seem to lie within the same range of opacities, and the distribution is more strongly peaked around the mean than the temperature distribution. However, the extreme values relative to the mean are much larger than in the case of temperature, with some points deviating by more than $500 [\text{cm}^2 \text{g}^{-1}]$, whereas the mean value at this depth is approximately $12 [\text{cm}^2 \text{g}^{-1}]$. This highlights how certain regions of the flow exhibit completely different behaviours. These extreme flows are hidden by the averaging process used in the 1D profile description, which explains, in particular, why distinct peaks are not visible in Fig. 4.19. Finally, the spread appears to be larger during the hot phase, which may be related to the greater number of downflows present during this phase. As emphasised several times, the most extreme behaviours appear to be associated with downflows, whereas upflows remain comparatively moderate.

A major conclusion emerges from this analysis: the differences in the properties of the two types

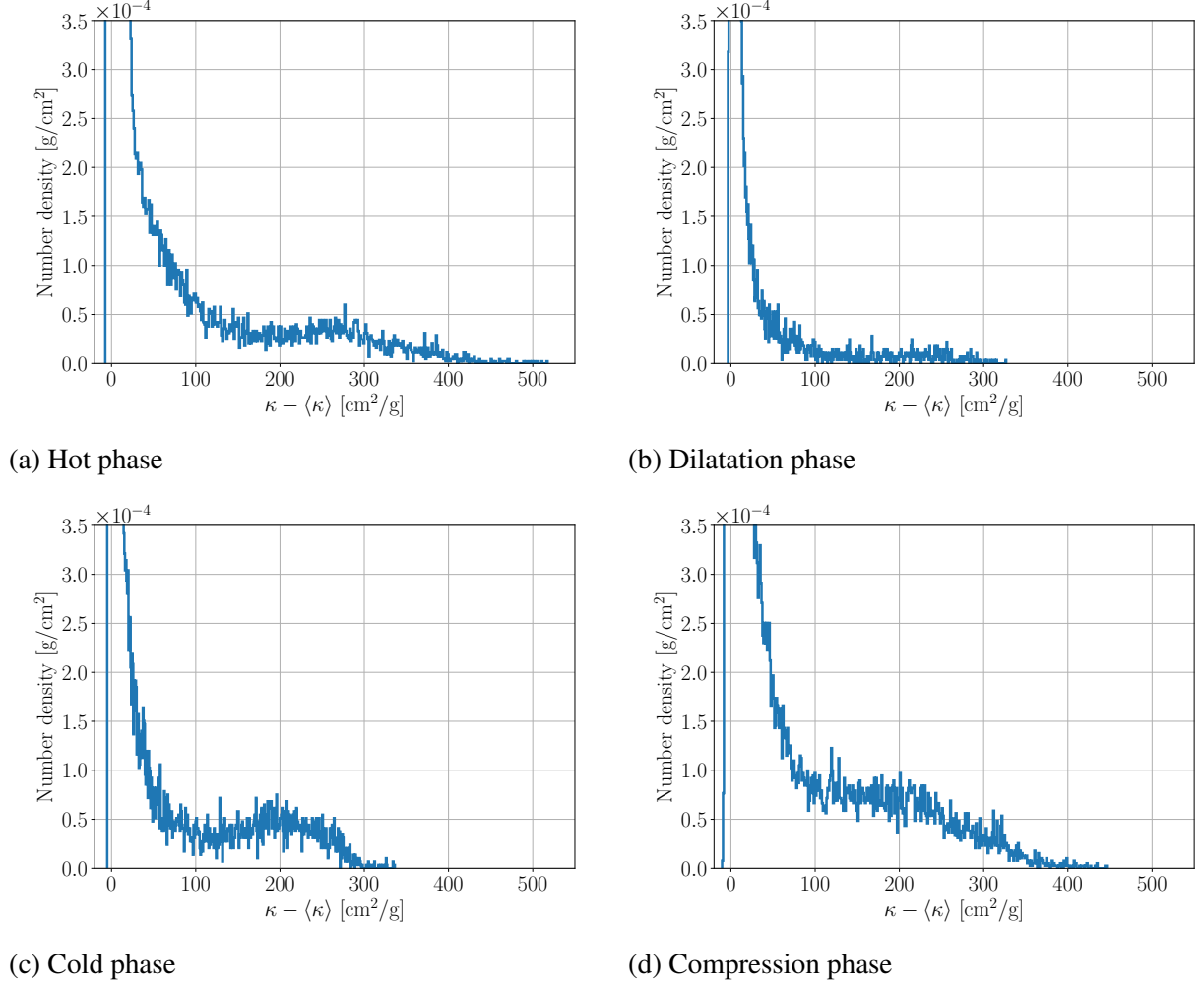


Figure 4.20: Distribution of the absolute opacity fluctuations $\kappa - \langle \kappa \rangle$ for the four main phases of the pulsation cycle at $z_0 \simeq -1.163 \times 10^{11} [\text{cm}]$.

of flow suggest that they are likely to behave very differently in terms of energy exchange. For instance, the κ -mechanism has no reason to operate in the same way for strong downflows exhibiting a wide range of opacities and for slower flows that remain at nearly uniform values. Separating these two behaviours therefore appears essential in order to properly understand the underlying physical processes. Moreover, attempting to interpret the system based on averaged quantities of these behaviours, especially when their relative proportions differ and vary in time, is not meaningful and prevents a proper physical understanding. It is also worth noting that this is in strong contrast with the classical assumptions often made in 1D models such as MLT, where a symmetry between upflows and downflows is generally assumed. Here, such a symmetry is clearly not observed, and the results rather suggest that different effective descriptions may be required for the two types of flows.

4.2.6 Energy transport

Another important point when addressing energy transport is to determine which energy transport mode, between radiation and convection, is dominant in each region of the simulation. It is already expected, due to the absence of convective patterns in the inner layers, that the deepest layers are not convective. To verify this, the most intuitive approach is to check where

the Schwarzschild criterion predicts convective zones by comparing the actual and adiabatic temperature gradients. This is illustrated in Fig. 4.21.

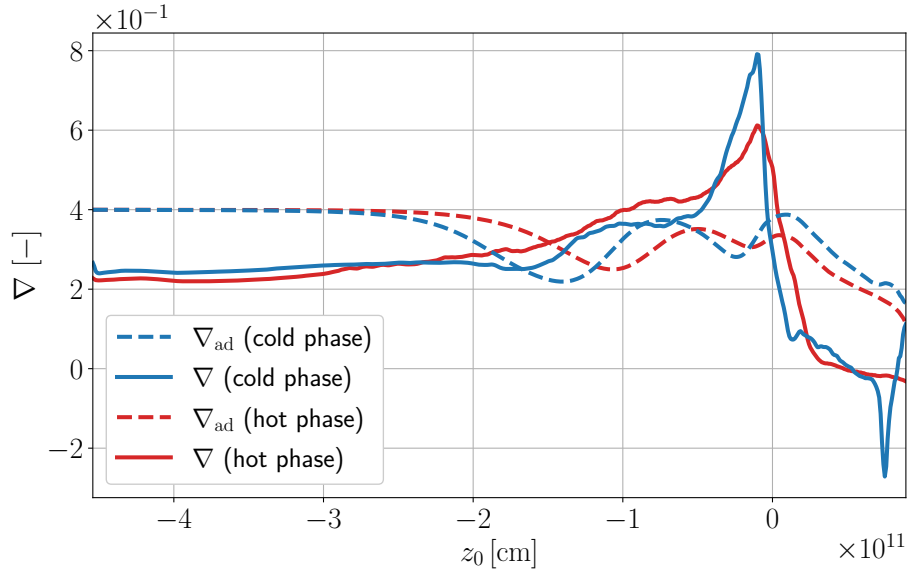


Figure 4.21: Comparison of the real and adiabatic gradient profiles as a function of the pseudo-Lagrangian radius z_0 for the 3D simulation during the hot and cold phases.

The figure shows that this local criterion predicts a convective zone extending over approximately one third of the simulation domain, since, as a reminder, convection is expected where the actual temperature gradient exceeds the adiabatic one. As expected, the inner layers are radiative, whereas the outer layers are convective. Concerning the adiabatic gradient, one can observe that it converges towards 0.4 in the deepest layers, which is the characteristic value for an ideal fully ionised gas. Two local minima are also visible, corresponding to the ionisation zones. Furthermore, according to this criterion, the convective region remains at roughly the same location and with a similar extent throughout the pulsation cycle, although some small variations can be observed. Finally, it is important to note that the difference between the actual and adiabatic gradients is smaller during the cold phase. In addition, a narrow region can be identified during the cold phase where the adiabatic gradient locally exceeds the actual gradient, indicating a stable stratification according to the Schwarzschild criterion.

However, this criterion does not guarantee that these predicted regions correspond to the actual convective zones. The limitations discussed in Sec. 2.3.2 remain present: this criterion is based solely on local values and does not account for the spatial extension of the convective envelope due to inertia (undershooting). It is thus necessary to check directly the value of the different fluxes to see where the convective flux is important. Unfortunately, the convective flux computed automatically from the mean files appears to be completely dominated by the pulsational component, rendering it unsuitable for a meaningful analysis. It is therefore necessary to find a way to circumvent this issue. In practise, this problem arises due to the difference in the definition of the enthalpy flux which is in the code:

$$F_e = \langle \rho v_z h \rangle, \quad (4.9)$$

and decomposing the enthalpy into its spatial mean and fluctuating components:

$$h = \langle h \rangle + \Delta h, \quad (4.10)$$

one obtains

$$F_e = \langle \rho v_z (\langle h \rangle + \Delta h) \rangle. \quad (4.11)$$

Expanding this expression yields

$$F_e = \langle h \rangle \langle \rho v_z \rangle + \langle \rho v_z \Delta h \rangle, \quad (4.12)$$

so that the last term is very close to the definition of the convective flux given in Eq. 2.73. The first term on the right-hand side can therefore be readily subtracted from the enthalpy flux output by the code, as it is simply the product of the mean enthalpy, available in the mean files, and the mean mass flux $\langle \rho v_z \rangle$, also available. It should be noted, however, that the remaining term does not exactly correspond to the definition of the convective flux. Indeed, the velocity entering this expression still contains both a pulsational component and a convective component, whereas only the latter should appear in the formal definition of the convective flux. Nevertheless, it is not possible to proceed further with the decomposition since the additional correlation terms that would arise from separating the velocity into mean and fluctuating components cannot be computed from the quantities available in the mean files. Consequently, subtracting $\langle h \rangle \langle \rho v_z \rangle$ from the enthalpy flux represents the only feasible approach for estimating the convective flux from the mean-file data.

