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RELATIVISTIC FLUID MODELLING OF GAMMA-RAY
BINARIES

RELATIVISTIC FLUID MODELLING OF GAMMA-RAY BINARIES

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Unfortunately, I'm still not a fashion expert.

— GM Magnus Carlsen

PREFACE

In this dissertation, I developed a novel model for the non-thermal emission of wind-driven High-Mass Gamma-Ray Binaries (HMGBs) based on extensive numerical simulations treating the relativistic fluid interaction and the dynamically coupled particle transport. The presented work was carried out from October 2017 to the summer of 2021 at the Institute for Astro- and Particle Physics at the University of Innsbruck.

The thesis consists of an introduction that intends to provide a broader overview on the modelling of HMGBs and related concepts: introducing the basic physical principles, observational methods, past modelling approaches and the issues that have been encountered thereby. Further, I provide prospects and potential points of contact for future work that can tie in with the work presented in this thesis.

This is followed by three research articles that have been published (or accepted for publication) in major peer-reviewed astrophysical journals.

- D. Huber and R. Kissmann (2021). *Special Relativistic Hydrodynamics with CRONOS*. A&A **in press**. arXiv: [2107.10644 \[astro-ph.HE\]](#), henceforth also referred to as [Article I](#) (see [Chapter 4](#))
- D. Huber et al. (2021b). *Relativistic fluid modelling of gamma-ray binaries. I. The model*. A&A **646**, A91, A91. DOI: [10.1051/0004-6361/202039277](#). arXiv: [2012.04975 \[astro-ph.HE\]](#), henceforth also referred to as [Article II](#) (see [Chapter 5](#))
- D. Huber et al. (2021a). *Relativistic fluid modelling of gamma-ray binaries. II. Application to LS 5039*. A&A **649**, A71, A71. DOI: [10.1051/0004-6361/202039278](#). arXiv: [2103.00995 \[astro-ph.HE\]](#), henceforth also referred to as [Article III](#) (see [Chapter 6](#))

My contribution to each of the articles is specified at the end of this thesis in [Appendix A](#).

ABSTRACT

Gamma-ray binaries are among the most extreme astronomical objects. They consist of a massive star and a compact object and radiate the major part of their emission in the gamma-ray band. In a wind-driven scenario, the compact object is presumed to be a pulsar whose highly relativistic outflow collides with the dense stellar wind. This wind interaction gives rise to a complex shock structure, where particles are thought to be accelerated to high energies and subsequently produce the observed radiation.

Since the high-energy emission of these objects cannot be spatially resolved by current and near-future instruments, understanding the involved physical processes requires modelling efforts that try to recover other, observable aspects. While past modelling efforts succeeded at recovering parts of the observed features, they fail at others due to the employed model simplifications and assumptions.

This dissertation aims to elevate the state-of-the-art by developing and implementing a comprehensive numerical model for the non-thermal emission of wind-driven gamma-ray binaries. For the first time, the wind interaction and the evolution of energetic particles are treated in a dynamically coupled, fully three-dimensional framework. This allows for a self-consistent prediction of the expected high-energy emission, including the combined effects of orbital motion, fluid instabilities, relativistic boosting and internal absorption of gamma radiation.

The capabilities of the presented model are demonstrated on the LS 5039 system, testing our model predictions against the wealth of available observational data for this source. The performed simulations make extensive use of modern high-performance-computing infrastructure and thereby enable insights with unprecedented dynamical complexity into this intriguing, astrophysical environment. The obtained results help in advancing our current understanding of gamma-ray binaries in wind-driven scenarios.

KURZFASSUNG

Gamma-Ray Binaries zählen zu den extremsten bekannten astronomischen Objekten. Sie bestehen aus einem massereichen Stern und einem kompakten Objekt, welche den größten Teil ihrer nichtthermischen Emission in Form von Gammastrahlen emittieren. In einem windgetriebenen Szenario wird angenommen, dass es sich bei dem kompakten Objekt um einen Pulsar handelt, dessen hochrelativistischer Ausfluss mit dem dichten Sternwind kollidiert. Diese Windwechselwirkung führt zu einer komplexen Schockstruktur, worin Teilchen auf höchste Energien beschleunigt werden können, um anschließend die beobachtete Strahlung zu erzeugen.

Da die hochenergetische Strahlung dieser Objekte mit heutigen und aktuell geplanten Instrumenten nicht räumlich aufgelöst werden kann, erfordert das Verständnis der beteiligten physikalischen Prozesse Modellierungen, welche beobachtbare Aspekte zu reproduzieren versuchen. Während es den bisherigen Modellen gelang Teile der beobachteten Eigenschaften zu beschreiben, scheitern sie aufgrund der verwendeten Vereinfachungen und Annahmen bei anderen.

Diese Dissertationsschrift zielt darauf ab den Stand der Technik zu verbessern und beschreibt die Entwicklung und Implementierung eines umfassenden, numerischen Modells für die nichtthermische Emission von Gamma-Ray Binaries. Zum ersten Mal wird die Windwechselwirkung und der Transport energetischer Teilchen in einem dynamisch gekoppelten, dreidimensionalen Modell behandelt. Dies ermöglicht eine selbstkonsistente Vorhersage der zu erwartenden hochenergetischen Emission, einschließlich der kombinierten Effekte der Orbitalbewegung, der Fluidinstabilitäten, des relativistischen Beamings und der internen Absorption von Gamma-Strahlung.

Das Potential des vorgestellten Modells wird am Beispiel des LS 5039 Systems demonstriert, wobei die Vorhersagen des Modells mit der Fülle an verfügbaren Beobachtungsdaten dieser Quelle verglichen werden. Die durchgeführten Simulationen nutzen moderne Hochleistungs-Recheninfrastrukturen und ermöglichen dadurch Einblicke mit einer bisher unerreichten dynamischen Komplexität in diese faszinierenden, astrophysikalischen Umgebungen. Die erzielten Ergebnisse tragen dazu bei unser gegenwärtiges Verständnis von Gamma-Ray Binaries in windgetriebenen Szenarien zu verbessern.

*No one who achieves success does so without the help of others.
The wise and confident acknowledge this help with gratitude.*

— Alfred North Whitehead

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Part I

INTRODUCTION

COSMIC RAYS

Unlike the title of this thesis might suggest, the first chapter in this introduction will not be devoted to gamma-ray astronomy. Instead, I will make a small detour to the beginning of the last century and the foundation of the field of astroparticle physics, which opened an important window to high-energy physics that is flourishing to this day. Since this thesis is fundamentally rooted in this field, we should start our journey from there.

1.1 DISCOVERY

In the early twentieth century, the Austrian physicist Viktor Franz Hess discovered during his series of iconic balloon flights (see [Figure 1.1](#)) that the flux of ionizing radiation increases with altitude (Hess, [1912](#)). Since this behaviour could not be reconciled with a terrestrial source, the origin of the radiation was concluded to be extraterrestrial and the radiation was henceforth referred to as Cosmic Rays ([CRs](#)) (Millikan and Cameron, [1928](#)).

It is important to clarify that [CRs](#) are not radiation in the classical sense, which usually refers to electromagnetic waves. Quite on the contrary, it was found later in the 1930s that [CRs](#) are corpuscular and carry electric charges interacting with the Earth's magnetic field.

Thanks to the pioneering work of Pierre Auger and the many modern ground- and space-based instruments, the properties of [CRs](#) could in the meantime be measured

Figure 1.1: Victor Franz Hess (second from left in the balloon basket) and his colleagues before one of their balloon flights in 1912. Image Credits: Victor F. Hess Archiv, Universität Innsbruck.

in great detail. Today we know that **CRs** are a mixture of highly energetic particles that is composed of protons, electrons, and heavier nuclei, which permeate the cosmos (see e.g. Blasi, 2013; Bell, 2013, for a review). **CRs** cover an enormous range in energy spanning from $\sim \text{MeV}$ to $\sim 100 \text{ EeV}$ as shown in Figure 1.2. The **CR** spectrum can be well described by a broken powerlaw with three prominent features where the spectral index changes: the knee at $\sim \text{PeV}$, the ankle at $\sim \text{EeV}$ and the toe cutoff $\sim 100 \text{ EeV}$.

According to simple arguments relating to estimates of the galactic magnetic field strength, **CRs** with energies below the knee remain confined within our Galaxy. Hence, **CRs** below $\sim \text{PeV}$ are thought to be mainly of Galactic origin, whereas the ones with higher energies are thought to stem from extragalactic sources.

The detection of **CRs** and their extreme energies sparked several questions: Where do **CRs** come from, i.e. what are the environments where particles can be accelerated to such high energies? How are these particles accelerated, i.e. what are the mechanisms that transfer energy from the environment to the **CR** particles and can reach up to these extreme energies? However, to this day, these questions remain partially unanswered and are still subject to actively ongoing research.

1.2 FERMI ACCELERATION

In the decades following the detection of **CRs**, the processes responsible for their acceleration remained widely unknown. This was changed by the publication of the landmark work by Fermi (1949), who established the fundamental physical principles for the acceleration of charged particles in astrophysical plasmas.

Figure 1.2: A compilation of the cosmic-ray energy spectrum measured by several experiments (after 2000). Image Credits: Evoli (2020).

Such plasmas are characterised by a very high conductivity that leads to the immediate short-circuit of any possibly occurring electric fields by the freely moving charges constituting the plasma – a property that is fundamental to ideal Magneto-Hydrodynamics (MHD). Consequently, electric fields vanish in the frames comoving with the plasma flow, leaving only magnetic fields. Magnetic fields by themselves, however, are unable to increase the energy of charged particles but can only deflect them. Fermi, therefore, argued that the acceleration process has to be rather viewed as a scattering process on turbulent magnetic-field irregularities, which for instance occur naturally in interstellar space in the form of Alfvén waves.

Another, more modern view promoted by Lemoine (2019) is to understand Fermi-acceleration by following a particle through a continuous sequence of rest-frames that are comoving with the bulk fluid flow. Again, particles cannot gain energy in these rest-frames due to the vanishing electric field but suffer from pitch angle scattering that induces their spatial diffusion. Depending on the velocity profile of the fluid and the trajectory of the particle, the frame changes can be non-inertial. The particles will therefore experience associated inertial forces, which finally provide the energy gains or losses. In its essence, Fermi-acceleration is therefore

tightly related to the diffusion of particles and the inertial forces provided by changing fluid velocities.

1.2.1 Diffusive shock acceleration

Important examples for the application of Fermi acceleration that involve rapid changes in fluid velocities are shocks. Shocks are a particular type of waves that are characterised by a steep jump in density, pressure and speed. They emerge naturally from the solution of the classical or relativistic Euler equations and occur in nature in a multitude of different environments. The most prominent of these are Supernove Remnants (SNRs), where the expanding material launched by a supernova explosion drives a shock into the interstellar medium. Due to estimates of their frequency of occurrence and average energetics, SNRs were soon suspected to provide the bulk of the power required to drive the observed CR luminosity observed at Earth (see e.g. Baade and Zwicky, 1934; Blandford and Ostriker, 1978).

Fermi acceleration at shocks is often also referred to as Diffusive Shock Acceleration (DSA) or first-order Fermi acceleration. Due to the strongly compressive fluid motion at shocks, these environments pose particularly efficient accelerators (see e.g. Krymskii, 1977; Blandford and Ostriker, 1978; Bell, 1978). There exists a broad variety of different approaches and methods to quantify the acceleration characteristics at shocks, ranging from the tracing of individual particles or the solution of particle transport equations to a perturbative analysis of the fundamental Boltzmann equation (see e.g. also Drury, 1983; Blandford and Eichler, 1987). For the purpose of illustration, I will closely follow the test particle approach presented by Bell, 1978 in the following.

Let's consider an infinitely extended planar shock that moves with speed β_s in $-x$ -direction, separating a homogeneous, upstream medium at rest and the shocked, downstream material that moves with a speed β_d in the same direction. In our case, the laboratory frame coincides with the upstream rest-frame (denoted without superscript). In the following, it will be necessary to relate various quantities to other frames such as the downstream rest-frame (denoted by $\tilde{\cdot}$) and the shock rest-frame (denoted by $\cdot^*$) depicted in Figure 1.3.

On the upstream side, a particle with energy E will undergo multiple scatterings on magnetic irregularities until it might eventually cross the shock and enter the downstream side as depicted in Figure 1.3. In the rest-frame of the downstream flow, the energy of the particle is given by the Lorentz transformation

$$\tilde{E} = \gamma_{\text{rel}} (E + \beta_{\text{rel}} p_x), \quad (1.1)$$

Figure 1.3: Schematic representation of Diffusive Shock Acceleration (DSA) in the shock rest frame. An upstream particle with initial energy E_i crosses the shock to the downstream side, is scattered and eventually comes back to the upstream side again, gaining energy depending on the shock-crossing angles θ .

where $\beta_{\text{rel}} = \frac{\beta_u - \beta_d}{1 - \beta_u \beta_d}$ is the relative speed between the up- and downstream flow in natural units ($c = 1$) and $\gamma_{\text{rel}} = (1 - \beta_{\text{rel}}^2)^{-1/2}$ the corresponding Lorentz factor. The relative speed is Lorentz invariant and can thus be computed independently of the considered rest-frame. Using the particle's shock-crossing angle $\mu_{\rightarrow d} = \cos \theta_{\rightarrow d}$ and assuming that it is ultra-relativistic $p \approx E$, the momentum along the shock normal is given by $p_x = E\mu_{\rightarrow d}$, yielding the energy

$$\tilde{E} = \gamma_{\text{rel}} E (1 + \beta_{\text{rel}} \mu_{\rightarrow d}). \quad (1.2)$$

In analogy, the particle on the downstream side is scattered and might eventually cross the shock again under an angle $\tilde{\mu}_{\rightarrow u}$, yielding the energy in the upstream frame

$$E = \gamma_{\text{rel}} \tilde{E} (1 - \beta_{\text{rel}} \tilde{\mu}_{\rightarrow u}) \quad (1.3)$$

After a full shock-crossing cycle, a particle with initial energy E_i in the upstream medium thus ends up with energy E_f that is on average given by

$$\left\langle \frac{E_f}{E_i} \right\rangle = \gamma_{\text{rel}}^2 (1 + \beta_{\text{rel}} \langle \mu_{\rightarrow d} \rangle) (1 - \beta_{\text{rel}} \langle \tilde{\mu}_{\rightarrow u} \rangle) \quad (1.4)$$

From this equation, it is obvious that whether or not a particle gains energy in such a cycle strongly depends on the statistics of the shock-crossing angles. In the subrelativistic regime $\beta_{\text{rel}} \ll 1$, the particle density n scattered on either side can be assumed to be isotropic $dn \propto \frac{1}{2} d\mu$ in the respective rest-frames before crossing the shock. The crossing rate ζ for a given angle is thus given by $d\zeta \propto (\mu - \beta_s) dn$, which yields the average crossing angle

$$\langle \mu \rangle = \int_{\mu_{\min}}^{\mu_{\max}} \mu d\zeta = \frac{\int_{\mu_{\min}}^{\mu_{\max}} \mu (\mu - \beta_s) d\mu}{\int_{\mu_{\min}}^{\mu_{\max}} (\mu - \beta_s) d\mu} \quad (1.5)$$

after normalisation of the distribution. The minimum and maximum angles $\mu_{\min}, \mu_{\max}$, for which a particle is still able to cross the shock, depend on the shock speed in the respective frames $\beta_s < \mu_{\rightarrow d} < 1$, $-1 < \tilde{\mu}_{\rightarrow u} < \tilde{\beta}_s$. Combining this with Equation 1.5 yields the average crossing angles

$$\langle \mu_{\rightarrow d} \rangle = \frac{2}{3} + O(\beta_s); \quad \langle \tilde{\mu}_{\rightarrow u} \rangle = -\frac{2}{3} + O(\tilde{\beta}_s), \quad (1.6)$$

which implies that particles performing a full cycle indeed gain energy on average by a factor of

$$\left\langle \frac{E_f}{E_i} \right\rangle \approx \gamma_{\text{rel}}^2 \left(1 + \frac{2}{3} \beta_{\text{rel}} \right)^2 \approx 1 + \frac{4}{3} \beta_{\text{rel}} \quad (1.7)$$

in the sub-relativistic limit.