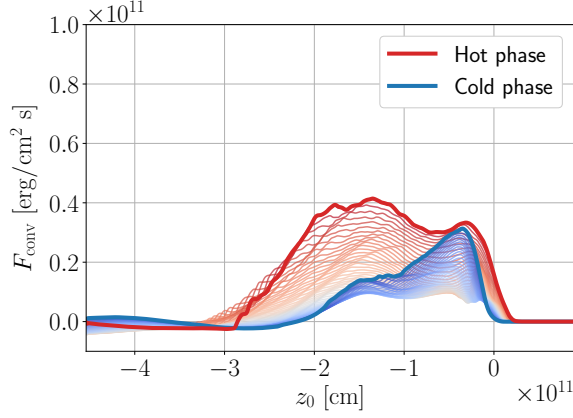
The constructed convective flux and the radiative fluxes are compared in Fig. 4.22. For now, the constructed convective flux is assumed to be the real convective flux. It will be of course checked while analysing the full files.

This figure contains a large amount of relevant information. Focusing first on the radiative flux, it can be seen that it remains non-zero throughout the entire simulation domain. This highlights the fact that even convectively unstable regions continue to transport a fraction of their energy through radiation. The radiative flux varies significantly across the different layers of the model, while remaining comparatively weak in the regions where convection is expected to dominate. Turning now to the convective flux, it exhibits a complex and strongly time-dependent profile, reflecting the well-known difficulties associated with modelling convective transport. The convective zone is identified as the region where the convective flux takes non-zero values, and this zone appears to be more important during the hot phase. What also immediately stands out is that this region is much larger than the one predicted by the Schwarzschild criterion in Fig. 4.21. The origin of this difference lies in fact in the intrinsically non-local nature of convection. The limitations associated with the local character of the Schwarzschild criterion have already been discussed, and this figure clearly demonstrates that they can lead to a radically different estimate of the extent of the convective zone. Predicting convection only using variables evaluated at a single point appears to be completely incorrect.

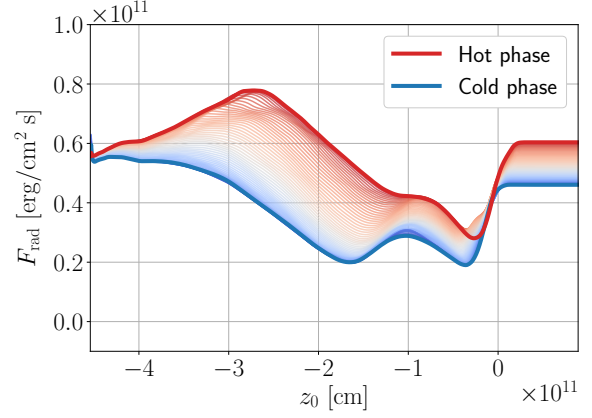
4.2.7 Conclusion on 1D limitations

To conclude this first part of the analysis, several important points should be kept in mind for the remainder of the study. First, comparisons with 1D models remain difficult and limited due to the fundamentally different structures, boundary conditions and model assumptions of the 1D models. Secondly, it has been emphasised that downflows and upflows are strongly asymmetric and that the average of those two dynamics makes the interpretation of the averaged profile limited.

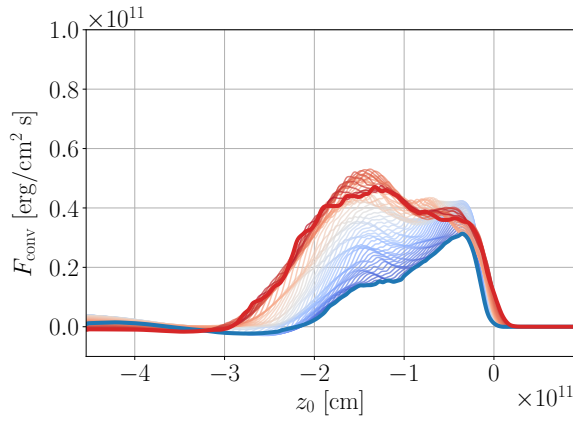
As a consequence, it is necessary to switch into a description where flows will be separated.



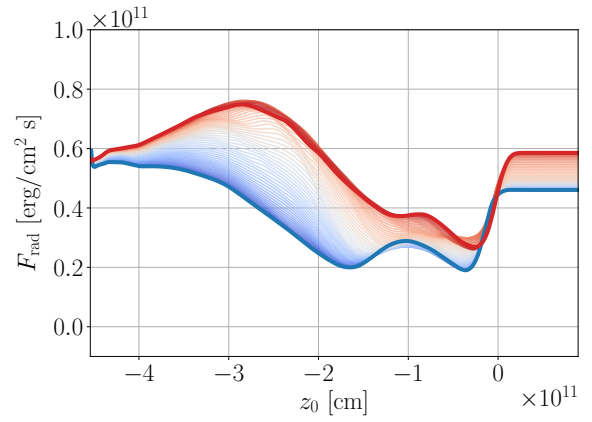
(a) Convective flux, dilatation



(b) Radiative flux, dilatation



(c) Convective flux, compression



(d) Radiative flux, compression

Figure 4.22: Temporal evolution of the convective and radiative fluxes during the main pulsation cycle. The expansion and compression phases are shown separately.

Such a separation is straightforward to perform on full snapshots, as it only requires classifying the flow according to the sign of the relative velocity. The drawback, however, is that it will not be possible to follow the complete temporal evolution of each type of flow, since only selected full snapshots are analysed. This separation is performed in the next section and will enable one to get closer to the understanding of the pulsational behaviour.

4.3 Upflow and downflow decomposition

4.3.1 Asymmetry origin

Before trying to better understand the differences between the two fluxes, it is first important to interpret the origin of such a strong asymmetry. In practice, the degree of symmetry of a convective flow depends on several physical parameters and cannot be attributed to a single mechanism alone. It is, however, possible to provide hints that may explain such a behaviour. For instance, the density and temperature stratifications of the medium play a significant role: a stronger density gradient tends to inhibit the lateral expansion of descending flows, while rising flows can more easily expand as they move towards regions of lower density.

Another key parameter governing the flow symmetry is the thermal diffusivity, χ , defined in Eq. 2.46. In Sec. 2.3.1, this quantity was introduced and compared with inertial effects through the definition of the Péclet number. To better understand its influence on the flow asymmetry, it is instructive to consider the case of solar convection. As shown in Fig. 2.5, convection in the Sun is also asymmetric, although the asymmetry is much less pronounced than in our simulations. It is therefore interesting to compare the Péclet numbers of the Cepheid model with those characteristic of solar convection. To make this comparison possible, a $1 M_{\odot}$ stellar model was computed using CLÉS, and the Péclet number is compared for this model and the Cepheid 3D simulation in Fig. 4.23. For both models, constant reference values for the convective velocity and the characteristic length scale were adopted. For the solar model, these values were estimated from snapshots of 3D solar convection simulations. The adopted values are $v_z = 3 \times 10^5$ [cm/s] and a characteristic cell size of 2×10^8 [cm]. For the Cepheid model, the radial velocity field can be decomposed into a pulsational (mean) and a convective component:

$$v_z = v_{z,\text{puls}} + v_{z,\text{conv}}, \quad (4.13)$$

with $v_{z,\text{puls}} = \langle v_z \rangle$. A typical value of $v_{z,\text{conv}}$ within the convective region was adopted as the reference convective velocity, while a characteristic length scale of 4×10^{11} [cm] was used.

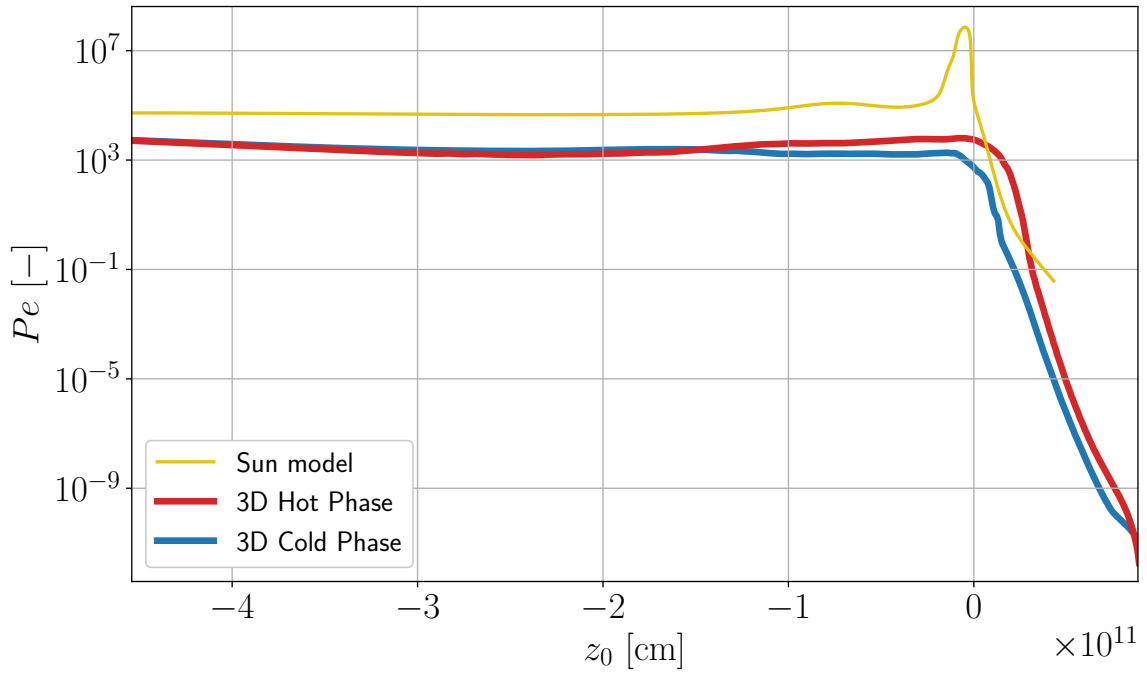


Figure 4.23: Comparison of the Péclet number Pe during the hot and cold phases with a 1D solar model.

In this Fig. 4.23, one can first observe the large values of the Péclet number, confirming the dominance of advection over thermal diffusion. Nevertheless, the Péclet number is significantly larger in the solar model than in the Cepheid model. This indicates that thermal diffusivity is relatively more important in the Cepheid. This may help explain the stronger asymmetry of the flow, as rising plumes can more easily diffuse their thermal excess and release their heat to the surrounding medium. Furthermore, since the Péclet number quantifies the efficiency of convective heat transport, the lower values found in the Cepheid model suggest that convection

is less efficient there than in the Sun. It is worth noting, however, that the Péclet number reaches its maximum values close to the stellar surface for the solar model, where convection is generally expected to be less efficient. This apparent contradiction highlights one of the limitations of interpreting such a dimensionless number in isolation. In the present case, it is mainly caused by the strong dependence of the thermal diffusivity on the $\kappa\rho^2$ term (Eq. 2.46), whose behaviour in the superficial layers artificially increases the Péclet number. The same term then drops rapidly above the photosphere, as both κ and ρ decrease sharply.