If the shock is strongly relativistic $\gamma_{\text{rel}} \gg 1$, it can be shown that an initially isotropic distribution of particles can gain energy by a factor of $\sim \gamma_{\text{rel}}^2$ in the first shock-crossing. For subsequent cycles, the particle distributions remain highly anisotropic while crossing the shock, which consequently reduces the gains to a factor of ~ 2 per cycle (see e.g. Gallant and Achterberg, 1999; Achterberg et al., 2001).

To obtain a differential energy spectrum for particles performing repeated Fermi acceleration cycles, one commonly considers that a constant fraction of particles $\mathcal{P}_{\text{esc}}$ escapes the system and is lost at each cycle. The probability for a particle performing k cycles is therefore given by $\mathcal{P}_{\text{cycle}}^k = (1 - \mathcal{P}_{\text{esc}})^k$. An initial population of N_0 particles with uniform energy E_0 is therefore reduced to $N_k = N_0 \mathcal{P}_{\text{cycle}}^k$ particles, which will have the average energy $E_k = E_0 \langle \frac{E_f}{E_i} \rangle^k$. After eliminating k , one finds that the differential distribution of particles asymptotically approaches a power-law of the form

$$dN \propto E^{-s} dE, \quad (1.8)$$

with spectral index $s = 1 - \log \mathcal{P}_{\text{cycle}} / \log \langle \frac{E_f}{E_i} \rangle$.

To compute the spectral index, some knowledge of the escape probability is required. It can be obtained by considering the system in the shock rest-frame and assuming that the scattering kernels are advected approximately with the fluid flow, i.e. that the shock is much faster than the Alfvén speed. This implies that particles cannot escape the system on the upstream side since the scattering kernels are advected towards the shock with speed β_u^* and the particles will thus eventually be overtaken by the shock. The particle flux crossing the shock from

upstream to downstream can be computed from similar arguments leading up to Equation 1.5 yielding

$$f_{\rightarrow d} = \int_{\beta_s}^1 \frac{n}{2} (\mu - \beta_s) c d\mu = \frac{1}{4} nc + O(\beta_s). \quad (1.9)$$

In contrast, on the downstream side, the flow moves away from the shock and some particles will eventually escape the system and not be available for further Fermi-acceleration cycles. Considering a steady state, the advection away from the shock has to be balanced by the diffusion of particles. In the subrelativistic limit, the corresponding advection-diffusion equation takes the form (Bell, 1978)

$$\beta_d^* c \partial_x n = D_d^* \partial_x^2 n, \quad (1.10)$$

where D_d^* is the respective diffusion coefficient. The above differential equation can be readily solve using the Ansatz

$$n = k_1 + k_2 \frac{D_d^*}{\beta_d^* c} \exp\left(\frac{\beta_d^* c}{D_d^*} x\right), \quad (1.11)$$

where $k_2 = 0$ to maintain finite values at $x \rightarrow \infty$, which consequently implies $n \propto \text{const}$. The flux of particles escaping the systems is thus given by $f_{\text{esc}} = \beta_d^* cn$. Balancing it against the incoming particle flux yields the escape probability

$$\mathcal{P}_{\text{esc}} = \frac{f_{\text{esc}}}{f_{\rightarrow d}} \approx \frac{\beta_d^* nc}{\frac{1}{4} nc} = 4\beta_d^*. \quad (1.12)$$

The up- and downstream states of shocks are not independent of each other but are related by the Rankine-Hugoniot jump conditions. In the case of Newtonian hydrodynamics, they connect the plasma speeds on both sides by $\beta_u^* = r\beta_d^*$, where r is the compression ratio of the shock. Consequently, one finds that $\beta_{\text{rel}} \approx (r-1)\beta_d^*$, which can be combined with Equation 1.8 to obtain the well-known result for the spectral index of particles accelerated at subrelativistic shocks

$$s = 1 - \frac{\log \mathcal{P}_{\text{cycle}}}{\log \langle \frac{E_f}{E_i} \rangle} \approx 1 + \frac{4\beta_d^*}{\frac{4}{3}\beta_{\text{rel}}} = 1 + \frac{3}{r-1} = \frac{r+2}{r-1}. \quad (1.13)$$

Strong hydrodynamical shocks exhibit compression ratios up to $r = 4$, which yields the commonly used standard value for DSA of $s = 2$.

In the relativistic case $\gamma_{\text{rel}} \gg 1$, the assumption of a super-Alfvénic shock is no longer valid and particles can escape the system also on the upstream side. Combined with the highly anisotropic distribution of particles due to less efficient

Figure 1.4: Different modifications to the standard Diffusive Shock Acceleration (DSA) scenario.

scattering and deflection mechanisms, the resulting spectrum is expected to be slightly softer with $s \sim 2.2 - 2.3$ (see e.g. Gallant and Achterberg, 1999; Achterberg et al., 2001).

On the other hand, DSA in principle can also produce even harder spectra. This could for example be realised in the interaction of multiple shock waves as shown in Figure 1.4a, where indices up to $s \sim 1$ were reported (see e.g. Melrose and Pope, 1993; Bykov et al., 2013; Vieu et al., 2020), or through non-linear DSA, where the accelerated particles provide additional pressure and modify the shock structure as depicted schematically in Figure 1.4b (see also e.g. Malkov and Drury, 2001; Blasi, 2013, and references therein).

Together with the processes involved in the transport of the accelerated particles through the galaxy, DSA is able to produce particle spectra that are quite close to the observed power-law distributions (see also e.g. Amato and Blasi, 2018). DSA or Fermi-acceleration in general, therefore gives a quite simple but very reasonable explanation for the acceleration of CR particles to very high energies. Due to these qualities, Fermi-acceleration has ever since served as a guide in high-energy astrophysics, with DSA sitting at the very heart of our current understanding for the origin of CRs.

As a final note, it should be mentioned that next to the DSA many other acceleration mechanisms can work alongside in different environments. To name a few, they include shear acceleration (another manifestation of the Fermi-process, see e.g. Berezhko and Krymskii, 1981; Jokipii and Morfill, 1990; Rieger and Duffy, 2006), the acceleration at magnetic reconnections (see e.g. Arzner and Vlahos, 2004;

Matthews et al., 2020) or the espresso acceleration mechanism (Caprioli, 2015; Mbarek and Caprioli, 2019).

Due to the presence of cosmic magnetic fields, the accelerated, charged CRs are continuously deflected on their journey from their origin to their detection at Earth. This makes it virtually impossible to reconstruct their trajectories and thus to identify their source environments directly. To circumvent this issue, one has to rely on secondary, neutral messengers that remain unaffected by magnetic fields.

2

THE GAMMA-RAY SKY

A classical neutral messenger that has been exploited for centuries to study astronomical objects are photons. Since we are interested in processes at the highest energies, the photons produced in these environments have also to be searched at the highest energies, in the so-called gamma-ray regime. The transition from X-rays to gamma-rays is not strictly defined, however, a value of 511 keV corresponding to the energy of photons generated in the electron-positron annihilation is commonly used. In contrast to lower energetic radiation, gamma-ray photons cannot be produced through thermal processes but are generated through the interaction of relativistic particles with their environment in high-energy processes (Morrison, 1958). The production of gamma-rays is thus closely entwined with the presence of non-thermal particles and is hence a smoking gun for the acceleration of CRs.

For completeness, it should be mentioned that gamma-ray photons are by no means the only messengers that can be used to study such highly energetic environments. Next to other bands of the electromagnetic spectrum, also other neutral particles such as neutrinos can be used to gain valuable insights that could not be obtained with photons alone. Due to great technological advances in the past years, also an entirely different type of waves, namely gravitational waves, was made accessible, which opened yet another window to astrophysical objects and processes that could not be tapped before.

These different messengers complement each other by being sensitive to various aspects of a given system. Combining all these messengers into a single picture can

therefore lead to great advances in our understanding. This lead to a flourishing of multi-messenger astronomy in recent years that will surely continue for many years to come (see e.g. Mészáros et al., 2019, for a review).

2.1 PRODUCTION OF GAMMA-RAYS

In this section, I will briefly introduce selected radiative processes that produce parts of the gamma radiation measurable at Earth. Due to the nature of the objects that lie at the heart of this dissertation (introduced later in Chapter 3), I will solely focus on leptonic emission processes. For hadronic emission channels or more detailed descriptions in general, I refer the interested reader to the wealth of literature available on this subject (e.g. Rybicki and Lightman, 1979; Aharonian, 2004; Longair, 2011; Ghisellini, 2013).

2.1.1 Synchrotron Process

In the presence of magnetic fields, moving charged particles are continuously deflected due to the arising Lorentz force. Since this force always acts perpendicular to a particle's instantaneous direction of motion, the particle is forced on a spiral trajectory around the magnetic field lines and gyrates with an angular frequency of $\omega_g = \frac{qB}{\gamma mc}$, where q, m, γ are the particle's charge, mass, and Lorentz factor, respectively, and B the magnetic field.

Due to the continuous acceleration by the Lorentz force, the particle will also continuously emit electromagnetic waves that are also known as synchrotron radiation as shown schematically in Figure 2.1. In doing so, the particle loses energy and releases a radiant flux (energy per unit time) of

$$\mathcal{P}^{\text{sync}} = 2c\sigma_T w_{\text{mag}} \gamma^2 \sin^2 \alpha \left(\frac{q}{e}\right)^4 \left(\frac{m_e}{m}\right)^2, \quad (2.1)$$

where α is the pitch angle between the particle and the magnetic field and $w_{\text{mag}} = \frac{B^2}{2\mu_0}$ the magnetic field's energy density (see e.g. Longair, 2011). From the above expression, it is immediately visible that electrons lose their energy much quicker than protons due to their much lower mass causing stronger acceleration in the same magnetic field.

For relativistic particles, the produced radiation is strongly beamed into a cone with an opening angle $\sim \gamma^{-1}$ along the direction of motion. This produces repeated, lighthouse-like emission pulses that are responsible for the resulting synchrotron

Figure 2.1: Schematic production of synchrotron radiation due to the gyration of a relativistic electron with Lorentz factor γ and inclination angle α relative to the magnetic field lines. In the far field, the angular radiation characteristics take the form of a hollow cone.

emission spectrum. The spectral flux (power per unit photon energy) of a single particle can be obtained by a Fourier analysis (see Longair, 2011, for more detail) and takes the form

$$\mathcal{P}_\epsilon^{\text{sync}} = \mathcal{P}^{\text{sync}} \frac{9\sqrt{3}}{8\pi} \frac{1}{\epsilon_c} F_{\text{sync}} \left(\frac{\epsilon}{\epsilon_c} \right), \quad (2.2)$$

where $F_{\text{sync}}(x) = x \int_x^\infty K_{5/3}(y) dy$ with $K_{5/3}$ denoting the modified Bessel function of the second kind. Due to the properties of F_{sync} , the emission is peaked around the critical photon energy

$$\epsilon_c = \frac{3e\hbar}{2m_e} \gamma^2 B \sin \alpha = 1.74 \times 10^{-8} \text{ eV} \frac{B \sin \alpha}{1 \text{ G}} \gamma^2. \quad (2.3)$$

Depending on the magnetic field strength and the energy of the electrons, synchrotron emission can be produced in virtually every band of the electromagnetic spectrum. Therefore, the study of synchrotron emission has ever since been an important cornerstone for investigating non-thermal processes.

2.1.2 Inverse-Compton scattering

Apart from interactions with magnetic fields, electrons can also interact with radiation fields and scatter on the photons therein (see also Aharonian, 2004; Longair, 2011, and references therein). Compton (1923) observed that high-energy photons can scatter on low-energy electrons and transfer a fraction of their energy and momentum to the electrons in the process. In doing so, the photon is left with less energy and is therefore shifted to larger wavelengths, whereas the electron has gained energy. This process is also known as Compton scattering.

Figure 2.2: Schematics of the Inverse-Compton (IC) scattering process, where energy is transferred from highly energetic, relativistic particles to lower energetic seed photons, which are consequently transformed into gamma-rays.

The energy ϵ of the photon after a collision with an electron can be calculated straightforwardly through relativistic kinematics. This yields the expression

$$\epsilon = \frac{\gamma \epsilon_0 (1 - \beta \cos \alpha)}{\gamma (1 - \beta \cos(\theta - \alpha)) + (\epsilon_0 / m_e c^2) (1 - \cos \theta)} \quad (2.4)$$

$$\approx \frac{\epsilon_0}{1 + (\epsilon_0 / m_e c^2) (1 - \cos \theta)}, \quad \text{for } \beta \ll 1 \quad (2.5)$$

where α denotes the incident angle between the photon and the electron, θ the scattering angle of the photon (see also Figure 2.2), ϵ_0 the incident photon energy and β, γ the initial electron speed and corresponding Lorentz factor, respectively. In the sub-relativistic limit, the photon always loses energy depending on its scattering angle as seen in Equation 2.5, whereas this is not the case in general.

Naturally, equation Equation 2.4 also accounts for inverted scenarios, where relativistic electrons transfer a part of their energy to lower energetic photons as shown schematically in Figure 2.2. This process is commonly referred to as Inverse-Compton (IC) scattering and is responsible for a large part of the gamma-ray signal that is detected at Earth. The maximum energy is transferred from the electron to the photon in a head-on collision ($\alpha = \pi$) that completely reverses the photon's trajectory ($\theta = \pi$). Following Equation 2.4, the upscattered photons can thus reach energies up to

$$\epsilon_{\max} = \frac{4\gamma^2 \epsilon_0}{1 + (4\gamma \epsilon_0 / m_e c^2)}. \quad (2.6)$$

This implies that in the Thomson regime $\gamma \epsilon_0 \ll m_e c^2$, photons can gain energy by up to a factor of $\epsilon_{\max} / \epsilon_0 \sim \gamma^2$ and can hence be scattered to very high energies. For example if we consider an electron population at TeV energies ($\gamma \sim 10^6$), photons from the Cosmic Microwave Background (CMB) with an energy $\epsilon_0 \sim \text{meV}$ can be scattered up to GeV gamma-ray energies and more energetic stellar photons ($\epsilon_0 \sim \text{eV}$) can even reach up to TeV energies.