4.3.2 Energy fluxes decomposition

The differences between the properties of upflows and downflows can be better understood by revisiting the quantities analysed previously and separating the contributions from each flow. To this end, it is convenient to begin with the different energy fluxes and examine the contribution of upflows and downflows separately for the four full time steps for which snapshots are available. With those full files, it becomes possible to compute properly the convective flux as wanted. For this purpose, the convective flux is identified with the enthalpy flux as in Eq. 2.73:

$$F_{\text{conv}} = \langle \rho c_p (v_{z,\rho} - \langle v_{z,\rho} \rangle) (h - \langle h \rangle) \rangle. \quad (4.14)$$

The convective flux is shown in Fig. 4.24, together with the contributions of the upflows and downflows to this convective flux.

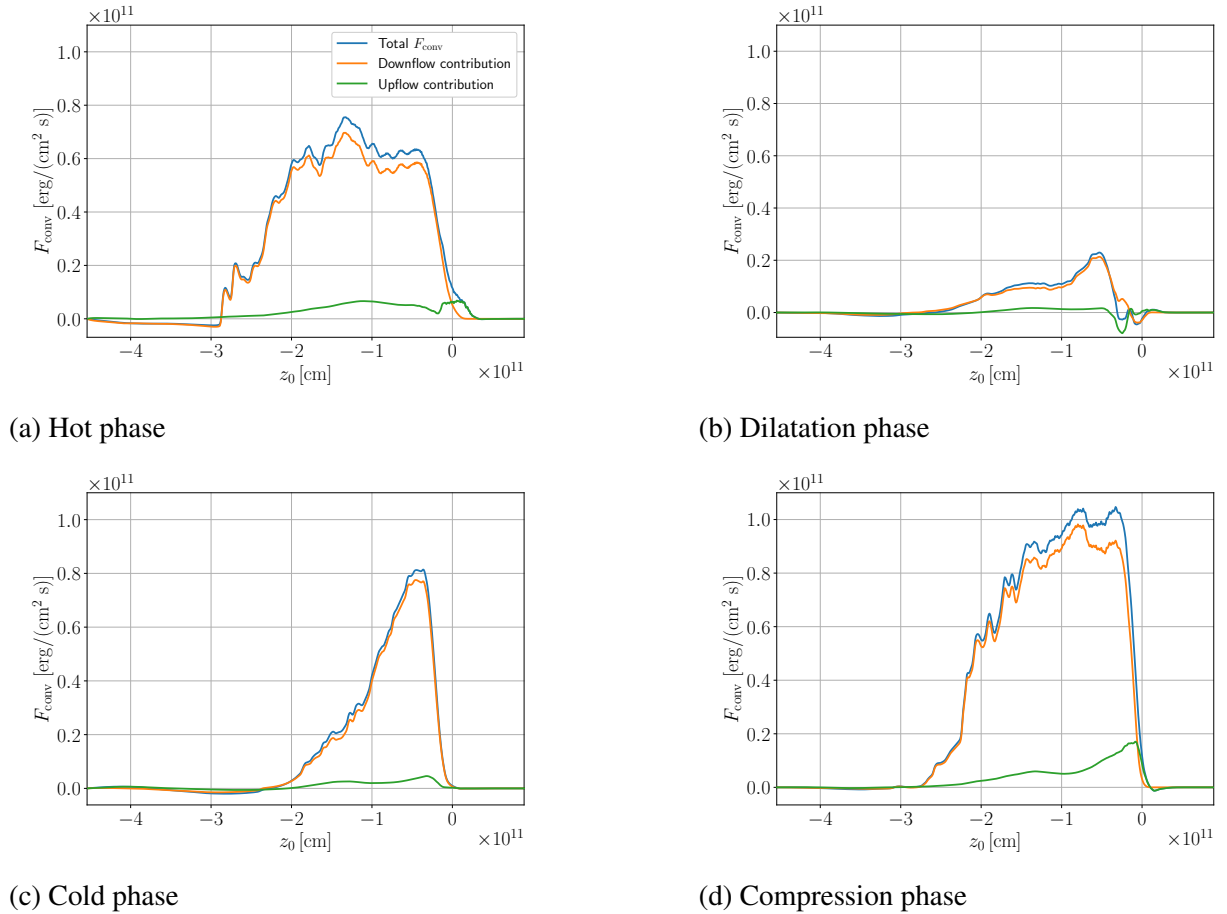


Figure 4.24: Separation of the contributions of upflows and downflows to the total convective flux F_{conv} during the four main phases of the pulsation cycle.

Moreover, the contribution of each flow component is evaluated separately. For instance, the upflow contribution is obtained by averaging the flux over the entire domain, while setting it to zero in regions where the vertical velocity is negative. Conversely, the downflow contribution is computed by setting the flux to zero wherever the vertical velocity is positive. By construction, the sum of the upflow and downflow contributions is equal to the total convective flux.

First, one can verify that Fig. 4.24 shapes are very similar to the evolution of the constructed convective flux displayed in Fig. 4.22a, although the flux is now a little bit stronger, confirming that the general behaviour of the constructed convective flux from the mean files was relevant to the analysis. The flux appears to be even more strongly time-dependent in this case, with significant differences between the hot and cold phases. In particular, the convective zone extends much deeper during the hot phase than during the cold phase. Furthermore, the figure reveals another striking result. Although downflows occupy only a small fraction of the volume, their strength makes them overwhelmingly dominant, and they are responsible for almost the entire convective flux. The profile of the convective flux is therefore entirely determined by the downflows, while the upflows provide only a minor contribution. This highlights again the total invalidity of the assumption of symmetry of the convective flux with respect to the opposite flows. Moreover, this analysis remains valid for all the phases of the pulsation.

The same analysis can be performed for the radiative flux and is shown in Fig. 4.25. The radiative flux has here been calculated using the definition of Eq. 2.40:

$$F_{\text{rad}} = -\frac{4acT^3}{3\kappa\rho} \frac{dT}{dr}, \quad (4.15)$$

where in practice the gradient is obtained by finite differences of first order. Note that, because of the use of spatial derivatives in this method, the outer layers are strongly affected by numerical noise. The large gradients present in these regions amplify the fluctuations and lead to unrealistically large values. For this reason, the radial range shown in the figure has been restricted, while still retaining all the layers relevant to the present analysis. Moreover, Eq. 4.15 is, as already said in Sec. 2.2.6, an approximation commonly referred to as the diffusion approximation. It assumes that the photon mean free path is much smaller than the local scale heights. It is a simplified approach compared to CO5BOLD that performs a much more sophisticated treatment of radiative transfer. In fact, this assumption is more likely to be violated in the atmospheric layer, where the mean free path is larger. This may thus also explain why such unrealistic values are obtained at those layers.

A first noticeable feature in Fig. 4.25 is that the radiative flux associated with the downflows remains relatively small, especially in the regions where the convective flux is strongest. Furthermore, its profile remains roughly unchanged throughout the pulsation cycle. The energy transport in the downflows is therefore predominantly convective. In contrast, the radiative flux is significantly larger in the upflows and accounts for a large fraction of the total radiative flux. Additionally, this flux undergoes substantial changes during the pulsation cycle. In particular, one can focus on the region between $z_0 \simeq -1.5 \times 10^{11}$ [cm] and $z_0 \simeq -10^{11}$ [cm]. During the hot phase, the radiative flux decreases outward, corresponding to a negative flux gradient. This implies that radiative energy is deposited in these layers. During the cold phase, the gradient reverses sign, indicating that these layers radiate away more energy than they receive. Such behaviour is qualitatively consistent with the expected signature of the κ -mechanism. Indeed, this mechanism relies on a phase-dependent modulation of the radiative energy transport, whereby energy is preferentially stored during compression and released during expansion. Since the

process is fundamentally radiative in nature, the observed variations of the radiative flux in this region provide evidence that radiative driving may contribute to the excitation of the pulsations.

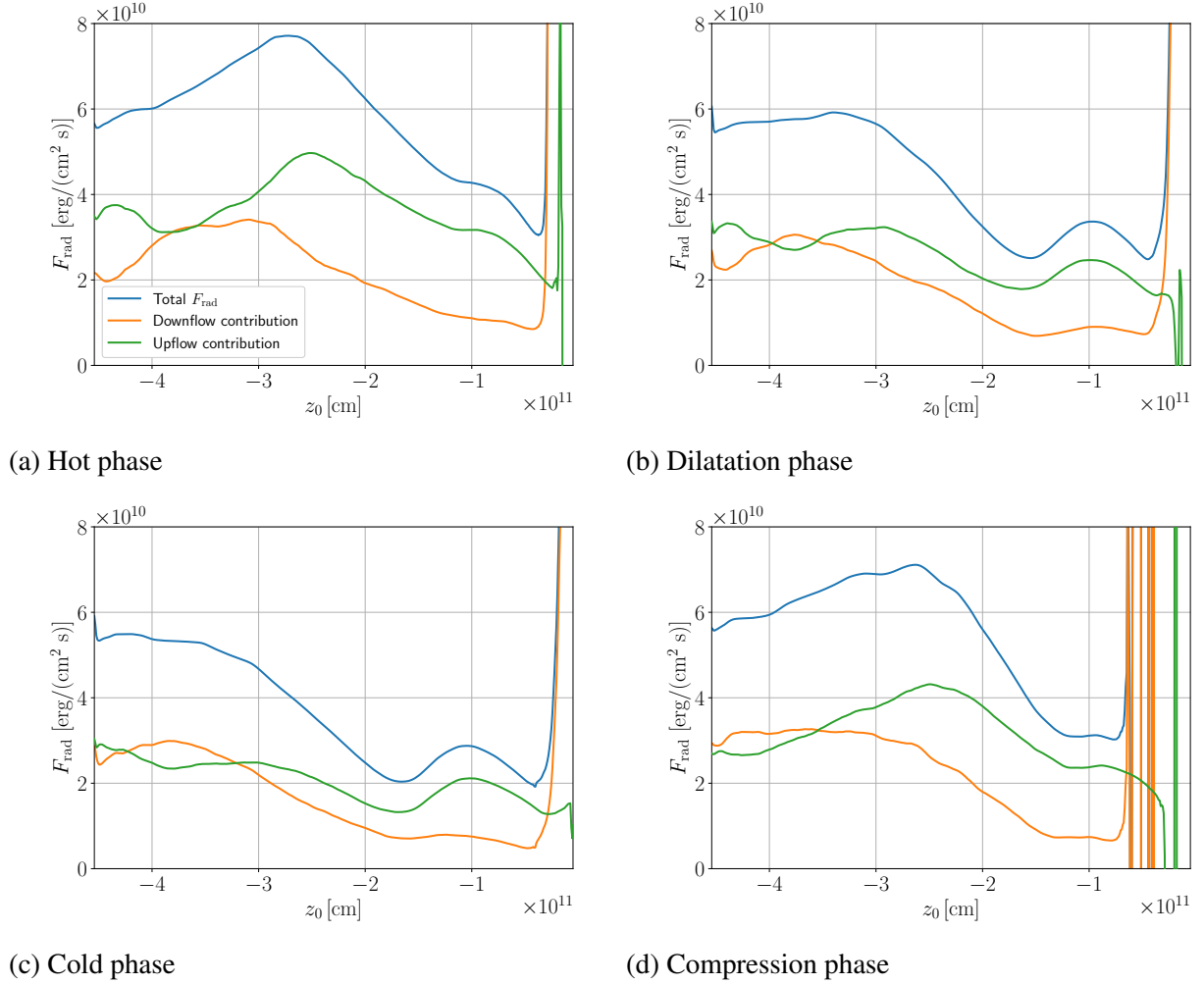
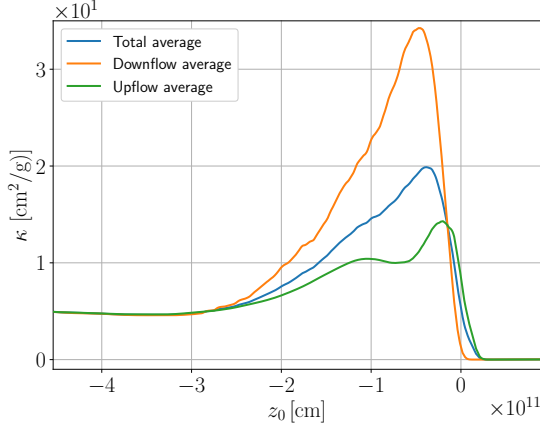


Figure 4.25: Separation of the contributions of upflows and downflows to the total convective flux F_{rad} during the four main phases of the pulsation cycle. The radial domain is shorter due to too much noise near and above the photosphere.