As for all scattering processes, also IC scattering is best described by a scattering cross-section σ_{IC} . In the non-relativistic, low-energy case, where the electron's Lorentz factor $\gamma \sim 1$ and the energy of the incoming photon is negligible against the electron mass $\epsilon_0 \ll m_e c^2$, IC scattering is well described by classical Thomson scattering with $\sigma_{\text{IC}} \sim \sigma_T$. For higher photon energies and relativistic electrons, however, quantum-relativistic effects have to be included. The respective differential cross-section was derived by Akhiezer and Berestetskii (1965) and is commonly also referred to as Klein-Nishina cross-section. An approximation to the total (angle averaged) Klein-Nishina cross-section, that is frequently used in literature, was formulated by Coppi and Blandford (1990) and reads as

$$\sigma_{\text{IC}} = \frac{3\sigma_T}{8x} \left[\left(1 - \frac{2}{x} - \frac{2}{x^2} \right) \log(1+2x) + \frac{1}{2} + \frac{4}{x} - \frac{1}{2(1+2x)^2} \right]. \quad (2.7)$$

The approximation depends only on the term $x = \gamma\epsilon_0/m_e c^2$ and gives good estimations with an accuracy better than 10 per cent over a wide range of scattering parameters. From the above expression, it is visible that the scattering cross-section decreases with increasing energy, separating the Thomson from the Klein-Nishina regime at $\gamma\epsilon_0 \sim m_e c^2$.

To obtain the energetic and angular distribution of the upscattered IC photons, the differential Klein-Nishina cross-section has to be considered. This was, for example, done by Aharonian and Atoyan (1981) assuming an isotropic distribution of relativistic electrons and a monochromatic beam of target photons, yielding the spectral intensity

$$\mathcal{P}_{\epsilon, \Omega}^{\text{ic}} = \frac{3}{16\pi} c \sigma_T \frac{1}{\gamma^2} \frac{\epsilon}{\epsilon_0} n_{\epsilon_0} f_{\text{ic}}(\epsilon, \epsilon_0, \gamma, \theta), \quad (2.8)$$

where ϵ_0, ϵ again denote the initial and the scattered photon energies and n_{ϵ_0} the target photon density. The scattering kernel f_{ic} for energies in the range of $\epsilon_0 \ll \epsilon \ll \epsilon_{\text{max}}$ is given by

$$f_{\text{ic}}(\epsilon, \epsilon_0, \gamma, \theta) = 1 + \frac{w^2}{2(1-w)} - \frac{2w}{b_\theta(1-w)} + \frac{2w^2}{b_\theta^2(1-w)^2}, \quad (2.9)$$

with $b_\theta = 2(1 - \cos \theta)\epsilon_0\gamma/m_e c^2$ and $w = \epsilon/\gamma m_e c^2$. One finds that the emission is strongly anisotropic with the minimum or maximum fluxes being reached in the direction parallel or antiparallel to the beam, respectively (see e.g. also Dubus et al., 2008).

2.2 OBSERVING GAMMA-RAYS

Unlike photons at other wavelengths, gamma-rays cannot be observed directly at ground level on Earth. Due to their large interaction cross-section with nuclei in the atmosphere, they will inevitably scatter and be destroyed. This made the detection of gamma-rays technically very challenging (see e.g. Degrange and Fontaine, 2015, for a historical review) and decades of development were needed until the necessary technologies became available.

The detection of gamma-rays can be subdivided conceptually into direct space-based and indirect ground-based approaches - both having their distinct characteristics, advantages and shortcomings. In the next sections, I will give a brief overview of the underlying detection principles and the observation missions that provided parts of the data used in this work.

2.2.1 *Space-based observatories*

The most direct way to circumvent the absorption of gamma-rays in the Earth's atmosphere is to launch gamma-ray detectors into space. After the first pioneering phase in the 1970s and significant technological advances in the 1980s, the first major gamma-ray observatory, the Compton Gamma-Ray Observatory (CGRO), was launched into space in 1991. Onboard were instruments such as the Compton Telescope (COMPTEL) and the Energetic Gamma-Ray Experiment Telescope (EGRET), which enabled observations in the low-energy (LE) gamma-ray band (1 – 100 MeV) and beyond, up to energies of 30 GeV.

Currently, there are two more modern satellite missions in operation: the Astro-rivelatore Gamma ad Immagini Leggero (AGILE) and the Fermi Large Area Telescope (Fermi-LAT). Both telescopes are built on the same basic detection principles and access the observational window between 100 MeV and 100 GeV, which is commonly referred to as high-energy (HE) gamma-rays. Throughout this section, the Fermi-LAT will serve as an example for the introduction of these principles.

One of the principal components of the Fermi-LAT is the tracker, which is composed of interleaving layers of tungsten converter-foils and silicon strip-detectors shown schematically in Figure 2.3b. When a gamma-ray photon enters the detector, it is converted to an electron-positron pair at one of the converter layers. Unlike the uncharged photon, the trajectories of the charged leptons can now be measured by the detectors, which allows a reconstruction of the arrival direction of the incoming gamma-ray photon.

(a) The [Fermi-LAT](#) instrument (silvery box at the top) is shown integrated with the spacecraft. Image Credits: NASA/General Dynamics Advanced Information Systems

(b) Schematic cross-section of the [Fermi-LAT](#) showing how the conversion foils in the tracker transform an incoming gamma-ray photon into an electron/positron pair and how they are stopped in the calorimeter. Image Credits: NASA's Goddard Space Flight Center

Figure 2.3: The Fermi gamma-ray space telescope with special focus on the [Fermi-LAT](#) instrument.

For highly energetic photons, the created lepton pair will be highly relativistic. As a consequence, their opening angle in the detector will be relatively small, which allows for a more accurate reconstruction of the photon's arrival direction, i.e. a lower Point Spread Function ([PSF](#)) with increasing incident photon energy. Typical values for the [Fermi-LAT](#) are for example around 5° at 100 MeV and 0.2° at 10 GeV (at 68% containment) ([Abdollahi et al., 2020](#)).

Finally, the created electron-positron pair is stopped in the caesium-iodide absorption calorimeter at the bottom of the [Fermi-LAT](#). The deposited energy is measured, which directly relates to the energy of the incoming photon that can be reconstructed with an energy dispersion of $< 10\%$ between 1 GeV and 100 GeV.

In addition to gamma-ray photons, also [CR](#) particles enter and trigger the detector causing unwanted signals. To be able to identify and reject these tracks, the tracker is surrounded by an anticoincidence shield, which detects charged particles entering the instrument. It is therefore only sensitive to charged [CRs](#) but not gamma-rays, which enables effective discrimination between the signals.

Since in operation, [Fermi-LAT](#) continuously surveys the whole sky thanks to its large Field of View ([FOV](#)) of ~ 2 sr, which enabled the production of stunning all-sky maps such as the one depicted in [Figure 2.4](#). The exhibited features in the [HE](#) gamma-ray sky are quite different from the ones seen in other wavelengths. They include very bright diffuse emission around the Galactic plane together

Figure 2.4: The gamma-ray sky above 1 GeV as seen by Fermi-LAT after 12 years of observations. Image Credits: Fermi-LAT Collaboration.

with other Galactic sources, that are hard to distinguish in many cases due to the relatively large PSF. The point-like sources above and below the Galactic plane mainly correspond to extragalactic objects belonging to the broad class of Active Galactic Nuclei (AGNs).

2.2.2 Ground-based observatories

Even though gamma-rays cannot be observed directly at Earth due to their interactions with the atmosphere, they can be detected indirectly by exploiting these interactions and measuring the observable signal of their secondary particles. Using this concept, one effectively leverages a large part of the atmosphere as a detector.

After entering the atmosphere, a gamma-ray photon will scatter on the nuclei of air molecules and produce electron-positron pairs in a process known as Bethe-Heitler pair-production (Bethe and Heitler, 1934). Since the incoming gamma-ray photons are highly energetic, the produced leptons are highly relativistic and suffer severe energy losses due to the emission of Bremsstrahlung. This process again generates gamma-ray photons, which will once more create additional pairs, initiating a cascading production of particles known as Extensive Air Showers (EASs).

The produced particles can then be measured either directly or indirectly to infer the properties of the incident gamma-ray photon. The former case is realised in so-called EAS arrays, which are typically built at higher altitudes to be located

Figure 2.5: The schematic measurement principle of Imaging Atmospheric Cherenkov Telescopes (IACTs). An incoming [VHE](#) gamma-ray photon produces an air shower that emits Cherenkov light upon interaction with the atmosphere, which is observed via detectors at the ground. Image Credits: R. White (MPIK) / K. Bernlöhr (MPIK) / DESY

within the showers initiated by gamma-ray photons. The [EAS](#) particles are detected using, for example, water-Cherenkov tanks as in the case of the High Altitude Water Cherenkov Observatory ([HAWC](#)), scintillation counters as in the Tibet Air Shower Array ([Tibet AS Array](#)) or a mixture of both as in the Large High Altitude Air Shower Observatory ([LHAASO](#)).

Indirect [EAS](#) detection techniques are based on the principle that most of the produced air-shower particles move faster than the phase velocity of light in the surrounding air. In analogy to the amplification of acoustic waves by objects travelling faster than the speed of sound, this leads to a build-up of electromagnetic waves known as Cherenkov radiation (Čerenkov, 1934). Due to this mechanism, [EAS](#) produce very short flashes (~ 2 ns) of blue light ($\sim 300 - 350$ nm) that can be detected at ground-level as shown schematically in [Figure 2.5](#) using specifically designed, very sensitive cameras often composed of arrays of photomultiplier tubes.

Figure 2.6: The [H.E.S.S.](#) telescope array located on the Khomas Highlands in Namibia. Image Credits: C. Föhr (MPIK) / [H.E.S.S.](#)

This concept for detecting gamma-rays at Earth is realised in so-called Imaging Atmospheric Cherenkov Telescopes ([IACTs](#)), such as the High-Energy Stereoscopic System ([H.E.S.S.](#)), the Major Atmospheric Gamma Imaging Telescopes ([MAGIC](#)) and the Very Energetic Radiation Imaging Telescope Array System ([VERITAS](#)) that are currently in operation, and the next-generation Cherenkov Telescope Array ([CTA](#)), which is already in construction. To produce a Cherenkov signal that is strong enough to be detected at ground level, very high incident gamma-ray energies are needed. The typical observational window accessible by [IACTs](#) was thus consequently dubbed as very-high-energy ([VHE](#)) gamma-rays with photon energies $> 100 \text{ GeV}$. Since all of these telescopes are based upon the same basic, technical principles, I will pick out [H.E.S.S.](#) as an example for their introduction in this section. Further, as a member of the [H.E.S.S.](#) collaboration, I had the chance to carry out an observational shift at [H.E.S.S.](#) during my early time as a PhD student.

[H.E.S.S.](#) consists of an array of five telescopes as shown in [Figure 2.6](#): four smaller ones (CT1-4) with an effective mirror diameter of 12 m (in operation since 2004) and a larger one (CT5) with diameter 28 m that was added at a later stage (since 2012). Depending on the mode of operation, multiple telescopes will observe the same [EAS](#) produced by an incident gamma-ray photon from different angles. Combining the data from different telescopes, especially the different orientations of the shower recorded by the cameras, allows for an accurate reconstruction of

Figure 2.7: The Galactic plane in gamma-rays above 1 TeV as seen through the eyes of [H.E.S.S.](#). The map was created as a result of the [H.E.S.S.](#) Galactic Plane Survey ([HGPS](#)) and is only filled where the point-source sensitivity for a 5σ detection is better than 2.5% of the flux of the Crab nebula (see Aharonian et al., [2006b](#)). Image Credits: H.E.S.S. Collaboration et al. ([2018b](#)) reproduced with permission from © ESO.

the arrival direction of the incident gamma-ray photon and its energy. With this, [H.E.S.S.](#) can achieve [PSFs](#) as small as 0.05° (at 68% containment) and typical energy resolutions of $\sim 20\%$.

Like space-based instruments, [IACTs](#) also suffer from background signals produced by [CRs](#), which trigger the formation of [EASs](#). The shape of the signal in the telescope cameras, however, is different and provides information on the nature of the incident particle that can be used to discern these background signals in a statistical sense.

The exact process for the photon reconstruction, however, is quite complex and requires a very precise understanding of the detector's response to the signals produced by the various showers. The instrument response is subject to a multitude of influences. Next to instrumental parameters like pointing position and broken pixels, they include environmental conditions, such as the night-sky background, temperature, humidity, and other atmospheric qualities. To minimise and control the impact of many of the latter factors, [H.E.S.S.](#) is located on the Khomas highlands near Windhoek (Namibia) at an altitude of 1800 m above sea level, which provides

night-sky conditions that are among the clearest on Earth together with low levels of light pollution and precipitation.

Even though the environmental effects are as small as possible due to the chosen location, they are still non-negligible in the analysis of the data. One of the approaches within the [H.E.S.S.](#) collaboration to account for the whole range of influences is to simulate a multitude of showers and their detector signals for the exact conditions of the observation run and to infer the instrument response therefrom; a procedure known as run-wise simulations (Holler et al., 2020). This technique provides a significant improvement of the instrument's [PSF](#) over conventional methods based on pre-generated lookup tables, which enabled the first measurement of the extension of the Crab nebula at TeV energies (H.E.S.S. Collaboration, 2020b) and the detection of extended [VHE](#) emission along the jets of the radio galaxy Centaurus A (H.E.S.S. Collaboration, 2020a).

In contrast to space-based telescopes such as the [Fermi-LAT](#), [H.E.S.S.](#) has a significantly smaller [FOV](#) of ~ 0.006 sr that renders extensive sky surveys very expensive. However, after many years of observations, the [H.E.S.S.](#) collaboration was able to compile the data collected for the Galactic plane into the [H.E.S.S.](#) Galactic Plane Survey ([HGPS](#)) and produce stunning images of the sky through the eyes of [H.E.S.S.](#) such as the one shown in [Figure 2.7](#).

Again, the observed features in [VHE](#) gamma-ray are quite different from what was seen in other wavelengths. In comparison to the [HE](#) gamma-ray sky, the diffuse emission is significantly fainter at [VHE](#) energies making it easier to discern individual sources. Also, thanks to the higher angular resolution as compared to [Fermi-LAT](#) below 100 MeV and the much higher effective area, many new, previously unknown sources were discovered.

It is important to note that neither of the two observational principles for gamma-rays is superior. Instead, they complement each other by providing valuable data at different energies that, combined, provide deeper insights into the high-energy processes at play in the observed sources and eventually bring us one step closer to the understanding of the origins of [CRs](#).

2.3 DETECTION OF BINARIES

As highlighted in the previous sections, gamma-ray observations suffer from fairly large instrumental [PSFs](#) as compared to observations at longer wavelengths. This makes the firm identification of sources and assignment to sources observed at other wavelengths challenging.

A class of objects that allows circumvention of this issue is binary systems. Due to the periodical orbital motion of the two constituents, these systems produce periodically reoccurring emission patterns. One can thus leverage the timing information of the detected gamma-ray photons in addition to their arrival direction to establish unambiguous associations with objects seen at other wavelengths.

The study of gamma-ray-emitting binary systems is also intriguing from a physical point of view. Not only are these systems amongst the most extreme astrophysical objects known and involve a great range of high-energy non-thermal processes, but they offer a window to study these processes in a dynamical environment. This is something that is not possible in the study of SNRs since they evolve on much longer timescales that are not easily accessible to humans.