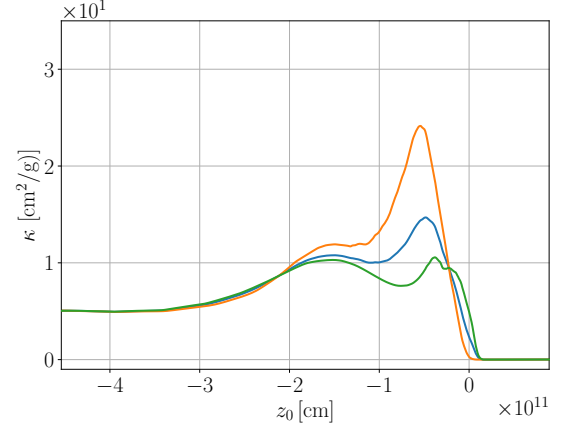
4.3.3 Opacity effects

To further investigate the possibility of a κ -mechanism, it is instructive to examine the opacity structure of the flow. However, the mean opacity profile shown in Fig. 4.19 is strongly affected by the large differences between upflows and downflows, which tend to smooth out the individual opacity peaks. As a result, several features become difficult to identify in the averaged profile. To circumvent this issue, the opacity is separated according to the flow direction, in the same manner as for the fluxes. The resulting profiles, corresponding to the total average, the upflows only, and the downflows only, are presented in Fig. 4.26.

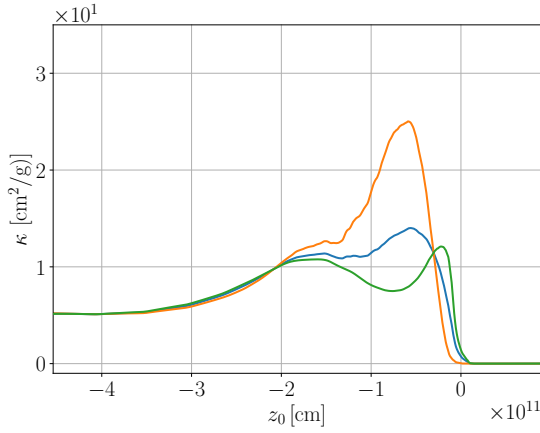
This opacity separation allows a clearer interpretation of the underlying physical processes. A notable feature is that, for the upflows, the second helium ionisation peak is now clearly separated from the combined hydrogen and first helium ionisation contribution, and two distinct peaks can be identified, although the first remains relatively weak. It is worth recalling that the



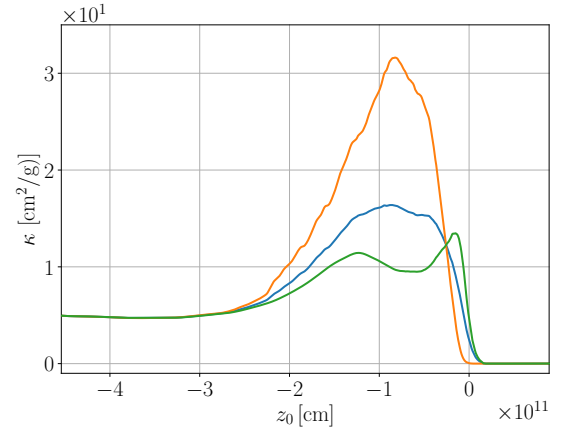
(a) Hot phase



(b) Dilatation phase



(c) Cold phase



(d) Compression phase

Figure 4.26: Comparison of the mean opacity profiles κ during the four main phases of the pulsation cycle and computed over the entire domain, over the upflows only, and over the downflows only.

second helium ionisation zone is responsible for the κ -mechanism, and that this peak is located in a region close to where a change in the radiative flux gradient was previously observed, thereby supporting the κ -mechanism hypothesis.

Regarding the downflows, only a single dominant peak remains, which is not surprising. As already mentioned, downflows span a wide range of temperatures and opacities, as shown in Fig. 4.20. In the present separation, only the average over upflows and downflows has been distinguished, while the internal variability within the downflow population remains large, which explains why the individual opacity peaks remain unresolved in this component.

4.4 Thermodynamic cycle

4.4.1 Work

Now that the properties of the convective flow have been clearly characterised, the important question of pulsation excitation can be addressed. The goal here is to investigate whether the gas motions within the star act to excite the pulsation modes or, conversely, contribute to their

damping. A global excitation, or at least a maintenance of the modes, is of course expected, since the modes are observed. To verify this, one can examine the work performed by the gas over one oscillation cycle. As presented in Sec. 2.4.2, a positive work over a cycle leads to mode excitation, whereas negative work results in damping.

Since the work (by unit mass) is essentially given by $\int P dv$ over one oscillation cycle, the first step is therefore to visualise the P - v diagrams in different regions of the star in order to analyse their shapes. In such diagrams, the area enclosed by the cycle corresponds to the work per unit mass, since the specific volume is used here. A clockwise cycle corresponds to positive work, while an anticlockwise cycle indicates negative work. It is important to emphasise that the results presented in this section are obtained from a work integral computed at constant pseudo-Lagrangian coordinates using averaged quantities at each layer. As already discussed, although this approach relies on a simplifying assumption, it is difficult to define a more rigorous alternative in the presence of turbulent convection. Indeed, following individual fluid elements over a pulsation cycle is not feasible, as turbulent motions continuously mix the flow and prevent the identification of a unique trajectory. Moreover, a fluid element would not, in general, return to its initial position after one pulsation cycle. It is nevertheless important to remain aware of this strong assumption associated with those calculations since it implies directly that only a part of the real work is successfully computed.

The $P - v$ diagrams are shown in Fig. 4.27 for a selection of stellar layers. The deeper layers are not shown since they exhibit the same behaviour as the deepest layer shown in this figure. All of them correspond to the main oscillation cycle (defined in Sec. 4.1.2), since a single pulsation period must be considered.

Before interpreting these results, it is interesting to recall the classical behaviour that can be observed in such diagrams. For perfectly linear adiabatic oscillations, the P - v diagram reduces to a single line, corresponding to a simple back-and-forth motion. This therefore produces zero net work. For linear non-adiabatic oscillations, the constant phase shift between pressure and specific volume leads to non-zero work. In this case, the trajectory forms an ellipsoid, whose enclosed area corresponds to the work (with the sign depending on the direction of the cycle). Finally, more complex non-linear behaviours lead to more intricate P - v diagram shapes, reflecting the departure from simple harmonic motion.

Thus, Fig. 4.27 exhibits a wide range of different cycles depending on the layer. In the inner region, the cycles exhibit a familiar shape, tending towards a line form. This is explained by the fact that, as discussed earlier, the oscillation amplitudes are much smaller in this region so that the system approaches the linear regime. As one moves towards the surface, the shapes become increasingly complex, eventually reaching strongly distorted forms in the near-atmosphere layers, where pulsation velocities are large and non-linear effects become significant. Another issue arises in this figure. Due to the non-perfectly periodic and oscillatory nature of the pulsations, as well as the difficulty in defining a strictly consistent oscillation cycle, the curves do not always form closed loops, since the initial and final points do not exactly coincide. This is problematic for the evaluation of the work, which requires integration over a closed cycle. To remedy this, it is necessary to define more robust methods to compute the work, and two approaches have been considered.

The first method that was considered is to assume the case of linear non-adiabatic oscillations. For this purpose, the pressure and specific volume are approximated as presented in Sec. 2.4.2

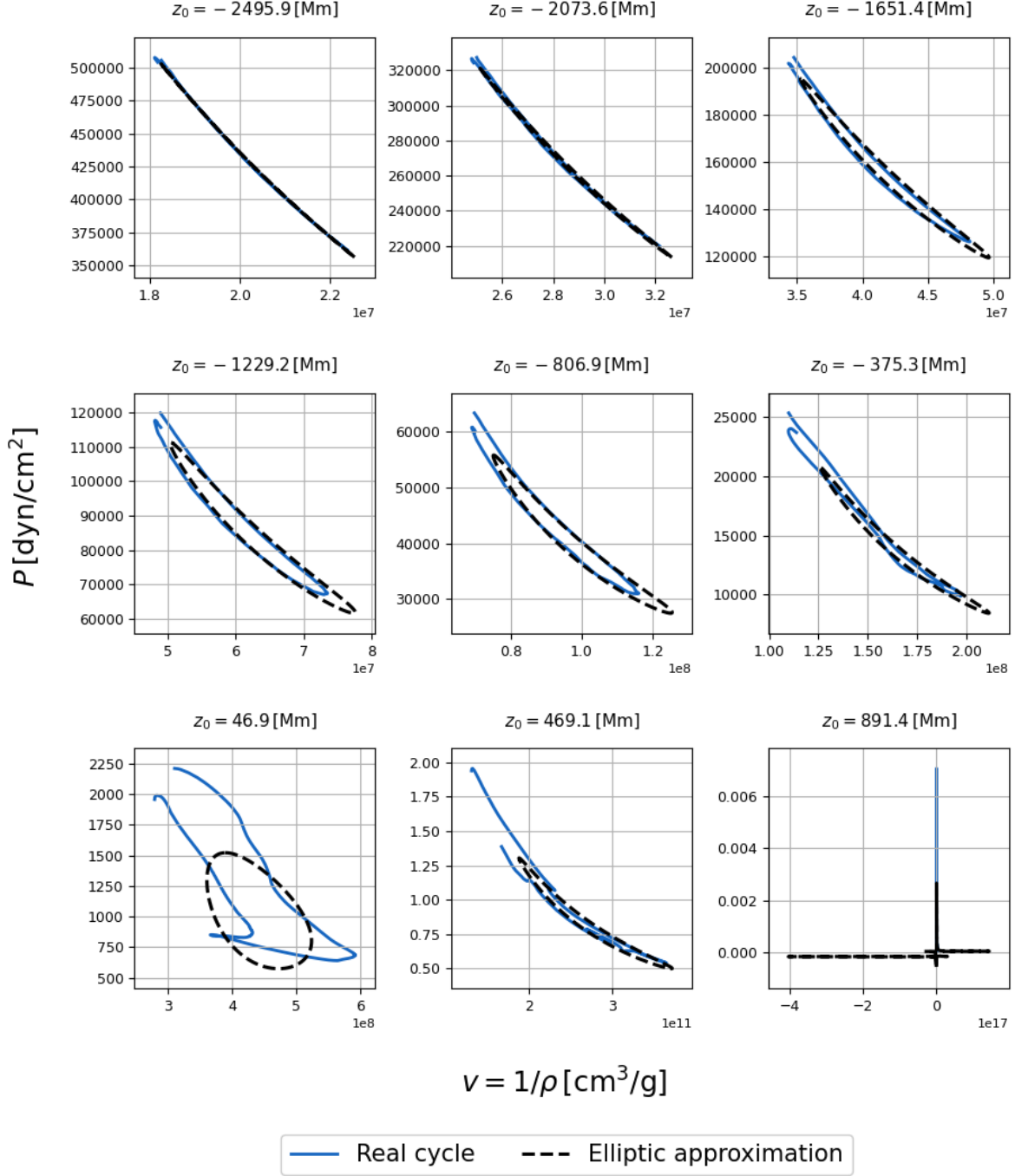


Figure 4.27: $P - v$ diagram of the main cycle for a selection of layers. The real cycle and the approximated elliptic cycle are also compared.

in Eqs. 2.111 and 2.112, which is equivalent to the following form:

$$P = P_0 + P_1 \sin(\omega t) + P_2 \cos(\omega t), \quad (4.16)$$

$$v = v_0 + v_1 \sin(\omega t) + v_2 \cos(\omega t), \quad (4.17)$$

For each layer, P and v are thus approximated by these forms, with coefficients determined using a least-squares method. Once these coefficients are known, computing the work by unit mass for the layer is done by recalling Eq. 2.115 and with a few trigonometric transformations,

it becomes

$$\begin{aligned}
dW &= -\pi |\delta P| |\delta v| \sin(\phi_v - \phi_P) \\
&= -\pi \sqrt{P_1^2 + P_2^2} \sqrt{v_1^2 + v_2^2} \sin \left[\arctan \left(\frac{v_2}{v_1} \right) - \arctan \left(\frac{P_2}{P_1} \right) \right] \\
&= -\pi \sqrt{P_1^2 + P_2^2} \sqrt{v_1^2 + v_2^2} \left[\frac{v_2}{\sqrt{v_1^2 + v_2^2}} \frac{P_1}{\sqrt{P_1^2 + P_2^2}} - \frac{v_1}{\sqrt{v_1^2 + v_2^2}} \frac{P_2}{\sqrt{P_1^2 + P_2^2}} \right] \quad (4.18) \\
&= -\pi (v_2 P_1 - v_1 P_2) \\
&= \pi (P_2 v_1 - P_1 v_2).
\end{aligned}$$

This method is useful since it is very simple to implement but might have difficulties of evaluating the work in regions where the pulsations are strongly non-linear. To see this, the trajectory predicted by this method is also displayed in Fig. 4.27, where, indeed, the simplified trajectories seem not to match perfectly in the superficial layers.

The second method will be called the method of the real cycle, it consists of trying to get as close as possible to the real shape of the cycle by closing it through a direct connection between the first and last points, thereby creating a fictitious closure. This has the advantage of preserving the overall shape of the cycle and improving the match compared to the first method, but it may introduce errors by creating loops in the opposite direction (if the trajectory already crosses itself) or, conversely, by including portions of the curve that should not contribute to a single closed cycle. Here again, its simplicity remains an advantage since the work is simply integrated numerically.

The results provided by the two methods are gathered in Fig. 4.29, where the work per unit volume, ρdW , is displayed as a function of the radius. In this figure, the two methods yield similar trends, which is already reassuring regarding their construction and their ability to approximate the "true" work, which is not uniquely defined in this context.

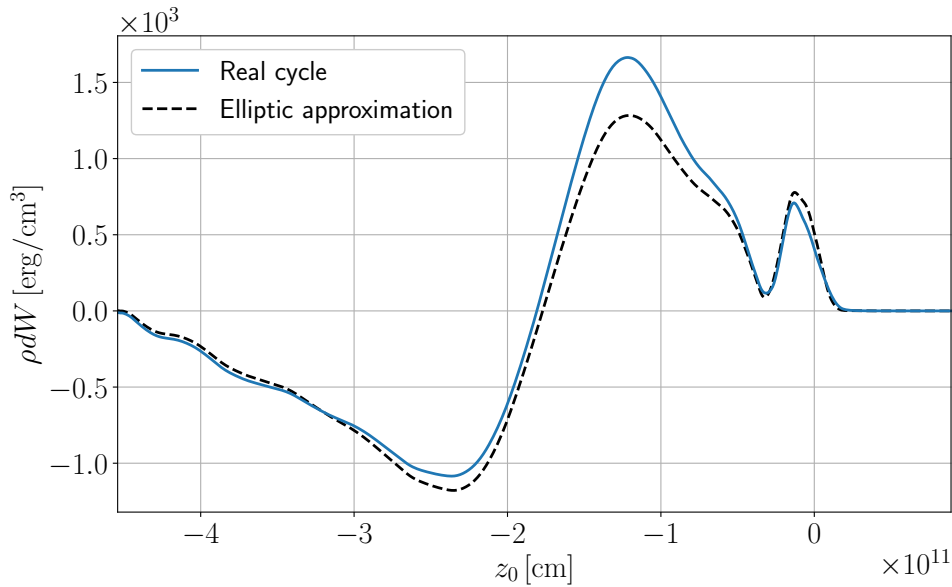


Figure 4.28: Work by unit volume ρdW as a function of the layer depth for the two different methods of real cycle and elliptic approximation.

In the innermost layers, the work is negative, meaning that these regions tend to damp the pulsational motion. In the same zones, the two methods provide quasi-identical results, as expected due to the near-elliptical shape of the P - v diagrams. As one approaches the surface and the motions become strongly non-linear, the values of the work start to differ between the two methods. However, they both exhibit two excitation regions (with positive work), with a main excitation peak located near $z_0 \simeq -1.2 \times 10^{11}$ [cm]. The crucial point is now to assess the global effect by integrating over all layers in order to determine whether the overall gas motions excite or damp the pulsations. This is done by integrating the work over the entire volume. In Fig. 4.29, this volume integration is performed from the bottom of the box z_{bot} up to the considered radius so that the value at the stellar surface corresponds to the total work integrated over the entire star. The comparison with the 1D eigenmodes non-adiabatic linear model is also done.

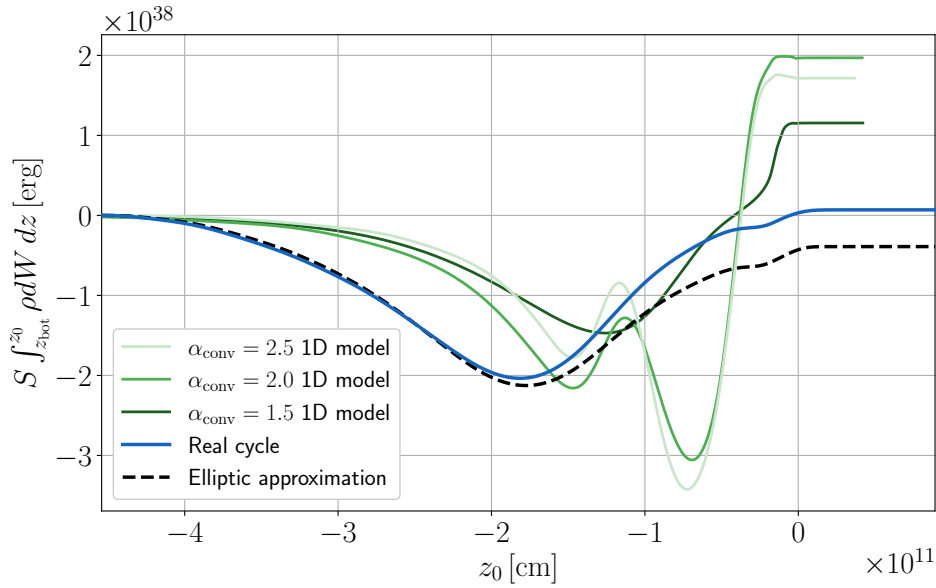


Figure 4.29: Integrated work $S \int_{z_{\text{bot}}}^{z_0} \rho dW dz$ as a function of the layer depth for the two different methods of real cycle and elliptic approximation. The comparison is also made with the eigenmodes of the three 1D models with $\alpha_{\text{conv}} = 1.5, 2$, and 2.5 .

Unfortunately, the discrepancy in the work amplitude in some layers for the two methods leads to a different sign of the total work. The first method therefore predicts a negative work, meaning a global damping of the pulsations, while the second method predicts an overall excitation. Although it can be expected that the second method is less affected by numerical errors than the first one, it is not possible at this stage to draw any definitive conclusion. However, the spatial distributions in both cases consistently show that the innermost layers strongly damp the motion, such that in the middle of the simulation domain the pulsation is significantly attenuated before being re-excited in outer layers, which tends to compensate for the inner damping. Once again, the comparison with 1D models gives very different behaviour, showing again that these models are too different to be compared. It is however interesting to note that these three models predict a positive net work.

4.4.2 Heat exchanges

The analysis of the work integrals does not allow a firm conclusion to be drawn regarding the excitation or damping of the pulsations, as the two methods considered lead to opposite signs for

the net work. In addition, because of the approximation of constant pseudo-Lagrangian coordinates, only part of the actual work can be evaluated. Furthermore, it was not possible to obtain a perfectly closed pulsation cycle. Since the positive work accumulated during the expansion phase is nearly balanced by the negative work accumulated during the compression phase, the net work results from the difference between two much larger quantities. As a consequence, even small uncertainties in the calculation can significantly affect the final result, limiting the precision and reliability of the derived net work.