Over the years, different subclasses to gamma-ray emitting binaries have emerged. They include Novae (e.g. Chomiuk et al., 2020; H.E.S.S. Collaboration, 2021a), Microquasars (e.g. Zhang, 2013), Millisecond Pulsars (MSPs) (with their especially interesting subclasses of redback and black-widow systems) (e.g. Torres and Li, 2020), Colliding-Wind Binaries (CWBs) (e.g. Eichler and Usov, 1993; De Becker and Raucq, 2013), and High-Mass Gamma-Ray Binaries (HMGBs) (e.g. Dubus, 2013). HMGBs compose the most extreme subclass and lie at the very heart of this work, devoting them a separate, more dedicated introduction in the following Chapter 3.

With the exception of MSPs for which about ~ 100 representatives have been found (see e.g. Torres and Li, 2020), each of the other classes contains only up to a handful of firmly identified objects (see e.g. Wakely and Horan, 2008; Abdollahi et al., 2020; H.E.S.S. Collaboration, 2021b). Considering that more than 50% of stars occur in binary systems (Karttunen, 2007), it is astonishing that only so few binaries emit at gamma-ray energies. This observation, together with the extreme energetics of these sources, raised the need for a better understanding of the physical processes at play in these systems.

HIGH-MASS GAMMA-RAY BINARIES

In comparison to the other classes of gamma-ray-emitting binary systems, [HMGBs](#) are distinguished by releasing most of their radiative luminosity in the gamma-ray regime (see Dubus, [2013](#); Paredes and Bordas, [2019](#), for a review). These systems consist of an early-type star (O-, B-type) in orbit with a Compact Object ([CO](#)), since no second thermal emission component could be found in any of these systems. [HMGBs](#) are among the most extreme astronomical objects in the gamma-ray sky and have been observed at many different wavelengths, ranging from radio through X-rays up to [HE](#) and [VHE](#) gamma-rays, providing a wealth of observational data.

At the time of writing only 9 [HMGBs](#) could be firmly identified:

- 1FGL J1018.6-5856 (Fermi LAT Collaboration et al., [2012](#); H.E.S.S. Collaboration et al., [2015b](#)),
- 4FGL J1405-6119 (Corbet et al., [2019](#)),
- HESS J0632+057 (Aharonian et al., [2007](#)),
- HESS J1832-093 (H.E.S.S. Collaboration et al., [2015a](#); Martí-Devesa and Reimer, [2020](#)),
- LMC P3 (Corbet et al., [2016](#); H.E.S.S. Collaboration et al., [2018a](#)),
- LS 5039 (Paredes et al., [2000](#); Aharonian et al., [2005a](#), [2006a](#)),
- LS I +61 303 (Kniffen et al., [1997](#); Albert et al., [2006](#)),

Figure 3.1: Multiband lightcurves of LS 5039 obtained from different instruments. From top to bottom: X-rays from *Suzaku* (purple triangles, Takahashi et al., 2009) and *INTEGRAL* (red stars, Chang et al., 2016) in units of counts s^{-1} ; *LE* gamma-rays from *COMPTEL* (blue dots, Collmar and Zhang, 2014) in units of $10^{-5} \text{ ph cm}^{-2} \text{ s}^{-1}$; *HE* gamma-rays from *Fermi-LAT* (green crosses, Chang et al., 2016) in units of $10^{-6} \text{ ph cm}^{-2} \text{ s}^{-1}$; and *VHE* gamma-rays from *H.E.S.S.* (purple downwards triangles, Aharonian et al., 2006a) in units of $10^{-12} \text{ TeV}^{-1} \text{ cm}^{-2} \text{ s}^{-1}$. Image Credits: Chang et al. (2016) reproduced with permission from OUP.

- PSR B1259-63 (Aharonian et al., 2005b),
- PSR J2032+4127 (Abeysekara et al., 2018).

In the Milky-Way, the total number of *HMGBs* is expected to be around 101^{+89}_{-52} (Dubus et al., 2017) and they are commonly understood to correspond to a preced-

Figure 3.2: The multiband SEDs of LS 5039 at inferior (red) and superior conjunction (blue). Image Credits: Chang et al. (2016) reproduced with permission from OUP.

ing stage in the evolution of High-Mass X-Ray Binaries (HMXBs). This estimation, however, might be too pessimistic because it is mainly based on systematic studies of Fermi-LAT and H.E.S.S. data that are most sensitive to bright systems and could hence miss a potential, additional population of GeV faint HMGBs (Martí-Devesa and Reimer, 2020).

Phenomenologically, HMGBs share two key aspects: the temporal correlation (or anti-correlation) of the orbital modulation in certain bands, and the spectral shape of the non-thermal emission components (see also Dubus, 2013).

Regarding the former, in Figure 3.1 we can see typically observed multiband lightcurves, in this case of LS 5039, which show a pronounced correlation of the X-ray to LE gamma-ray band with VHE gamma-rays. The HE gamma-ray emission, in contrast, is anti-correlated, peaking when the fluxes in the other bands are lowest. The flux extrema do not coincide with orbital extrema, that are periastron and apastron, but rather with inferior and superior conjunction when the CO passes in front or behind its stellar companion as seen from Earth. This hints at strongly anisotropic, line-of-sight dependent effects to be the dominant cause for the orbital modulation, rather than the changing intra-binary distance.

Regarding the latter, the gamma-ray emission from HMGBs exhibits two distinct spectral components as seen for example in Figure 3.2. The first component is found in the HE band with an exponential cutoff at a few GeV, whereas a second component arises in the VHE band. Due to the GeV spectral cutoff, the two components are disconnected and therefore hard to reconcile with a common origin,

hinting for example at different radiative processes and/or different emitting particle populations. Additionally, for many systems, the luminosity is approximately one order of magnitude higher in the [HE](#) than in the [VHE](#) band (Dubus, 2013), with the exceptions being HESS J0632+057 (Li et al., 2017) and HESS J1832-093 (Martí-Devesa and Reimer, 2020), where the [HE](#) band is one order of magnitude lower.

3.1 EMISSION SCENARIOS

Explaining the observed temporal variability of [HMGBs](#) together with their distinct spectral characteristic has ever since their detection been a challenging task. Their discovery sparked a still ongoing discussion on the origin of their non-thermal emission (see e.g. Mirabel, 2006; Romero et al., 2007, and references therein), discriminating two principle scenarios depending on the nature of the [CO](#): A jet-related emission scenario, where the [CO](#) accretes matter from its stellar companion and releases the accretion energy in the form of relativistic jets with high-energy particles (see e.g. Bosch-Ramon and Khangulyan, 2009); or a wind-driven scenario, commonly assuming the [CO](#) to be a pulsar, whose rotational energy is dissipated as a relativistic pair plasma that interacts with the dense stellar wind (see Maraschi and Treves, 1981; Dubus, 2006). This interaction leads to the formation of an extended Wind-Collision Region ([WCR](#)) terminating both the supersonic pulsar and stellar winds by shocks (see e.g. Bogovalov et al., 2008; Bosch-Ramon et al., 2012). At these sites, electrons and positrons from the pulsar wind can be accelerated to ultra-relativistic energies via [DSA](#) and other processes (see e.g. also Bosch-Ramon and Rieger, 2012; Sironi and Spitkovsky, 2011) and subsequently produce the observed non-thermal radiation.

Unfortunately, discerning between the two scenarios by attempting to determine the nature of the [CO](#) directly from observations remains inconclusive for most systems. For example, the detection of jets or a very high mass of the [CO](#) would be a strong indication for the presence of a black hole and hence the realisation of a microquasar scenario. So far, however, no jets could be detected for any of these systems. Although there are indications for high [CO](#) masses from optical measurements of the binary's orbital solution (see e.g. Sarty et al., 2011), they do not allow to rule out neutron stars. The detection of pulsations, on the other hand, would firmly establish a pulsar as [CO](#) and imply a wind-driven interpretation. Until now, this was only possible in the cases of PSR B1259-63 and PSR J2032+4127, which both have a relatively large orbit with periods on the order of several years. In compact-orbit [HMGBs](#), potential radio pulsations might be absorbed in the dense

stellar-wind plasma and hence only hardly be detectable at Earth (e.g. Chen et al., 2021). Tentatively, X-ray pulsations have also been found for LS 5039 (Yoneda et al., 2020), which, however, were recently disputed (Volkov et al., 2021).

A discrimination between the scenarios and an advance in our understanding of HMGBs thus relies on indirect evidence provided by comprehensive modelling efforts that try to recover other, observable aspects such as orbital modulations and spectral characteristics.

3.2 WIND-DRIVEN MODELS

Although both of the scenarios can explain at least some of the observational aspects reasonably well, a wind-driven interpretation is commonly favoured for most HMGB systems since the observed, modulated emission remained very stable over a vast number of orbits. Also, observations in entirely different bands, such as radio and X-ray, point towards scenarios harbouring a pulsar (see e.g. Moldón et al., 2012; Torres et al., 2012; Volkov et al., 2021).

Wind-driven models also possess fewer degrees of freedom as compared to models containing jets. They are therefore also favoured by Occam’s razor and offer a bigger constraining potential. Correspondingly, the work presented in this dissertation is strongly focused on furthering wind-driven models, especially with an application to LS 5039 in mind. In the following section, I will therefore present the wind-driven scenario in more detail using LS 5039 as an example - summarising the basic physical principles behind the related models.

3.2.1 Physical Principles

Wind interaction

As mentioned before, the interaction between the stellar and the pulsar wind gives rise to an extended WCR that is delimited by strong shocks (see e.g. Bogovalov et al., 2008; Bosch-Ramon et al., 2012) as depicted schematically in Figure 3.3. These shocks constitute the key locations within the systems, where the power of the winds, essentially driven by the pulsar’s spindown, can be converted to non-thermal emission by accelerating highly energetic, non-thermal particles.

The most pronounced shock is the bow shock, which is the part of the pulsar-wind termination shock situated between the star and pulsar, where both winds

Figure 3.3: Sketch of the Wind-Collision Region (WCR) at periastron for a close-orbit system similar to LS 5039. The region of the Contact Discontinuity (CD), where significant turbulence, and therefore wind mixing, is expected to take place is indicated with a wavy line. The red regions indicate the presumed emitter locations for non-thermal radiation. Image Credits: Zabalza et al. (2013) (cropped) reproduced with permission from © ESO.

collide approximately head-on. The location of the head of the bow shock can be approximated by the wind standoff point, where the ram pressure of both winds are in equilibrium (see e.g. Zabalza et al., 2013). It is located at a distance of $x_{\text{so}} = d / (1 + \sqrt{\eta})$ from the stellar companion, where d is the orbital separation and η the pulsar-to-stellar wind momentum flux ratio. Since the stellar wind usually has a higher momentum flux than the pulsar wind ($\eta < 1$), the wind standoff is located closer to the pulsar producing a cone-like WCR structure that engulfs the pulsar as shown in Figure 3.3.

On scales larger than the orbital separation, the WCR structure significantly deviates from the stationary scenario neglecting orbital motion. Due to the orbital motion, the WCR is bent sideways, facing in the opposite direction to the rotation (Bosch-Ramon and Barkov, 2011, see e.g.). The additional pressure provided by the Coriolis force leads to a second termination of the pulsar wind behind the pulsar, as seen from the star, and thereby to the formation of a so-called Coriolis shock (Bosch-Ramon et al., 2012, see e.g.) as shown in Figure 3.3.

The large velocity shear and density gradient between the shocked stellar and pulsar winds at the Contact Discontinuity (CD) triggers the development of instabilities and turbulent mixing, which significantly affect the shape of the WCR (see e.g. Lamberts et al., 2013; Bosch-Ramon et al., 2015). On even larger scales, the flow continuously loses coherence and eventually becomes an expanding, disrupted structure that interacts with the interstellar medium (see e.g. Bosch-Ramon and Barkov, 2011; Barkov and Bosch-Ramon, 2021).

Figure 3.4: Schematic representation of different geometry-dependent emission processes in **HMGBs**. Image Credits: Dubus et al. (2010) reproduced with permission from © ESO.

Interplay between production and absorption

The majority of the models that try to explain the multiband, non-thermal radiation from LS 5039 are purely leptonic, considering the accelerated electrons and positrons from the pulsar wind to be the dominant emitters thereof. Anisotropic Inverse-Compton (IC) emission (see also [Section 2.1.2](#)) was established as the dominant radiative process for HE and VHE gamma-rays (see e.g. Zabalza et al., 2013; Dubus et al., 2015). In this picture, the massive, stellar binary companion provides a dense seed photon field for the IC process as depicted in [Figure 3.4a](#). Ultra-relativistic electrons and positrons, that are accelerated in the vicinity of the pulsar, scatter these photons to higher energies producing the observed HE and VHE gamma-rays (see e.g. Dubus et al., 2008). The scattering process is most efficient at superior conjunction, i.e. when the stellar photons are back-scattered in the direction of the observer (see [Section 2.1.2](#)).

The γ radiation generated at this orbital phase, however, has to propagate through the binary system before it can escape (see also [Figure 3.4b](#)). Since the photons

Figure 3.5: The absorption maps around two **HMGBs**, that are LS5039 (left) and PSR B1259-63 (right), for a 1 TeV gamma-ray photon. The observer is positioned at the bottom of the figure. The orbit of the compact object is given by a solid white line with the companion star to scale. The colour scale corresponds to the attenuation factor $\exp(-\tau_{\gamma\gamma})$, where $\tau_{\gamma\gamma}$ is the optical depth. Image Credits: du Plooy and van Soelen (2021) (reprinting only two selected systems) released under **CC BY-NC-ND 4.0**.

produced in the **VHE** regime are above the threshold for pair-production with the Ultraviolet (**UV**) stellar radiation field, their flux is strongly attenuated by the $\gamma\gamma$ pair-production process (see e.g. Dubus, 2006; du Plooy and van Soelen, 2021) as shown in Figure 3.5. The $\gamma\gamma$ -absorption is at its maximum at superior conjunction and reaches its minimum at inferior conjunction. This interplay between the generation of **IC** emission and its absorption by pair-creation with the same seed photon field is commonly used to explain the observed anti-correlation between **HE** and **VHE** gamma-rays (e.g. Zabalza et al., 2013).

In the case of LS 5039, the $\gamma\gamma$ -opacity is so high that effectively no **VHE** gamma-ray photon, produced close to the pulsar, can escape the system at superior conjunction (see e.g. also Böttcher and Dermer, 2005). While the source becomes fainter at this orbital phase, it is still detectable at **VHE** (see Figure 3.1). This indicates that the region emitting the **VHE** gamma-rays is rather extended and located farther away from the star, because an alternative explanation via an electromagnetic cascade initiated by the $\gamma\gamma$ -pair-production turned out to be incompatible with observations (see e.g. Bosch-Ramon et al., 2008; Cerutti et al., 2010). Studies using an analytical model for the structure of the **WCR**, therefore, applied models involving multiple emission zones and established the Coriolis shock as a viable source for **VHE** gamma-rays (see, e.g., Zabalza et al., 2013; Molina and Bosch-Ramon, 2020).