To overcome this limitation, an alternative way to determine whether the thermodynamic cycle is driving or damping the pulsation is to analyse the heat exchange term Dq/Dt (per unit mass). This quantity has the advantage of changing sign completely between a driving and a damping cycle, making its interpretation more straightforward than that of the work integral. In particular, a pulsation is expected to be driven if heat is preferentially absorbed during the hot phase and released during the cold phase. Conversely, if heat is absorbed during expansion and released during compression, the pulsation is damped. The heat exchange term is defined as

$$\frac{Dq}{Dt} = T \frac{Ds}{Dt}. \quad (4.19)$$

From Eq. 2.23, it directly follows that

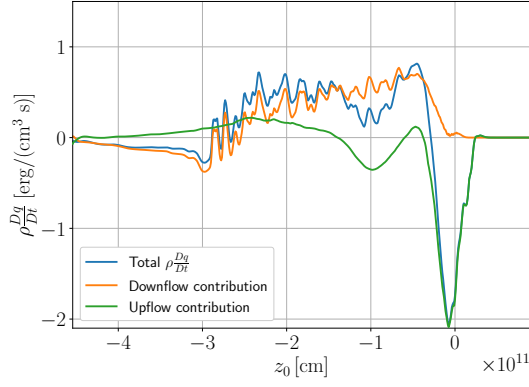
$$\frac{Dq}{Dt} = \frac{Du}{Dt} + P \frac{Dv}{Dt}, \quad (4.20)$$

so that the two contributions correspond, respectively, to the variation of internal energy and to the mechanical contribution. Note that, recalling Eq. 2.29, this can also be written as

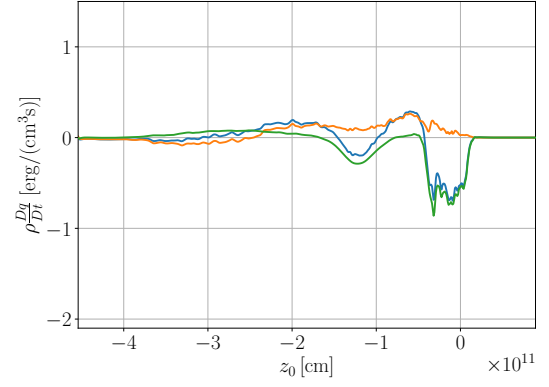
$$\frac{Dq}{Dt} = -\varepsilon_{\text{grav}}. \quad (4.21)$$

A positive value of this quantity therefore indicates that energy is supplied to the gas, whereas a negative value means that the gas loses energy. The value of this heat-exchange (or calorific exchanges) term per unit volume, together with the contribution of each flux component, is shown in Fig. 4.30. It was computed from Eq. 4.19. The entropy and temperature were obtained from the equation of state, while the time derivative of the entropy was evaluated using a centred finite-difference scheme based on the snapshots immediately preceding and following the analysed time step.

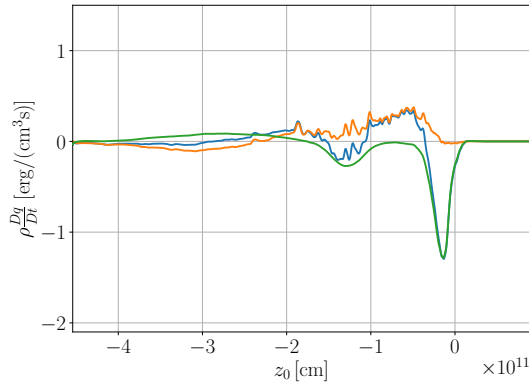
Fig. 4.30 is probably the most informative figure for understanding the results presented in this thesis. First, the total value of $\rho Dq/Dt$ appears to be larger during the hot phase than during the cold phase. This confirms that heat is supplied during the hot phase and lost during the cold phase, suggesting that the gas contributes to the excitation of the pulsation. This dynamic is dominated by the downflows, and this figure also reveals two distinct behaviours depending on the type of flow. Starting with the downflows, one can see that they receive more heat during the hot phase than during the cold phase, indicating that they participate in the thermodynamic driving cycle. This behaviour can be explained using several elements that have already been emphasised previously, and it is therefore worth highlighting them again. First, the snapshots showed that more convective structures are visible during the hot phase than during the cold phase, as illustrated for example in Fig. 4.9. This behaviour was confirmed by the temperature distribution shown in Fig. 4.10, which exhibited a much broader distribution together with a larger fraction of downflows during the hot phase. These observations suggest that the convec-



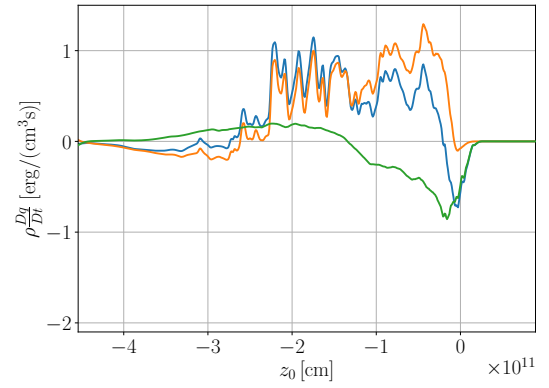
(a) Hot phase



(b) Dilatation phase



(c) Cold phase



(d) Compression phase

Figure 4.30: Separation of the contributions of upflows and downflows to the calorific exchanges $\rho \frac{Dq}{Dt}$ during the four main phases of the pulsation cycle.

tive instability is stronger during the hot phase than during the cold one. This can also be seen by comparing the relative density variations during the two phases, as done in Fig. 4.31 for a layer for which the heat supply change significantly with the phase.

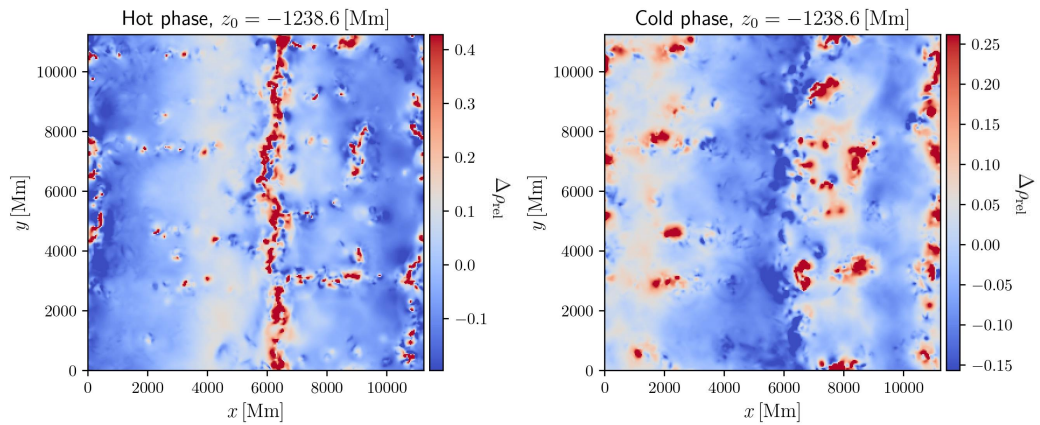


Figure 4.31: Snapshots of the spatial relative density variation $\Delta\rho_{\text{rel}}$ with respect to the mean value of the considered layer at $z_0 \simeq -1.238 \times 10^{11}$ [cm] during the hot and cold phases. The limits of the colour-bar scale are set to the 2nd and 98th percentiles of the data in each snapshot.

These variations appear to be larger during the hot phase, confirming the hypothesis of a stronger convective instability. This strengthening of the instability is further supported by the shape of the convective flux in Fig. 4.24, which exhibits both a larger extent and a greater amplitude during the hot phase. Finally, the comparison between the actual and adiabatic gradients through the Schwarzschild criterion also supports this interpretation, as shown in Fig. 2.51. For convenience, these gradients are shown again in Fig. 4.32 but this time taking the difference between those two. A clear decrease in this difference is observed during the cold phase in the middle of the convective zone, further emphasising the weaker convective instability present during this stage of the pulsation cycle.

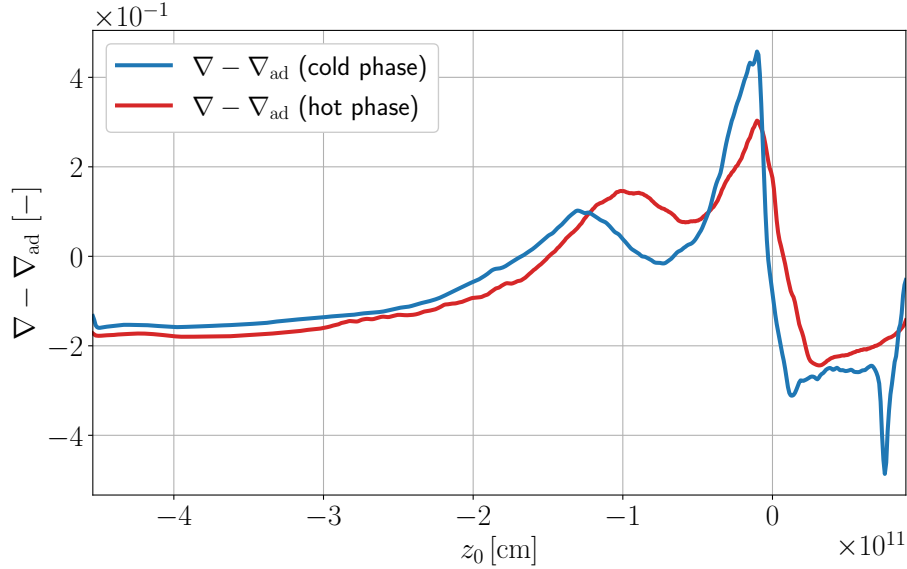


Figure 4.32: Comparison of the difference between the actual and adiabatic temperature gradients, $\nabla - \nabla_{\text{ad}}$, as a function of radius during the hot and cold phases.

In practice, this stronger instability during the hot phase can be explained as the cause of the observed higher calorific exchange during this phase. To understand this, Eq. 2.24, the energy equation, can be recalled. Since no nuclear reactions take place here, it directly gives the following:

$$\rho \frac{Dq}{Dt} = \rho T \frac{Ds}{Dt} = -\nabla \cdot \mathbf{F}. \quad (4.22)$$

Developing the divergence gives

$$\begin{aligned} -\nabla \cdot \mathbf{F} &= -\nabla \cdot (\mathbf{F}_{\text{conv}} + \mathbf{F}_{\text{rad}}) \\ &= -\nabla \cdot \mathbf{F}_{\text{rad}} - \nabla \cdot \mathbf{F}_{\text{conv}} \\ &= -\left(\frac{\partial F_{\text{rad},x}}{\partial x} + \frac{\partial F_{\text{rad},y}}{\partial y} + \frac{\partial F_{\text{rad},z}}{\partial z} \right) - \left(\frac{\partial F_{\text{conv},x}}{\partial x} + \frac{\partial F_{\text{conv},y}}{\partial y} + \frac{\partial F_{\text{conv},z}}{\partial z} \right). \end{aligned} \quad (4.23)$$

From this, since the convective instability is stronger during the hot phase, the downflows are more numerous, extend over a larger fraction of the domain, and extract more heat from their surroundings. This results in a larger convective flux during the hot phase and, consequently, in a larger divergence of the convective flux. The convective flux divergence term appearing in Eq. 4.23 is therefore stronger during the hot phase, leading to enhanced heat exchanges.