The spectral cutoff

A caveat in this description, however, relates to the spectral cutoff observed at a few GeV. In the modelling presented by Zabalza et al. (2013), the Coriolis shock is thought to accelerate a second particle population that is mainly responsible for the VHE emission, whereas the electrons at the wind-standoff produce the HE emission. Consequently, in their model, they found the accelerator at the latter location to be significantly less efficient than the one at the Coriolis shock. This is somewhat counterintuitive since one would expect a more efficient particle acceleration to occur at the wind-standoff, where the winds collide head-on.

This also poses further implications for the lower energetic part of the non-thermal emission in the X-ray and LE gamma-ray band, which is commonly interpreted as synchrotron emission from the same accelerated electrons (see also Section 2.1.1). A less efficient accelerator at the bow shock prevents the electrons from reaching high enough energies there to significantly contribute to the X-ray emission despite the increased magnetic field due to the proximity of the pulsar (Zabalza et al., 2013). This hence suggests that the electron population responsible for most of the X-ray emission is produced at the Coriolis shock, which is in line with the arguments by Takahashi et al. (2009), who proposed a common origin for the X-ray and VHE emission due to their correlated orbital modulation. However, the magnetic field strengths required to reach the observed X-ray fluxes at the Coriolis shock would introduce a softening in the VHE spectrum above 100 GeV that is hard to reconcile with observations (Zabalza et al., 2013; Molina and Bosch-Ramon, 2020).

There is, therefore, some tension in the opposing magnetic field requirements. It was argued that this disagreement could potentially be resolved by considering that the synchrotron emission is produced further downstream, where particles encounter a magnetic field that is amplified by the turbulent fluid motion (Zabalza et al., 2013). In this picture, however, the processes responsible for the observed X-ray modulation remain mostly unknown since the photons in this band are not modulated by $\gamma\gamma$ -absorption like VHE gamma-rays.

Relativistic boosting

In contrast, a quite natural explanation for the X-ray modulation can be found by relativistic Doppler-boosting, assuming that the emission indeed produced by synchrotron radiation. This effect is mainly present in the wings of the WCR, where the flow retains moderately relativistic speeds even after being shocked (Bogovalov et al., 2008; Dubus et al., 2010). The modulation introduced by relativistic boosting is therefore line-of-sight dependent. The boosted fluxes are increased towards

inferior conjunction, when the relativistic cometary downstream flow points towards the observer (shown schematically in [Figure 3.4b](#)), and reach their minimum around superior conjunction. The resulting modulation is effectively similar to the one introduced by $\gamma\gamma$ -absorption. Assuming a synchrotron emissivity that remains constant over the orbit, the modulation from Doppler-boosting alone can explain the observed X-ray lightcurve reasonably well ([Dubus et al., 2010](#)). Since relativistic boosting does not distinguish between different photon energies, this process will also have an impact on other bands and can therefore not be neglected in comprehensive modelling approaches.

Assuming that the X-ray emission is produced by relativistically boosted synchrotron emission, however, implies that the responsible electron population has to be accelerated at the bow shock since the turbulent fluid motion in the downstream region behind the Coriolis shock prevents coherent boosting. Consequently, this suggests that the accelerator at the bow shock has to be quite efficient to reach the required electron energies. On the other hand, this assessment somewhat contradicts the one made earlier, where a lower acceleration efficiency is required to produce the GeV emission component via [IC](#) scattering.

This tension can be resolved by considering a second particle distribution to emerge at the shocks that consist of electrons from the pulsar wind that are isotropised at the shock ([Dubus et al., 2015](#)). This additional population follows a narrow Maxwellian distribution and can naturally account for the cutoff at GeV energies. While this interpretation explains the observed [HE](#) modulations and spectral shape reasonably well, it yields a cutoff that is modulated over the orbit because of the anisotropic [IC](#) scattering, whereas no such modulation is detected.

Further emission contributions

It is important to note that also other processes may yield a further contribution in the [HE](#) gamma-ray and other bands. This could e.g. include the magnetospheric emission by the pulsar itself, which would naturally yield a GeV emission with an unmodulated cutoff ([Takata et al., 2014](#)), and/or emission from the cold pulsar wind, which heavily depends on its widely unknown composition and properties ([Bosch-Ramon, 2021](#)).

In contrast to LS 5039, many other [HMGB](#) systems harbour Be-type stars with stellar disks. Their interaction with the pulsar wind can lead to transient phenomena upon crossing the decretion disk, such as the GeV flares in PSR B1259-63 (see e.g. [Chernyakova et al., 2020](#), and references therein) which interestingly appears to be increasingly delayed for the recent passage ([Johnson et al., 2021](#)), or superorbital

modulations as in the case of LS I +61 303 (see e.g. Xing et al., 2017, and references therein).

Further open questions relate to the nature of the LE gamma-ray emission observed by Comptel (Collmar and Zhang, 2014), whose fluxes have been problematic for past modelling efforts (Dubus et al., 2015; Molina and Bosch-Ramon, 2020). Together with the recently observed spectral hardening at hard X-ray energies (Falanga et al., 2021), this points in the direction that the LE emission may not just be an extension of the synchrotron process, that produces the lower energetic X-ray emission, but possibly an individual component, whose origin has yet to be determined.

3.2.2 *Current numerical modelling approaches*

As it was argued in the previous sections, precise knowledge on the wind interaction, especially concerning the emerging shock structure, is a crucial ingredient for wind-driven emission models in general. Most of the models, however, rely on semi-analytic estimations for the WCR shape (e.g. Zabalza et al., 2013; Takata et al., 2014; Molina and Bosch-Ramon, 2020) and therefore implicitly neglect most of the morphology and dynamics of the arising structures. To go beyond the usage of such estimations, the wind interaction in HMGBs has been investigated numerically by different groups in the past (see e.g. Bogovalov et al., 2008, 2012; Lamberts et al., 2013; Bosch-Ramon et al., 2012, 2015) using dedicated simulations with various degrees of complexity.

The provided multi-dimensional solutions for the developing WCR enabled in turn the building of more complex and comprehensive emission models. For example, fluid solutions can be used to estimate the fluxes of non-thermal radiation directly from the data (Bosch-Ramon et al., 2017; Barkov and Bosch-Ramon, 2018, e.g.), or as a steady-state background for particle transport models (e.g. Dubus et al., 2015). Such approaches successfully incorporate the morphology of the WCR in much greater detail than the ones relying on analytic parametrisations, which enables a more self-consistent treatment of processes such as relativistic boosting. However, since the emitters are commonly inferred in a post-processing step, they commonly neglect the impact of wind-interaction dynamics in the transport of the particles and their potential influence on the radiative output of the systems.

3.3 A NOVEL NUMERICAL MODEL

In this dissertation, I aim to build a more comprehensive, numerical model for wind-driven [HMGBs](#) that especially focuses on the transport of accelerated pairs within the system, taking the dynamical structure of the [WCR](#) into account. The corresponding objectives of this dissertation, therefore, are to:

1. Develop and implement a numerical model for the wind-interaction in [HMGBs](#) including dynamical fluid instabilities and the effects of orbital motion
2. Determine the relevant sites for particle acceleration in this system
3. Follow the evolution of accelerated electrons within the dynamical structure of the [WCR](#) and assess the importance of different transport processes
4. Determine where the non-thermal emission is produced and how different processes affect the signal observed at Earth (depending on the orbital phase and the dynamically changing transport of the particles).

To achieve this, I took an approach similar to the one taken for Colliding-Wind Binaries ([CWBs](#)), which were successfully modelled at our institute before (see e.g. [Reitberger et al., 2017](#)).

3.3.1 *Colliding wind binaries*

[CWBs](#) are very similar to [HMGBs](#) in terms of wind-interaction but, in contrast, harbour a second early-type star instead of the [CO](#). They can hence be viewed as non-relativistic counterparts of wind-driven [HMGBs](#). In the related numerical model, a Fokker-Planck-type transport equation for the shock-accelerated protons and electrons is solved simultaneously to the equations of magneto-hydrodynamics ([Reitberger et al., 2014a,b](#)) – therefore taking the full dynamics of the wind interaction into account in the particle-transport process.

For the numerical treatment of the equations, the [CRONOS](#) code was used, which is developed and maintained by our research group for computational astroparticle physics¹ at the University of Innsbruck ([Kissmann et al., 2018](#)). The [CRONOS](#) code is specifically designed to solve hyperbolic, partial-differential equations with a focus on fluid dynamics and applications from astrophysics and space physics in mind. [CRONOS](#) was successfully applied in a variety of different contexts by us and

¹ https://www.uibk.ac.at/astro/research_groups/ralf-kissmann

Figure 3.6: Schematic representation of a finite-volume, Godunov scheme. Left: A finite-volume discretisation of a two-dimensional, rectangular computational domain. The changes of the cell-averaged fluid variables are determined by the fluxes through the cell interfaces to neighbouring cells. Right bottom: Employing a spatially constant subgrid reconstruction for the fluid variables leads to jumps at the cell interfaces. Right top: These jumps can be construed as local Riemann problems that can be solved to obtain an approximation for the cell-interface fluxes.

our collaborators (e.g. Kopp et al., 2017; Wiengarten et al., 2016; Kissmann et al., 2016).

3.3.2 Extension to gamma-ray binaries

An extension of the approach pioneered for [CWBs](#) to [HMGBs](#) will enable simulations of the emitting particle distributions that are consistent with the full dynamics of the wind-interaction; something that has not yet been attempted in the case of [HMGBs](#). In a post-processing step, the obtained particle solutions will allow predictions of the system's non-thermal radiative output that are fully three-dimensional and thus naturally incorporate the anisotropic, position-dependent effects of [IC](#) scattering and $\gamma\gamma$ -absorption. The joint treatment of the simulations further also allows effects such as relativistic boosting to be included consistently, as they can be computed directly from the fluid solution.

To realise such an extension, the previously developed framework for [CWBs](#) needs to be translated to a fully relativistic setting. This is required by the pulsar wind that is launched at speeds very close to the speed of light, which renders a Newtonian treatment inadequate (see e.g. Bosch-Ramon et al., 2012). In the following sections, I will give a brief overview of the main steps that I took for the development of the framework, composing one of the main parts of this dissertation work.

Relativistic hydrodynamics

The first step of the extension consists in extending CRONOS to solve the equations governing Special-Relativistic Hydrodynamics (SRHD) – an effort that was started during my master thesis and finished in my early years as PhD student leading up to [Article I](#) (see [Chapter 4](#)). Within CRONOS, we treat the respective set of equations using a finite-volume, Godunov scheme on orthogonal grids (shown schematically in [Figure 3.6](#)). The scheme is based on approximate relativistic Riemann solvers and a second-order, slope-limited reconstruction of the fluid variables in space. The temporal integration is handled by an explicit, second-order Runge-Kutta integrator (see also Kissmann et al., 2018, for more details).

For the implementation in CRONOS, we widely rely on numerical schemes commonly found in the literature – although several components from different approaches had to be combined to obtain a robust framework suitable for the present use-case. Finally, the code was validated on an extensive set of test problems that can either be solved (semi-)analytically or suitably compared to literature solutions.

We plan for a possible extension of the SRHD code to Special-Relativistic Magneto-Hydrodynamics (SRMHD) in the future. The relevant interfaces have already been foreseen while implementing the current version of the code. With this, we will be able to additionally investigate the influence of the pulsar and stellar magnetic fields on the fluid flow (see also Dubus et al., 2015; Bogovalov et al., 2019).

Particle transport

The second step in the extension concerns revisiting the particle transport model – mainly relating to the work in [Article II](#) (see [Chapter 5](#)). In the case of HMGBs, we consider electron-positron pairs to be accelerated at the dynamically changing shock structure in the system. We identify these sites and inject particles into the simulations according to the local fluid conditions and the given acceleration model, which can be specified by the user. The accelerated electrons will then evolve through various transport processes following the relativistic transport equation presented by Webb (1989). Similar to other works in the field (Dubus et al., 2015; Vaidya et al., 2018; Molina and Bosch-Ramon, 2020), we neglect diffusion in space and momentum and viscous shear-acceleration in this first stage. The spatial transport of the particles is hence exclusively given by passive advection with the fluid flow, which can be readily treated by the hydrodynamics solvers in CRONOS.

Figure 3.7: Schematic representation of the semi-Lagrangian solver used to treat the energy part of the particle transport in CRONOS. The spectrum is subdivided into energy bins. Characteristic curves are evolved backwards in time to determine the energy range from which the particles of a given cell originated. The bin content at the next time step is obtained by integrating a given subgrid reconstruction over its corresponding range at the current timestep.

For the energetic transport, we consider the particle spectrum to be shaped by a set of energy-changing processes whose rate may depend on energy, location, and local properties of the fluid. To increase the modularity of the code, a generic interface for such processes has been implemented that allows the user to easily adapt and introduce new processes in the future. For the current application to [HMGBs](#), we consider adiabatic energy changes and radiative cooling through synchrotron and [IC](#) emission. The energy part of the transport equation is solved numerically using a conservative, semi-Lagrangian scheme (shown schematically in [Figure 3.7](#)) as detailed in [Article II](#) (see [Chapter 5](#)). In this process, the particle spectra in each spatial cell are treated individually and independently of each other. To advance the simulation in time, both the hydrodynamic and the semi-Lagrangian solvers are applied in an alternating fashion according to a Strang-splitting scheme.

The extended structure of the code is visualised schematically in [Figure 3.8](#). As for every CRONOS application, the heart of the simulation setup consists of implementing a specialisation of the Problem class. This interface class has been extended to accommodate the initialisation of the newly implemented particle transport framework. This includes specifying the simulated particles, the energy loss processes, the injection model, etc., which allows a flexible adaptation to other problems apart from [HMGBs](#) in the future.

Emission computation

The third and final step in the work consists of adapting and unifying the computation of the resulting non-thermal emission. This is done in a post-processing step using the simulated particle distributions and fluid solutions. The emission is calculated individually for every cell of the simulation, thus naturally incorporating the full extent of the three-dimensional [WCR](#) structure.

Figure 3.8: Schematic structure of the CRONOS code. An implementation of the Problem class is responsible to initialise the fluid variables and set up the particle transport framework, specifying the particle species (acting as an interface to the scalar tracer fields in which the particle distributions are stored) and energy-change processes. The fluid variables and particle spectra are updated at every time step by the hydrodynamics solver and the energy solver. Ultimately, the simulation results are stored as HDF5 files.

Previously in the case of [CWBs](#), this was done by a separate program independently from the CRONOS code. However, since many code components such as the ones involving the data handling, the magnetic field, the seed radiation field for [IC](#) scattering, and many more can be efficiently reused in the emission computation, I decided to treat also this part as an extension to the CRONOS framework. Next to effective reuse of the existing code base, which is preferable from a maintainability perspective, this approach also allows user specifications made for a given problem to be reloaded and thus naturally avoids inconsistencies in the solution of the particle transport and the subsequent computation of the corresponding emission.

A basic overview of the code structure is given in [Figure 3.9](#). Again, the code offers a flexible structure, such that more radiative processes can be added easily in the future. In this context, the emissivities of radiative processes are specified in the fluid frame. After their evaluation for a given observer direction, the resulting fluxes are automatically related to the observer’s frame by a Lorentz transformation depending on the local fluid velocity. Relativistic boosting is hence automatically included and accounted for and can easily be reused for radiative processes to be added in the future.

Before the emission is reduced to a single spectrum or a given projection, the effects of processes that further modify the radiation on its way to the observer, are applied. A representative of such is $\gamma\gamma$ -absorption, which attenuates [VHE](#) gamma-ray fluxes depending on the line-of-sight integral of its differential opacity through

Figure 3.9: Schematic structure of the code handling the computation of the radiative output from pre-computed particle distributions and fluid solutions, loaded from previous output files. To ensure consistency, wide parts of the CRONOS code are reused, including the setup of the particle transport. Next to the specification of radiative loss processes, also post-processes, such as absorption, and different observers, i.e. projection and reduction methods, can be supplied. The computed emission is again stored as an HDF5 file.

the stellar radiation field. Although $\gamma\gamma$ -absorption is currently the only use-case of such a process, the framework offers the possibility for future extensions, e.g. free-free absorption.

The parallelisation of the emission computation is implemented in analogy to the rest of CRONOS by a rectangular domain-splitting approach. Each rank loads a spatial part of the whole domain and handles the corresponding emission locally. At the end of the computation, the results are either broadcasted over the network using MPI for further processing or written in parallel to an HDF5 output file. This type of parallelisation might not be ideal for such an application because the workloads posed for the individual domain blocks might not be constant, e.g. if a given block contains no particles in the worst case. This can result in a sub-optimal distribution of the required work and thus in a significantly reduced parallel efficiency. In the future, this issue can be addressed, for example, by switching to a task-based parallelisation instead.

3.3.3 *Future Prospects*

In this work, I have developed and implemented a novel numerical model for the non-thermal emission from [HMGBs](#), whose capabilities have been demonstrated on the LS 5039 system. The related simulations provide deeper insights into the complex dynamics of such sources and yield emission predictions that are in good agreement with gamma-ray observations as discussed in [Article III](#) (see [Chapter 6](#)).

In the future, applications to many other systems are foreseen. These studies can, for example, include systems such as LMC P3, which has similar orbital and stellar parameters as LS 5039 but has not been modelled extensively yet, or PSR B1259-63 and LS I +61 303 to study the interaction of the pulsar wind with stellar disks with respect to GeV flares and superorbital modulations, respectively. Since the latter two have orbital periods on the order of years, a different simulation strategy might be required since the whole orbit might no longer be feasibly simulated in one run.

Already for the current application to LS 5039 performed in [Article III](#) (see [Chapter 6](#)), the computational resources available at the University of Innsbruck are barely enough to fulfil the requirements on the resolution and the extent of the computational domain. This has caused, for example, the Coriolis shock not to be formed consistently inside the simulation volume for orbital phases around inferior conjunction. To overcome this issue, we were able to obtain more computational resources in the context of a PRACE application proposal scaling the simulation accordingly and simulating two full orbits to investigate orbit-to-orbit variations in the radiative output of the system. At the time of writing, the production simulations are already running and upcoming, future work will be concerned with analysing the produced data.

A natural improvement of the developed model could consist in a further extension of CRONOS to incorporate [SRMHD](#). As it was suggested by various works including this one, the magnetisation of the pulsar wind is significant and should no longer be neglected in the dynamics of the wind interaction (Dubus et al., 2015; Bogovalov et al., 2019). Such an extension can be integrated seamlessly into the existing framework, as the respective interfaces have already been foreseen. Next to an obvious influence on the structure of the [WCR](#), the more realistic and self-consistent picture of the magnetic field will also affect the particle transport and the production of synchrotron radiation, which raised issues in the presented application to LS 5039. It remains to be seen in future works whether [SRMHD](#) is able to resolve the encounter issues.

Another possible path for future work could, for example, relate to the employed acceleration model. So far, we take a purely phenomenological approach and consider every shock to have the same acceleration efficiency producing power-law particle-spectra with a constant spectral index, treated as free parameters of the simulation. This might be different in reality, where the produced spectrum depends on properties of the shock such as its compression ratio or magnetic obliquity (see e.g. Keshet and Waxman, 2005; Takamoto and Kirk, 2015), which might again require a more accurate picture of the magnetic fields at the shocks. As it is not yet clear which processes are responsible for the particle acceleration in HMGBs, the presented work provides a framework to explore different more sophisticated acceleration models in the future and thus provide further insight into the processes at play.

The produced simulation data can also be used to further investigate emission processes that have been neglected in the presented work, so far. This could, for example, relate to the emission from the cold pulsar wind using the detailed, orbital-phase-dependent morphology of the unshocked pulsar wind region from the obtained solutions (see also Bosch-Ramon, 2021). Also inferring the fluxes of thermal X-rays from the shocked stellar wind is thinkable, which can be used, together with the non-detection of thermal emission features, to potentially provide improved constraints for the pulsar's spin-down luminosity (similar to Zabalza et al., 2011).

Since the developed framework is very generic and the implemented processes are ubiquitously found in astrophysical contexts, the code is also applicable to a wider range of dynamical phenomena that go beyond the current application to HMGBs and CWBs. This could, for example, involve entirely different physical environments, such as supernovae or gamma-ray bursts. The code might, therefore, be made available to a broader number of researchers in the future, once it has been sufficiently documented and refactored to ensure future usability and maintainability.

Part II

PUBLICATIONS

ARTICLE I

SPECIAL RELATIVISTIC HYDRODYNAMICS WITH CRONOS

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Special relativistic hydrodynamics with CRONOS

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ABSTRACT

We describe the special relativistic extension of the CRONOS code, which has been used for studies of gamma-ray binaries in recent years. The code was designed to be easily adaptable, allowing the user to easily change existing functionalities or introduce new modules tailored to the problem at hand. Numerically, the equations are treated using a finite-volume Godunov scheme on rectangular grids, which currently support Cartesian, spherical, and cylindrical coordinates. The employed reconstruction technique, the approximate Riemann solver, and the equation of state can be chosen dynamically by the user. Further, the code was designed with stability and robustness in mind, detecting and mitigating possible failures early on. We demonstrate the code’s capabilities on an extensive set of validation problems.

Key words. Hydrodynamics – Relativistic processes – Methods: numerical

1. Introduction

Relativistic hydrodynamics is one of the most successful tools to describe complex dynamical phenomena ranging from cosmological scales to those of colliding particles. General relativity is thereby a necessary ingredient to understand systems with strong gravitational fields, such as accretion discs and the launch of jets in active galactic nuclei (e.g. Mościbrodzka et al. 2014, 2016; Komissarov & Porth 2021) or the mergers of compact objects producing gravitational waves (e.g. Siegel & Metzger 2018). Many other phenomena, however, do not involve strongly bent spacetime but still flow velocities near the speed of light, for example gamma-ray bursts (e.g. Willingale & Mészáros 2017; Zhang 2018), systems with pulsar winds (e.g. Barkov et al. 2019), such as gamma-ray binaries (Huber et al. 2021a,b) and pulsar wind nebulae (e.g. Olmi & Bucciantini 2019), or interacting heavy-ion beams in collider experiments (e.g. Busza et al. 2018). Their dynamics can therefore be more suitably described in special relativistic frameworks, which we focus on in this work.

Due to the high complexity of many problems in current research, analytical approaches are no longer feasible to explain observed data. Numerical approaches (see Martí & Müller 2003, 2015, for a review) are therefore essential to further our understanding of the related systems. For this, many modern codes have been presented that treat the equations of special relativistic hydrodynamics (SRHD) and/or magnetohydrodynamics (SRMHD), such as PLUTO (Mignone et al. 2007, 2012), RAMSES (Teyssier 2002; Lamberts et al. 2013), ATHENA++ (Stone et al. 2008; White et al. 2016), AMRVAC (Meliani et al. 2007), and others.

In this paper, we present the special relativistic extension of CRONOS (Kissmann et al. 2018), which was used in comprehensive models for the emission of gamma-ray binaries (see Huber et al. 2021a,b). CRONOS is a finite-volume, Godunov-type code that was developed to solve hyperbolic systems of partial differential equations with astrophysical applications in mind. A key feature of CRONOS consists in its easy adaptability and extensibility, providing a framework with several interfaces for customisations by the user that allows for the straightforward incorporation of additional physics, such as the transport of energetic particles (see e.g. Reitberger et al. 2017), radiative cooling of the plasma (see e.g. Scherer et al. 2020), or the use of more general reference frames (see e.g. Huber et al. 2021a). Here we describe the extension of CRONOS to SRHD, where we did not introduce any new algorithms, but selected and combined different techniques that have been proven successful in literature.

The paper is structured as follows: in Sect. 2 we introduce the governing equations; the notations and general structure of the code are defined in Sect. 3; in Sect. 4 we describe the numerical scheme implemented in CRONOS; and we validate it on an extensive set of numerical tests in Sect. 5. Finally, we comment on the parallel performance of the code in Sect. 6 and give a summary in Sect. 7.

2. System of equations

The CRONOS code (Kissmann et al. 2018) was in general developed to solve a set of hyperbolic conservation laws of the form

$$\partial_t U + \nabla \cdot \mathbf{F}(U) = S, \quad (1)$$

where U denotes a set of conserved quantities, $\mathbf{F}$ the respective fluxes, and S an additional source term.

2.1. Special relativistic hydrodynamics

In analogy to classical hydrodynamics, the dynamics of a relativistic fluid can be expressed as such a system (Landau & Lifshitz 1959). The respective equations for the conservation of rest-mass, energy, and momentum read as follows:

$$\partial_t D + \nabla \cdot (D\mathbf{v}) = S_D, \quad (2a)$$

$$\partial_t \tau + \nabla \cdot ((\tau + p)\mathbf{v}) = S_\tau, \quad (2b)$$

$$\partial_t \mathbf{m} + \nabla \cdot (\mathbf{m} \otimes \mathbf{v} + p \mathbb{1}) = S_m, \quad (2c)$$

where $U = (D, \tau, m^j)$ correspond to the conserved variables, that is the mass, energy, and momentum density in the j -th coordinate direction, respectively, and $S = (S_D, S_\tau, S_m^j)$ correspond to their respective source terms. The fluxes further involve the fluid's three-velocity $\mathbf{v}$ and pressure p . All quantities are given in the laboratory frame and in natural units, that is with the speed of light $c = 1$.

It should be noted that the momentum fluxes in Eq. (2c) are given by the rank-2 stress tensor. Additional geometrical source terms might therefore arise implicitly when evaluating the divergence in non-Cartesian coordinates (see Sect. 3.1).

Other codes treat the conservation of energy by solving an equivalent equation for $E = \tau + D$ (see e.g. Mignone et al. 2007; Lamberts et al. 2013). In the low pressure, non-relativistic regime, the variables D and E , however, can take very similar values, which can lead to severe truncation errors. This can be avoided by evolving the variable $\tau = E - D$, instead, which we therefore also used in CRONOS. This choice was solely motivated by numerical reasons and therefore has been used in many codes (see e.g. Banyuls et al. 1997; Aloy et al. 1999; Baiotti et al. 2005; Meliani et al. 2007; Rezzolla 2013).

The conserved variables and the corresponding fluxes are further expressed in terms of the primitive fluid variables $w = (\rho, p, u^i)$, which are the fluid's mass density ρ , pressure p , and the spatial part of the four-velocity vector u^i , respectively. The relations read as follows:

$$U(w) = (D, \tau, m^j) \\ = (\rho u^0, \rho u^0 (h u^0 - 1) - p, \rho h u^0 u^j), \quad (3)$$

where the fluid's bulk Lorentz factor is denoted by u^0 and its specific enthalpy by h .

In contrast to other implementations that employ the three-velocity vector (e.g. Mignone et al. 2007; Lamberts et al. 2013) as a primitive quantity, we used the four-velocity vector instead and inferred the former via $\mathbf{v} = \mathbf{u}/u^0$. This choice is more natural for numerical purposes since $|\mathbf{u}|$ is not bound by the speed of light – a constraint that one would have to guarantee for $|\mathbf{v}|$ at all times. The computation of the Lorentz factor via $(u^0)^2 = 1 + |\mathbf{u}|^2$ is also more robust by naturally avoiding truncation errors as compared to $(u^0)^2 = (1 - |\mathbf{v}|^2)^{-1}$.

The presented system of five equations in six unknowns is closed by specifying an additional equation of state (EoS), which is usually provided in the form of $h = h(\Theta)$ with $\Theta = \frac{p}{\rho}$. In CRONOS we considered two EoSs: the ideal one, assuming a constant adiabatic index Γ and the Taub-Mathews (TM) EoS (Mathews 1971), which approaches $\Gamma \rightarrow \frac{4}{3}$ in the high-temperature

limit and $\Gamma \rightarrow \frac{5}{3}$ in the low-temperature limit. The specific enthalpies are given by

$$h(\Theta) = \begin{cases} 1 + \frac{\Gamma}{\Gamma-1} \Theta & \text{ideal EoS} \\ \frac{5}{2} \Theta + \sqrt{\frac{9}{4} \Theta^2 + 1} & \text{TM EoS,} \end{cases} \quad (4)$$

respectively. For our current purposes, these EoSs are sufficient, although it should be noted that many more are available in the literature (see e.g. Synge 1957; Rezzolla 2013). Due to the modular design of CRONOS, additional EoSs can be easily added in the future by supplying the relevant routines.

2.2. Passive tracer fields

CRONOS provides the option to solve user-defined conservation laws alongside the ones governing the fluid dynamics (see also Kissmann et al. 2018). A prominent use case for this is the treatment of tracers fields ψ , which are passively advected with the fluid flow. Their value remains constant along fluid lines, following the transport equation

$$(\partial_t + \mathbf{v} \cdot \nabla) \psi = 0. \quad (5)$$

A corresponding conservation equation for $\Psi = \psi D$ can be found by combining Eq. (2a) and Eq. (5), yielding

$$\partial_t \Psi + \nabla \cdot (\Psi \mathbf{v}) = 0. \quad (6)$$

This equation was treated in analogy to the mass-conservation equation Eq. (2a) by the fluid solvers.

3. Notation and general structure

3.1. Coordinate systems

In CRONOS, we employed orthogonal, curvilinear coordinate systems in three dimensions, which are expressed in the generic variables (x^1, x^2, x^3) and the corresponding spatial metric tensor $\gamma = \text{diag}(h_1^2, h_2^2, h_3^2)$ given by the scaling factors h_i . Specifically, we have implemented Cartesian, cylindrical, and spherical coordinates (see also Table A.1). For the latter two, the divergence of the rank-2 stress tensor in the momentum-conservation equation Eq. (2c) yields non-zero geometrical source terms G_m^j . The expression can be expanded component-wise in terms of the standard vector-divergence in the respective coordinate system, yielding

$$\partial_t m^j + \nabla \cdot (m^j \mathbf{v} + p \mathbf{e}_j) = S_m^j + G_m^j, \quad (7)$$

where $\mathbf{e}_j$ denotes the unit base vector along the j -th coordinate direction (see Appendix A).

3.2. Normalisation

For the numerical treatment of the equations, CRONOS uses normalised quantities internally in the form $X = X_0 \hat{X}$, where X is a physical quantity, X_0 a normalisation constant, and $\hat{X}$ the resulting unit-free, normalised quantity that is treated by the solvers (Kissmann et al. 2018). Our implementation foresees four base quantities that can be normalised independently, which correspond to the length, time, mass, and number density. The latter is not strictly necessary to have a complete system of units. However, it has been proven to be useful in practice since employing a normalisation derived from the length-scale can lead to unwieldy large values for the number density.