Returning to Fig. 4.30, the behaviour of the upflows can now be analysed. A strong decrease can be observed near the surface. More importantly, contrary to the downflows and to the global behaviour, the upflows do not receive more heat during the hot phase. The trend is even reversed. This result is somewhat surprising, since signatures of the κ -mechanism were identified in Secs. 4.3.2 and 4.3.3. Such a mechanism would be expected to produce a larger heat input during the hot phase, but this is not observed for the upflows. To clarify this point, it is useful to return to Eq. 4.23 and focus on the divergence of the radiative flux, more specifically on its radial component. This term is directly responsible for the κ -mechanism, since the latter is a purely radiative mechanism. Comparing this term with the total heat exchanges for the upflows therefore amounts to comparing the contribution of the κ -mechanism with the total heat exchanges. These two are compared in Fig. 4.33. Here, the z_0 -axis has been restricted because of noise issues, as was already done previously for the radiative flux. It should be noted that the quantity considered here involves the divergence of a gradient, which amplifies numerical noise and therefore leads to even larger problems.

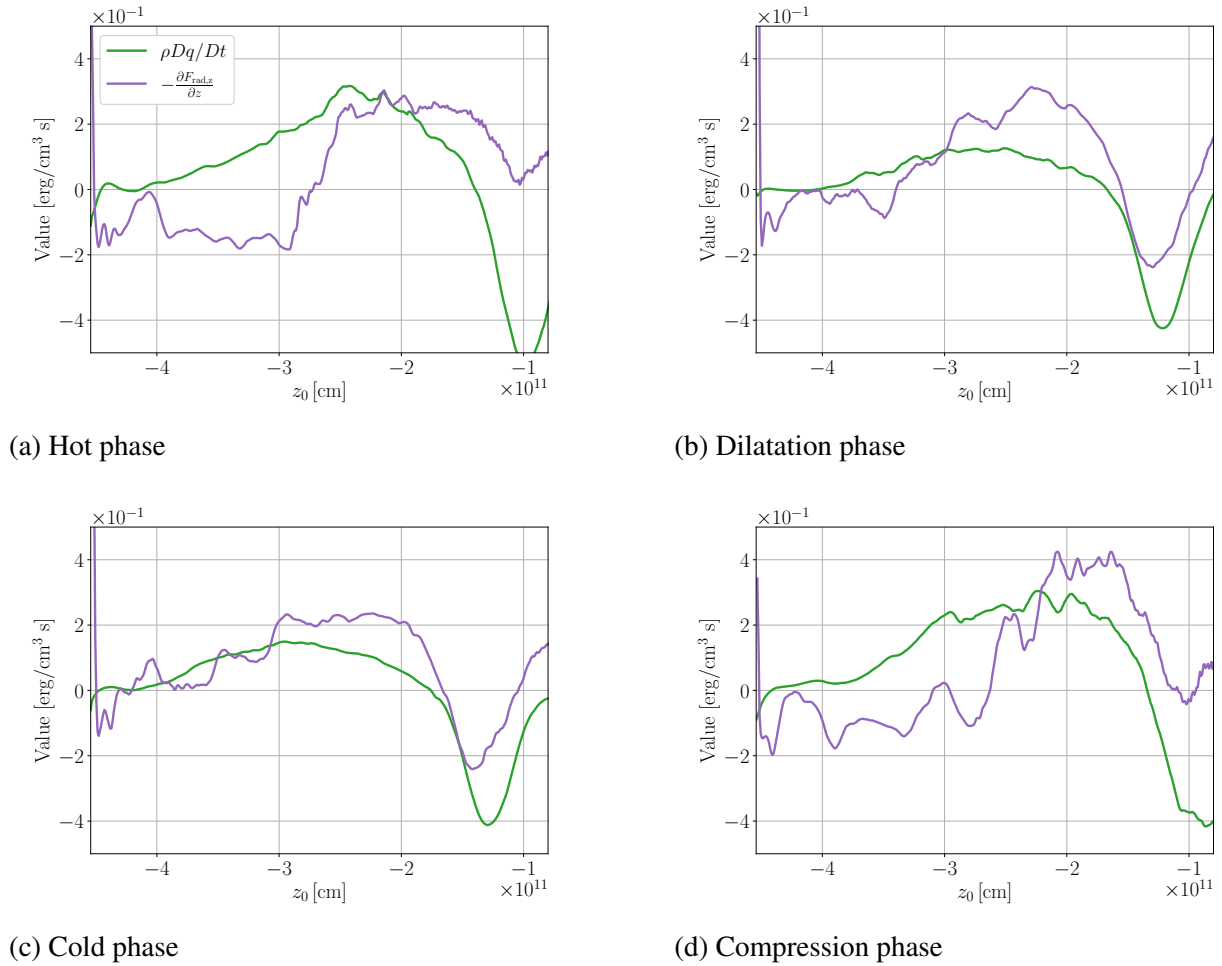


Figure 4.33: Comparison of the contribution of the κ -mechanism $-\partial F_{\text{rad},z}/\partial z$ to the total heat-exchange term of the upflows $\rho Dq/Dt$ during the four main phases of the pulsation cycle.

This figure makes the situation much clearer. It can be seen that the term associated with the κ -mechanism is indeed larger during the hot phase than during the cold phase in the region of the second ionisation zone (around $z_0 \simeq -1.5 \times 10^{11}$, [cm], see Fig. 4.26). This behaviour is consistent with a driving effect and therefore confirms the presence of the κ -mechanism in

the simulation. However, this term is largely dominated by the contributions of the other terms entering the heat-exchange equation since the total heat exchange does not follow the same trend. As a consequence, although the κ -mechanism is clearly present, its effect is largely overwhelmed by other physical processes and does not dominate the overall heat exchanges.

Another interesting figure to analyse is the calorific exchanges integrated over the star to the considered point, similarly to the previous integration of the work. This provides at the surface the total value received/lost by the box. This integration is performed and illustrated in Fig. 4.34.

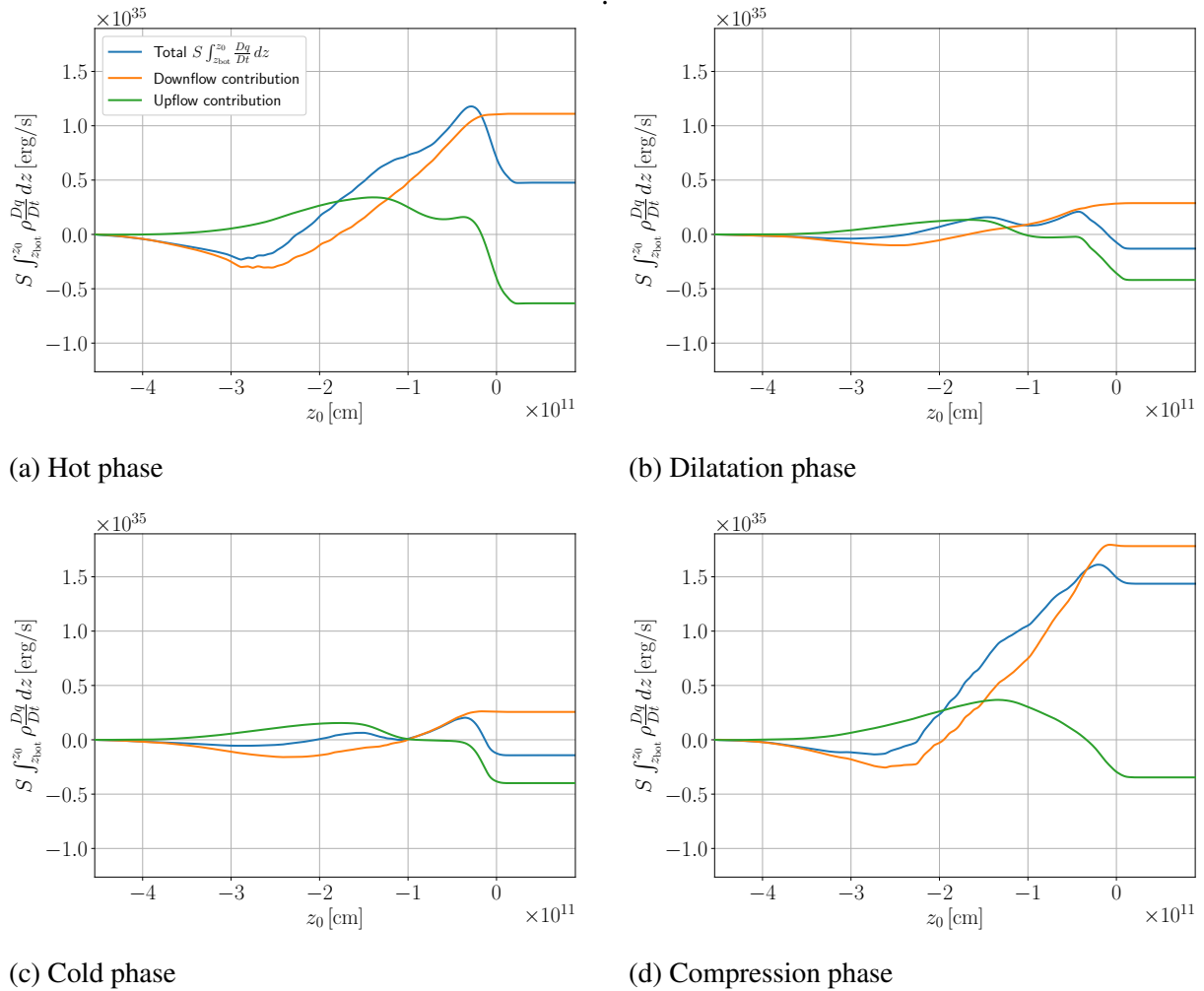


Figure 4.34: Separation of the contributions of upflows and downflows to the integrated heat supply $S \int_{z_{\text{bot}}}^{z_0} \rho \frac{Dq}{Dt} dz$ as a function of the layer depth during the four main phases of the pulsation cycle.

Fig. 4.34 again shows that the entire simulation domain receives more heat during the hot phase than during the cold phase. However, it is interesting to note that the oscillations of the total integrated heat-exchange term, evaluated at the surface, are not centred around zero. This means that the simulation domain receives more energy than it loses. In fact, this also indicates that the simulation has not yet reached a global mean steady state, in which the star would oscillate around an equilibrium structure whose average properties do not evolve with time. In such a state, the heat gained during the hot phase would be exactly balanced by the heat lost during the cold phase, resulting in a vanishing mean heat exchange over a complete pulsation cycle. An

analogy can be made with a car travelling at constant speed: although energy is continuously exchanged with the environment, there is no long-term accumulation or loss of energy, and the average energy balance remains zero.

To understand this more clearly, it is sufficient to integrate Eq. 4.20 over one pulsation cycle:

$$\int_0^{2\pi/\omega} \frac{Dq}{Dt} dt = \int_0^{2\pi/\omega} \frac{du}{dt} dt + \int_0^{2\pi/\omega} P \frac{dv}{dt} dt. \quad (4.24)$$

For a global mean steady-state situation, the first term on the right-hand side vanishes, since u is a state function, and the same state is recovered at the end of the cycle as at the beginning. Moreover, a global mean steady state implies that no net energy is either supplied to or extracted from the pulsational motion so that the work over a cycle is exactly zero. This directly implies that the integral of $\frac{Dq}{Dt}$ also vanishes.