The normalisations can be chosen freely by the user, depending on the problem at hand by specifying the normalisation constants for four different quantities, which can also include derived quantities (e.g. energy density, velocity, etc.). If constants for derived quantities are supplied, the normalisations for the non-specified base quantities are obtained automatically via physical relations. If the specified quantities form an inconsistent system of units, the procedure is aborted and the user is notified. In contrast to classical hydrodynamics, velocities are always normalised to the speed of light in the relativistic case, as implicitly imposed by Eq. (2). The user is hence only allowed to specify the three remaining normalisations to complete the system.

Finally, the normalised equations, corresponding to Eq. (2), that are solved by CRONOS are

$$\partial_t \hat{D} + \hat{\nabla} \cdot (\hat{D} \hat{\mathbf{v}}) = \hat{S}_D \quad (8a)$$

$$\partial_t \hat{\tau} + \hat{\nabla} \cdot ((\hat{\tau} + \hat{p}) \hat{\mathbf{v}}) = \hat{S}_\tau \quad (8b)$$

$$\partial_t \hat{m}^j + \hat{\nabla} \cdot (\hat{m}^j \hat{\mathbf{v}} + \hat{p} \hat{\mathbf{e}}_j) = \hat{S}_{m^j} + \hat{G}_{m^j}. \quad (8c)$$

For the rest of this work, we exclusively use normalised quantities and omit the hat sign on these for better readability. Once a solution in normalised quantities was obtained, physical quantities could be easily computed in a post-processing step using the corresponding normalisation constants, which are therefore stored together with the data in the output files.

3.3. Grid structure

To solve the set of equations Eq. (8), CRONOS employs a finite-volume scheme, decomposing the computational volume into a set of disjoint cells (see e.g. LeVeque 2002). While the shapes of the cells are in principle irrelevant for such a scheme, we restricted ourselves to three-dimensional, rectangular grids for practical reasons.

The division into cells is achieved by subdividing each coordinate axis $d \in \{1, 2, 3\}$ spanning the computational domain (x_b^d, x_e^d) into N^d intervals $\omega_{i^d}^d$, which are addressed by the index $i^d \in \{0, \dots, N^d - 1\}$. The edges of the individual intervals $\omega_{i^d}^d = (x_{i^d-1/2}^d, x_{i^d+1/2}^d)$ can be freely chosen as long as they are strictly increasing and first and last edges match the beginning and the end of the computational domain, that is $x_{-1/2}^d = x_b^d$ and $x_{N^d-1/2}^d = x_e^d$, respectively. Usually, the edges are chosen to be spaced linearly, however, non-linear options are also implemented (see Kissmann et al. 2018).

The individual cells are then given by $C_I = \omega_{i^1}^1 \times \omega_{i^2}^2 \times \omega_{i^3}^3$ and are correspondingly addressed by the index triplet $I = (i^1, i^2, i^3)$. The centre of a cell $x_I^d := (x_{i^d-1/2}^d + x_{i^d+1/2}^d)/2$ is defined to be located at the midpoint of each coordinate interval.

A cell C_I borders on a set of neighbouring cells with indices $J \in N(I)$. The interfaces to its neighbours $\Sigma_{I,J}$ can therefore be used to decompose the cell's surface as $\partial C_I = \bigcup_{J \in N(I)} \Sigma_{I,J}$. For rectangular grids, the cell interface normals $\mathbf{n}_{I,J}$ are further (anti-)parallel to the $d_{I,J}$ -th coordinate basis vectors, yielding $\mathbf{n}_{I,J} \cdot \mathbf{e}_{d_{I,J}} =: \sigma_{I,J} = \pm 1$.

In contrast to finite difference schemes, where the values of dynamical variables are stored as point values on a grid, in a finite-volume approach, cell-averaged values are stored. The averaged primitive variables $\bar{w}$, which are initially set by the user,

are defined by

$$\bar{w}_I := \frac{1}{\Delta V_I} \int_{C_I} w \, dV \quad \text{with} \quad \Delta V_I := \int_{C_I} dV. \quad (9)$$

The corresponding set of averaged conserved variables $\bar{U}$ is defined in analogy.

3.4. Semi-discrete finite-volume scheme

To obtain a numerical scheme to update the cell averages $\bar{w}$ or respectively $\bar{U}$, the set of conservation equations Eq. (1) was integrated over the extent of a cell C_I . Substituting the respective cell averages and applying Gauss's theorem yields

$$\frac{d}{dt} \bar{U}_I = \bar{S}_I - \frac{1}{\Delta V_I} \int_{\partial C_I} \mathbf{F} \cdot d\mathbf{A}, \quad (10)$$

where $\bar{S}$ denotes the cell averaged source term. Splitting the cell's surface into disjoint interfaces to its neighbours and using the interface-averaged fluxes defined as

$$\bar{F}_{I,J} := \frac{\sigma_{I,J}}{\Delta A_{I,J}} \int_{\Sigma_{I,J}} F^{d_{I,J}} dA, \quad \Delta A_{I,J} := \int_{\Sigma_{I,J}} dA \quad (11)$$

allows Eq. (10) to be rewritten as

$$\frac{d}{dt} \bar{U}_I = \bar{L}_I := \bar{S}_I - \frac{1}{\Delta V_I} \sum_{J \in N(I)} \Delta A_{I,J} \bar{F}_{I,J}. \quad (12)$$

With this, the initial system of partial differential equations in Eq. (1) has been cast into a system of ordinary differential equations (ODEs) for each grid cell. This is usually referred to as a semi-discrete scheme, since the problem was discretised in space but not in time, having the advantage that the spatial and temporal parts of the problem are conceptually decoupled (see e.g. also Kurganov & Tadmor 2000; LeVeque 2002).

4. Numerical scheme

In CRONOS we followed the general idea presented by Godunov (1959), but used higher-order schemes in both space and time, instead. First, we obtained interface-centred point values of the fluid variables at both sides of a given cell interface using a second-order spatial reconstruction (see Sect. 4.1). The resulting jump in the reconstructed quantities can be viewed as a local, one-dimensional Riemann problem, which was solved by approximate Riemann solvers (see Sect. 4.2) to obtain an estimation for the fluxes $\bar{F}_{I,J}$ in Eq. (12). Finally, advancing the solution in time was handled by a second-order Runge-Kutta scheme (see Sect. 4.3).

4.1. Reconstruction

To provide the initial data for the Riemann problems to be solved at the cell interfaces, a spatial reconstruction of the dynamical variables was used. The order of the reconstruction thereby critically determines the spatial accuracy of the overall method. In CRONOS we applied piecewise-linear reconstructions for every coordinate direction independently, using minmod (see van Leer 1979; Harten et al. 1983) and van-Leer (see van Leer 1977) slope limiters. The reconstruction methods employed for special relativistic hydrodynamics are identical to the ones for classical hydrodynamics (see Kissmann et al. 2018).

The reconstruction was applied for primitive variables, yielding the left- (L) and right-handed (R) states $w_{I,J}^L$ and $w_{I,J}^R$, respectively, at a given cell interface $\Sigma_{I,J}$. Therefrom, the corresponding point values of the conserved variables $U_{I,J}^{L/R}$ were computed subsequently. Since the flux function in Eq. (2) is expressed in terms of primitive variables, this approach has the additional advantage that the more expensive variable conversion from conserved to primitive ones (see Sect. 4.4) can be avoided.

As opposed to Newtonian hydrodynamics, where the fluid speed is generally not bound, it has to remain subluminal at all times for relativistic hydrodynamics. This constraint can be easily violated if three-velocity components are reconstructed independently of each other. In our case, related problems were avoided from the outset since we used and reconstructed spatial four-velocity components instead, which are not subject to such a constraint.

4.2. Approximate Riemann solvers

For a given cell interface $\Sigma_{I,J}$, the reconstructed states at both sides were used to define a local Riemann problem that can be formalised as

$$w(t_0, \xi) = \begin{cases} w_{I,J}^L & \xi < \xi_{I,J} \\ w_{I,J}^R & \xi > \xi_{I,J} \end{cases} \quad (13)$$

with $\xi = x^{d_{I,J}}$ denoting the coordinate aligned with the interface normal. Assuming the cell-interface to be flat, the conservation equations Eq. (1) governing the evolution of the Riemann problem reduce to

$$\partial_t U + \partial_\xi f(w) = 0, \quad (14)$$

where $f = \mathbf{e}_{d_{I,J}} \cdot \mathbf{F} = F^{d_{I,J}}$ corresponds to the flux through the interface.

Although relativistic Riemann problems cannot be solved in a closed analytic form, semi-analytic iterative solvers have been developed that can compute their solution to arbitrary precision (see e.g. Marti & Müller 1994; Pons et al. 2000). Employing such solvers, however, is cumbersome and computationally very expensive, which makes them unsuitable for an application in simulation codes.

Instead, approximate Riemann solvers have been developed, making simplifying assumptions on the waves emerging from the initial discontinuity. This significantly reduces the computational cost, while still yielding good approximations for the fluxes at the cell interfaces. In CRONOS we employed the HLL and the HLLC special-relativistic Riemann solvers (Mignone & Bodo 2005). Since every cell interface is treated individually and identically by the solver, we omit the cell indices, for example $w_L \equiv w_{I,J}^L$, for the remainder of this section for the sake of better readability.

4.2.1. HLL solver

One of the most commonly employed Riemann solvers is the HLL solver first proposed by Harten et al. (1983) for the classical Euler equations. The generalisation to the relativistic case is straightforward and was used in Schneider et al. (1993) for the first time. Here, we briefly summarise the expressions relevant for the implementation in CRONOS.

The solver assumes that the Riemann problem produces two shock waves propagating with speeds λ_L and λ_R computed from Eq. (27). Only one constant intermediate state U^* is considered

to be formed between both shocks, while the states ahead of the shocks remain unchanged. The intermediate state can be computed directly from the Rankine-Hugoniot jump conditions at both shocks

$$U^* = \frac{\lambda_R U_R - \lambda_L U_L + f_L - f_R}{\lambda_R - \lambda_L}, \quad (15)$$

using the fluxes of the undisturbed states at either side $f_{L/R} = f(w_{L/R})$. The corresponding fluxes in the intermediate region are then given by

$$f^* = \frac{\lambda_R f_L - \lambda_L f_R + \lambda_L \lambda_R (U_R - U_L)}{\lambda_R - \lambda_L}. \quad (16)$$

Depending on the signal speeds $\lambda_{L/R}$, the numerical cell-interface fluxes are ultimately given by

$$F^{\text{HLL}} = \begin{cases} f_L & \text{for } 0 < \lambda_L \\ f^* & \text{for } \lambda_L < 0 < \lambda_R \\ f_R & \text{for } \lambda_R < 0. \end{cases} \quad (17)$$

Although the HLL solver is quite simple and computationally inexpensive, it yields good and robust approximations for the cell-interface fluxes. In general, the solver has been found to perform well at shock and rarefaction waves. However, since contact discontinuities were not considered in the simplified wavefan, the HLL solver introduces additional numerical dissipation at such waves.

4.2.2. HLLC solver

A natural improvement to the HLL solver is to restore the neglected contact discontinuity. The corresponding approximate Riemann solver, which considers all physical intermediate states, is known as the HLLC solver and was first presented by Toro (1997) for the classical Euler equations and later extended to special relativistic hydrodynamics by Mignone & Bodo (2005). Again, we briefly summarise the quantities relevant for our implementation in CRONOS.

The solver assumes the emerging wavefan to be composed of two shocks together with a contact discontinuity in between, separating two intermediate states U_s^* with $s \in \{L, R\}$, respectively. Using the Rankine-Hugoniot jump conditions for both shock waves and assuming that the intermediate-state fluxes take the following form $f_s^* = f(w_s^*)$, which is not necessarily the case in general (Mignone & Bodo 2005), the speed of the contact discontinuity λ^* is given by

$$(\lambda^*)^2 [\lambda_L A_R - \lambda_R A_L] + [B_R - B_L] - \lambda^* [A_R - A_L + \lambda_L B_R - \lambda_R B_L] = 0, \quad (18)$$

with

$$A_s := \lambda_s (\tau_s + D_s) - m_s^x \quad (19)$$

$$B_s := m_s^x (\lambda_s - v_s^x) - p_s. \quad (20)$$

We solved this equation analytically, taking only the root with the minus sign into account since this is the only physically acceptable one (Mignone & Bodo 2005).

After computing the intermediate-state pressure for one side

$$p_s^* = \frac{\lambda^* A_s - B_s}{1 - \lambda_s \lambda^*} \quad (21)$$

and using the constant pressure over the contact discontinuity $p^* \equiv p_L^* \equiv p_R^*$, the remaining quantities of the intermediate states are given by

$$m_s^*(\lambda_s - \lambda^*) = m_s^x(\lambda_s - v_s^x) - p_s + p^* \quad (22)$$

$$\tau_s^*(\lambda_s - \lambda^*) = \tau_s(\lambda_s - v_s^x) - v_s^x p_s + \lambda^* p^* \quad (23)$$

$$\zeta_s^*(\lambda_s - \lambda^*) = \zeta_s(\lambda_s - v_s^x). \quad (24)$$

Here, ζ represents any passively advected, conserved quantity such as the mass density D , the momentum densities m^{t1}, m^{t2} tangential to the interface, or any generic tracer field Ψ . Finally, the numerical fluxes at the cell interfaces were obtained from

$$F^{\text{HLLC}} = \begin{cases} f_L & \text{for } 0 < \lambda_L \\ f_L^* & \text{for } \lambda_L < 0 < \lambda^* \\ f_R^* & \text{for } \lambda^* < 0 < \lambda_R \\ f_R & \text{for } \lambda_R < 0. \end{cases} \quad (25)$$

To avoid a direct evaluation of the flux function $f(w_s^*)$ for the intermediate states, which would require a variable inversion, the intermediate-state numerical fluxes were computed from the Rankine-Hugoniot conditions instead:

$$f_s^* = f_s + \lambda_s (U_s^* - U_s). \quad (26)$$

The HLLC solver has been shown to have superior performance compared to the more simple HLL solver. However, it has also been reported to potentially suffer from the carbuncle phenomenon (see e.g. Quirk 1994; Dumbser et al. 2004).

4.2.3. Wave speed estimates

Both the HLL and HLLC Riemann solvers require an estimate for the fastest signal speeds to the left and to the right of the discontinuity λ_L, λ_R , respectively (see also Toro 1997). They can be obtained from the smallest and largest eigenvalues of the system Eq. (14) and were first computed by Davis (1988) for the relativistic case. Although this is not the only possible estimate (e.g. the Roe average, see Roe 1981), it is commonly used in many codes (see e.g. Mignone et al. 2007; Lamberts et al. 2013). In CRONOS we used

$$\lambda_L = \min(\lambda_-(w_L), \lambda_-(w_R)) \quad (27a)$$

$$\lambda_R = \max(\lambda_+(w_L), \lambda_+(w_R)), \quad (27b)$$

where $\lambda_{\pm}$ are the smallest and largest eigenvalues of the system, respectively, which take the form

$$\lambda_{\pm}(w) = \frac{u^0 u^d \pm \sqrt{u_s^2 (u^{02} - u^{d2} + u_s^2)}}{u^{02} + u_s^2}, \quad (28)$$

with $d = d_{I,J}$ corresponding to the direction of the interface normal, $u_s^2 := c_s^2 / (1 - c_s^2)$, and the sound speed (taken from Mignone & McKinney 2007)

$$c_s^2(\Theta) = \begin{cases} \frac{\Gamma\Theta}{h} & \text{ideal EoS} \\ \frac{\Theta}{3h} + \frac{5h-8\Theta}{h-\Theta} & \text{TM EoS,} \end{cases} \quad (29)$$

with $h(\Theta)$ being computed from Eq. (4).