Here, the simulation domain receives more energy than it loses, implying that energy is accumulated within the box. This excess energy must therefore be stored in one or more reservoirs. Several possibilities exist, since the total energy of the simulation domain, E_{box} , can be decomposed as

$$E_{\text{box}} = E_i + E_{\text{kin}}, \quad (4.25)$$

where E_i is the total internal energy and E_{kin} is the total kinetic energy. The latter can itself be decomposed starting from its definition:

$$E_{\text{kin}} = \frac{1}{2} \int_V \rho v_z^2 dV. \quad (4.26)$$

The vertical velocity is then separated into a mean component, associated with the pulsational motion, and a fluctuating component:

$$v_z = \langle v_z \rangle + \Delta v_z. \quad (4.27)$$

This yields

$$E_{\text{kin}} = \frac{1}{2} \int_V \rho \langle v_z \rangle^2 dV + \int_V \rho \langle v_z \rangle \Delta v_z dV + \frac{1}{2} \int_V \rho (\Delta v_z)^2 dV. \quad (4.28)$$

The pulsational component is associated with the horizontally averaged vertical velocity and can be written as

$$E_{\text{puls}} = \frac{1}{2} \int_V \rho \langle v_z \rangle^2 dV, \quad (4.29)$$

and the convective or turbulent kinetic energy can therefore be estimated by subtracting this pulsational contribution from the total kinetic energy:

$$E_{\text{conv}} = E_{\text{kin}} - E_{\text{puls}}. \quad (4.30)$$

This quantity can be computed from the mean files by approximating the mean total kinetic energy using the term $\langle \rho \rangle \langle v_r^2 \rangle$. The pulsation energy can be exactly computed using $\langle \rho \rangle \langle v_z \rangle$.

These terms are then integrated over the radius to obtain the total associated energy.

Fig. 4.35 shows the evolution of the relative fluctuations of the different energy contributions. The quantities are presented in relative form because the internal energy is, in absolute terms, much larger than the kinetic energy. The mean value is 5.15×10^{41} [erg] for the internal energy, compared with only 2.31×10^{39} [erg] for the kinetic energy. Displaying relative variations therefore makes it possible to compare the temporal evolution of the different energy components on the same scale.

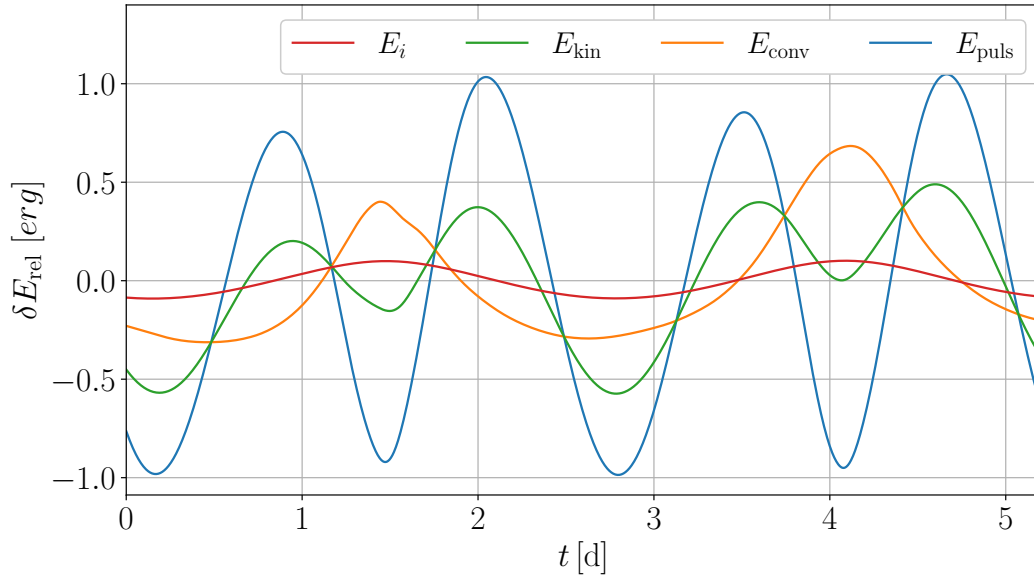


Figure 4.35: Temporal evolution of the relative energy variations δE_{rel} for the different contributions to the total energy of the system.

First, the increase of internal energy during the hot phase and its decrease during the cold phase can be clearly observed. The pulsational energy is also approximately in phase opposition with the internal energy, as it is expected to reach a minimum during the hot and cold phases, at least when neglecting possible phase shifts arising from the non-adiabatic nature of the pulsation. An interesting feature is that the turbulent kinetic energy is significantly larger during the hot phase than during the cold phase. This result further corroborates the previous evidence pointing towards a stronger convective instability during the hot phase.

Regarding the long-term evolution, the pulsational energy does not appear to increase significantly throughout the simulation. On the contrary, the convective or turbulent kinetic energy shows a substantial increase. The internal energy also increases, but this trend is less apparent in relative terms because its mean value is much larger. Consequently, the same amount of accumulated energy corresponds to a much smaller relative variation than in the case of the kinetic energies. These increases confirm that the simulation is still in a phase where its internal energy and turbulent kinetic energy are adjusting. One may expect this to correspond to a first stage of the relaxation process, while a later stage could involve a modification of the pulsational energy. The two components of the kinetic energy can also be analysed, this time in absolute terms. This is done in Fig. 4.36.

This figure allows one to see the weight of each contribution in the kinetic energy. Here, as expected, the two terms are of the same order.

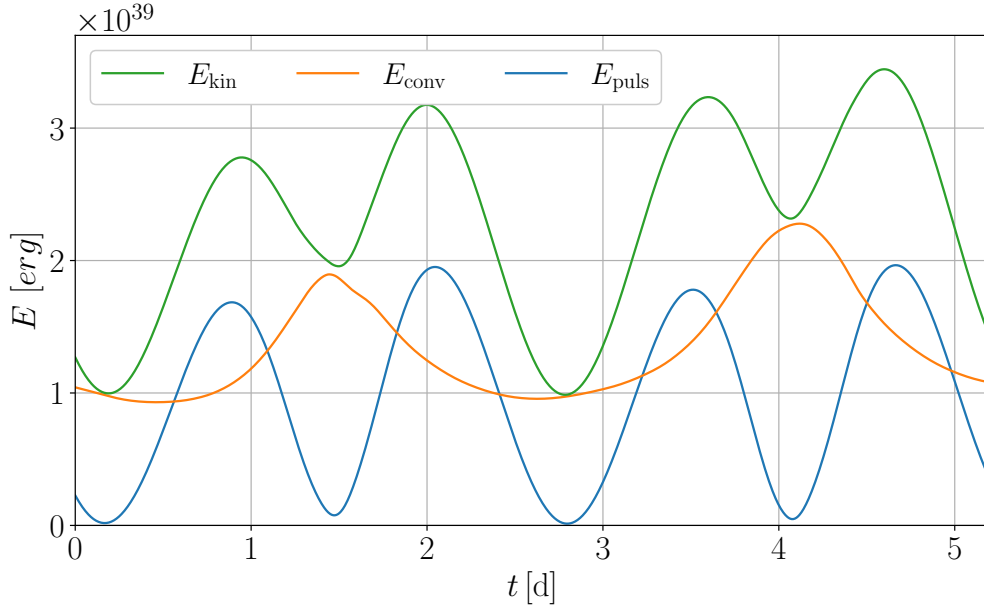


Figure 4.36: Temporal evolution of the kinetic energy E_{kin} and its two components: the pulsational energy E_{puls} and the turbulent energy E_{conv} .

Finally, the total estimated time required to reach a global mean steady state can be approximated by computing the thermal relaxation time τ_{th} , presented in Eq. 2.130, obtained by dividing the mean internal energy contained in the simulation domain by the mean radiated luminosity:

$$\tau_{th} = \frac{\overline{\int_V \rho u dV}}{\overline{L}} \sim 93 \text{ [d]}, \quad (4.31)$$

which shows that reaching such a state would be computationally extremely demanding and, in practice, likely unfeasible.

To conclude this final part of the analysis, the study of the pulsation cycle has shown that the pulsations are amplified by the gas through the action of the downflows, which dominate the dynamics of the system. Although signatures of the κ -mechanism are visible within the upflows, its contribution appears to be largely dominated by other terms. Furthermore, the simulation has not yet reached its global steady state and is still adjusting its internal and turbulent energy reservoirs throughout the evolution.

It should also be emphasised that the analysis presented here has been carried out by separating and examining the behaviour of each type of flow independently. In reality, these flows are coupled and continuously interact with one another. Additional physical mechanisms may therefore emerge from these interactions, potentially causing other contributions to the divergence of the total flux to become dominant. A complete understanding of the pulsational behaviour would thus require a more detailed investigation of these couplings and their role in the global energy balance.

Chapter 5

Conclusion and perspectives

5.1 Conclusion

This work has provided a comprehensive analysis of a three-dimensional simulation of a Cepheid variable star.

The first outcome of the analysis revealed the extreme conditions present in the star and the links between the different profiles. It also showed a clear discrepancy between the results obtained from three-dimensional simulations and those predicted by classical one-dimensional models, partly due to differing imposed conditions. In particular, this work has highlighted the intrinsic limitations of one-dimensional descriptions, especially models based on simplified treatments of convection, such as mixing-length theory. It also showed that the three-dimensional simulation remains limited by non-ideal boundary conditions and by its limited duration, which does not allow the system to reach a fully relaxed state.

A closer examination of the simulation reveals a pronounced dynamical asymmetry between upflows and downflows. The observed flow structure is characterised by narrow, fast, and intense downflows that dominate the convective transport, while upflows appear comparatively smoother and of lower amplitude. This asymmetry complicates the interpretation of one-dimensional averaged profiles, as the averaging process combines regions with markedly different dynamical behaviour, thereby underscoring the value of the full three-dimensional flow information.

Finally, the analysis of the thermodynamic evolution points towards the emergence of a self-sustained cycle with net positive work, associated with pulsational behaviour driven by alternating phases of heat gain during the hot phase and heat loss during the cold phase. While the κ -mechanism, commonly regarded as the primary driving mechanism in this context, is indeed present, it does not appear to play the leading role traditionally attributed to it and is instead largely overshadowed by other dynamical processes.

5.2 Perspectives

These conclusions open a range of possible directions for future work.

First, the clear dichotomy of the flows suggests moving away from the classical symmetric model of convection and instead considering more advanced descriptions that account for this

asymmetry, for example, by using different sets of governing equations depending on the direction of the flow.

Furthermore, several improvements could be made in hypothetical future simulations in order to reduce uncertainties and relax some of the assumptions made in this study. In particular, the assumption of constant gravity could be revisited, as well as the treatment of boundary conditions, which by construction constrain the mass flux. Longer-duration simulations would also help the system reach a more relaxed state, improving the robustness and reliability of the model. Although computationally expensive, simulations performed without some of these simplifying assumptions could significantly improve physical realism and potentially enable meaningful comparisons with observational data.

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