4.3. Time integration

In CRONOS, we treated the system of ODEs in time, arising in the semi-discrete framework in Eq. (12), using a second-order total-variation-diminishing Runge-Kutta scheme, that is Heun's method (see Shu 1988)

$$\bar{U}_I^* = \bar{U}_I^n + \bar{\mathcal{L}}_I(w^n) \Delta t \quad (30a)$$

$$\bar{U}_I^{n+1} = \frac{1}{2} (\bar{U}_I^n + \bar{U}_I^* + \bar{\mathcal{L}}_I(w^*) \Delta t), \quad (30b)$$

where the indices $n, n+1$, and $*$ indicate values at the current, the next, and an intermediate time-step.

The evaluation of the dimensionally unsplit operator $\bar{\mathcal{L}}_I$ for a given cell requires the computation of the numerical fluxes at every cell interface. This involves the solution of Riemann problems, which is the most expensive part of the scheme. Since $\bar{F}_{I,J} = -\bar{F}_{J,I}$ by construction, we iterated over interfaces in the computational domain instead of over cells to avoid unnecessary double computations. In practice, we further iterated over one-dimensional pencils for each coordinate, which allows for the efficient utilisation of the coordinate-wise nature of the reconstructions. This is followed by another iteration over the whole domain regarding the source term, where we evaluated the respective expressions at the cell centres as

$$\bar{S}_I = S(t, x_I, \bar{w}_I). \quad (31)$$

The step size for the numerical time integration was constrained by the CFL condition (see Courant et al. 1928) and was obtained from

$$\Delta t = C_{\text{CFL}} \min_{I,J} \left(\frac{\Delta L_I^{d(I,J)}}{\lambda_{I,J}^{\max}} \right), \quad (32)$$

where C_{CFL} is the Courant number and $\lambda_{I,J}^{\max}$ the largest absolute value of the signal speeds computed at the cell interface $\Sigma_{I,J}$, which was retrieved from the characteristic speeds that have been computed for the Riemann solvers. We allowed the user to set a specific value for C_{CFL} in each parameter file, individually. For dimensionally unsplit schemes, such as the one described here, the Courant number was chosen to be $C_{\text{CFL}} \leq 1/N_d$ to maintain stability in any case (see also Lamberts et al. 2013), where N_d is the dimension of the problem. Depending on the problem, however, the condition might be eased; for example, for radially symmetric flows, a Courant number of $C_{\text{CFL}} \leq 1/\sqrt{N_d}$ is sufficient. The time step is further adapted if an output checkpoint or the end of the simulation is reached.

In contrast to Newtonian hydrodynamics, where the signal speeds $\lambda^{\max}$ are not limited in general, they are bound by the speed of light in relativity. In practice, this implies that the step size computed from Eq. (32) does not become smaller than $\Delta t_{\min} = C_{\text{CFL}} \min_{d,I} (\Delta L_I^d) / c$, which only depends on the extension of the smallest cell. Such a lower bound has been proven to be useful in practice for the estimation of maximum simulation runtimes. After obtaining a solution at t^{n+1} , user-supplied routines are invoked, for example, to reset the solution in a given region, before the time integration procedure starts again.

4.4. Variable inversion

Since the fluxes are given in terms of the primitive fluid variables $w = (\rho, p, u^i)$ but the time integration has to be performed on conserved variables $U = (D, \tau, m^i)$ to obtain a shock-

capturing scheme, transformations between the two sets are required. While the conversion from primitive quantities to conserved ones is trivial and can be implemented in a straightforward manner, the conversion in the other direction is not and it involves solving non-linear equations for at least one of the quantities. For this, we closely followed the approach presented by Mignone & McKinney (2007), which was initially developed for relativistic MHD, and we adapted it for our purposes (similar to Lamberts et al. 2013). We solved the non-linear equation

$$f(W') := W' - \tau - p(\chi, \rho) = 0, \quad (33)$$

where $W' = D(hu^0 - 1)$ and $\chi = \rho(h - 1)$. The function $p(\chi, \rho)$ depends on the chosen EoS and can be found in Table 1 for the different cases implemented in Cronos. To evaluate f for a given W' , we first computed the corresponding four-speed via

$$|\mathbf{u}|^2(W') = \frac{|\mathbf{m}|^2}{(W' + D)^2 - |\mathbf{m}|^2}, \quad (34)$$

which was used to obtain (Mignone & McKinney 2007)

$$\chi(W', |\mathbf{u}|^2) = \frac{W'}{u^{02}} - \frac{D|\mathbf{u}|^2}{u^{02}(1 + u^0)} \quad (35)$$

and

$$\rho(W', |\mathbf{u}|^2) = \frac{D}{u^0} \quad (36)$$

employing the identity $(u^0)^2 = 1 + |\mathbf{u}|^2$.

We solved Eq. (33) numerically using an iterative Newton-Raphson scheme until the relative change was below a certain threshold ϵ , which can be set by the user depending on the problem (typically $\epsilon = 10^{-8}$). It can be shown analytically that the scheme is accurate in the ultra-relativistic limit as long as $u^0 \leq \epsilon^{-1/2}$ and $p/(\rho u^{02}) \gtrsim \epsilon$ (see Mignone & McKinney 2007), which might require an adjustment of ϵ for certain problems.

The derivative df/dW' required by the algorithm is expressed as

$$\frac{df}{dW'} = 1 - \frac{\partial p}{\partial \chi} \frac{d\chi}{dW'} - \frac{\partial p}{\partial \rho} \frac{d\rho}{dW'}, \quad (37)$$

where the kinematical derivatives are given by

$$\frac{d\chi}{dW'} = \frac{1}{u^{02}} + u^0 (D + 2u^0 \chi) \frac{|\mathbf{m}|^2}{(W' + D)^3} \quad (38)$$

$$\frac{d\rho}{dW'} = \frac{Du^0 |\mathbf{m}|^2}{(W' + D)^3}. \quad (39)$$

The derivatives involving the pressure $\partial_\chi p$ and $\partial_\rho p$ again depend on the chosen EoS and are also listed in Table 1.

The Newton-Raphson iteration is started using the initial value

$$W'_0 = \frac{1}{3} (2E + \sqrt{4E^2 - 3|\mathbf{m}|^2}) - D. \quad (40)$$

This choice guarantees pressure positivity given the conservative state is physically admissible (Mignone & McKinney 2007).

Once a sufficiently precise solution for W' is found, the primitive variables are given by Eq. (36), $p(\chi, \rho)$ supplied by the EoS, and by

$$\mathbf{u}(W') = \frac{\mathbf{m}}{(W' + D)^2 - |\mathbf{m}|^2}. \quad (41)$$

Table 1. Thermodynamical quantities for different EoS implemented in Cronos (see also Sect. 2) necessary for the variable inversion (compiled from Mignone & McKinney 2007).

	$p(\chi, \rho)$	$\partial_\chi p$	$\partial_\rho p$
Ideal EoS	$\frac{\Gamma-1}{\Gamma} \chi$	$\frac{\Gamma-1}{\Gamma}$	0
TM EoS	$\frac{2\chi(\chi+2\rho)}{5(\chi+\rho) + \sqrt{9\chi^2 + 18\rho\chi + 25\rho^2}}$	$\frac{2\chi+2\rho-5\rho}{5\rho+5\chi-8\rho}$	$\frac{2\chi-5\rho}{5\rho+5\chi-8\rho}$

4.4.1. Admissible conserved states

If a given conserved state is unphysical, the variable inversion fails and produces unphysical primitive states, for example, with negative density or pressure, superluminal speeds, etc., or the inversion does not converge at all. To avoid related problems, we checked the admissibility of a given conserved state $U \in \mathcal{G}_1$ before every inversion, relying on the set of physically admissible states formulated by Wu & Tang (2015):

$$\mathcal{G}_1 = \{U \mid D > 0, q(U) := \tau + D - \sqrt{D^2 + |\mathbf{m}|^2} > 0\}. \quad (42)$$

If the constraint is violated ($U \notin \mathcal{G}_1$), the user is informed and the simulation is aborted by default. Alternatively, the user can choose to overwrite the states in the concerned cells with new ones by supplying user-defined routines, for example, setting a lower limit for the pressure and computing other quantities accordingly.

4.4.2. Entropy inversion

In situations where the thermal energy is negligible compared to the kinetic energy, simple discretisation errors can lead to unphysical states ($U \notin \mathcal{G}_1$) for which the variable inversion will fail. To avoid related problems, we offer the user the possibility to solve an additional equation for the conservation of entropy in smooth flows

$$\partial_t \Sigma + \nabla \cdot (\Sigma \mathbf{v}) = 0, \quad (43)$$

next to the hydrodynamic equations (in analogy to our procedure for classical HD and MHD Kissmann et al. 2018), with $\Sigma = \sigma D$ and the entropy (Mignone & McKinney 2007)

$$\sigma = \begin{cases} \frac{p}{\rho^\Gamma} & \text{ideal EoS} \\ \frac{p}{\rho^{5/3}} (h - \Theta) & \text{TM EoS.} \end{cases} \quad (44)$$

Numerically, the equation was treated in analogy to passive tracer fields (see Sect. 2.2), which guaranteed that we maintained positive values for Σ using the implemented solvers. Although the conservation of energy might be slightly violated by employing Σ instead of τ in the variable inversion, the resulting scheme is much more stable, which can be necessary for certain applications.

When using Σ , the inversion was performed by numerically solving

$$g(\rho) = \rho u^0(h(\rho)) - D = 0, \quad (45)$$

where

$$u^0(h) = \sqrt{1 + \frac{|\mathbf{m}|^2}{D^2 h^2}} \quad (46)$$

and

$$h^2(\rho) = \begin{cases} \left(1 + \frac{\Gamma-1}{\Gamma} \sigma \rho^{\Gamma-1}\right)^2 & \text{ideal EoS} \\ \frac{(1+4\rho^{2/3}\sigma)^2}{1+3\rho^{2/3}\sigma} & \text{TM EoS.} \end{cases} \quad (47)$$

Table 2. Parameters for the Riemann problems according to Eq. (50) solved in Sect. 5.1 (taken from Mignone & Bodo 2005) together with the L_1 errors of the numerical solutions for the density and the pressure, respectively.

	P1	P2	P3	P4
w_L	(1, 0.9, 1)	(1, -0.6, 10)	(10, 0, 40/3)	(1, 0, 10 ³)
w_R	(1, 0, 10)	(10, 0.5, 20)	(1, 0, 2/3 × 10 ⁻⁶)	(1, 0, 10 ⁻²)
L_1^p	4.05 × 10 ⁻²	5.62 × 10 ⁻²	5.94 × 10 ⁻²	1.62 × 10 ⁻¹
L_1^ρ	6.88 × 10 ⁻²	1.14 × 10 ⁻¹	3.23 × 10 ⁻²	2.94

Although the derivative of Eq. (45) can be easily found and implemented for a Newton-Raphson scheme to solve the equation, we used a hybrid, bracketing, root-finding method, that is Brent's method (Brent 1972), instead. For our use cases, we found a comparable performance for both solvers, while the latter one is guaranteed to converge in any case. As an initial bracket for the scheme, we used $\rho_{\max} = D$ and $\rho_{\min} = D^2 / \sqrt{D^2 + |\mathbf{m}|^2}$. These limits were obtained from $\rho = D/u^0(h)$ using the asymptotic values of the specific enthalpy $1 < h < \infty$ in the ultra-cold and ultra-hot limit, respectively.

Once a sufficiently accurate value for ρ was found, the inversion was completed by computing the fluid velocity from $\mathbf{u} = \mathbf{m}/Dh(\rho)$ and the pressure according to

$$p = \begin{cases} \sigma \rho^\Gamma & \text{ideal EoS} \\ \frac{1}{2} \rho (h(\rho) - \sqrt{h^2(\rho) - 4\sigma \rho^{2/3}}) & \text{TM EoS.} \end{cases} \quad (48)$$

The conservation of entropy, however, only applies for smooth, non-compressive flows. To identify those cells for which this is the case and the variable inversion can be feasibly performed using Eq. (45), we flagged cells according to the following criteria (similar to Balsara & Spicer 1999; Mignone et al. 2020):

$$\mathcal{F}_I^\Sigma = \left(\|\nabla p_I\| \max_d \Delta L_I^d < \alpha_1 \min_{I,N(I)} p \right) \vee \left(-\alpha_2 \max_{I,N(I)} c_s < (\nabla \cdot \mathbf{v}) \min_d \Delta L_I^d \right). \quad (49)$$

The occurring gradient and divergence were approximated using central, finite differences and c_s denotes the local sound speed computed according to Eq. (29). We typically used values of $\alpha_1 = 0.05$ and $\alpha_2 = 0$. Further, if a given cell I did not qualify for the entropy inversion ($\mathcal{F}_I^\Sigma = 0$), we also disabled the flag for its direct neighbours for safety ($\mathcal{F}_J^\Sigma = 0$ for $J \in N(I)$).

Wherever $\mathcal{F}_I^\Sigma = 1$, we performed the variable inversion using Eq. (45). Otherwise, Eq. (33) was used and the corresponding value of σ was recomputed from the resulting state. The described procedure can be enabled or disabled by a compile-time switch set by the user.

5. Validation

In the following sections, we present the results from a variety of numerical tests to verify our implementations within the CRONOS code.

5.1. 1D Riemann problems

One-dimensional Riemann problems are particularly useful numerical tests for hydrodynamic codes since they can be solved by

semi-analytical methods to arbitrary precision (Marti & Müller 1994). The Riemann problems for the following tests are posed in the general form

$$(\rho, v^x, p) = \begin{cases} w_L & \text{for } x < 0.5 \\ w_R & \text{for } x > 0.5, \end{cases} \quad (50)$$

For comparison, we considered the same set of Riemann problems as in Mignone & Bodo (2005), summarised in Table 2 with zero fluid velocity tangential to the discontinuity and an ideal EoS with $\Gamma = \frac{5}{3}$. All numerical tests were performed using extrapolating boundary conditions.

In Fig. 1, we present the numerical evolution of the considered Riemann problems together with their exact solutions¹. In P1 and P2, two shock waves and two rarefaction waves are formed, respectively, which are in good agreement with the exact solutions. The tests P3 and P4 are characterised by large differences in pressure between the initial states and they evolve into a leftward-moving rarefaction and a rightward-moving shock wave, forming dense shells of material. These shells are also known as relativistic blast waves and pose notoriously difficult problems for numerical schemes. For P4, the numerical solution yields a shock position and a compression ratio that slightly differ from their exact locations and values. This is caused by an insufficient resolution of the blast wave in combination with the spatial reconstruction effectively reducing to first order in the vicinity of shocks. Overall, the numerical solutions obtained using CRONOS are in good agreement with the exact, semi-analytic solutions, which validates the implemented solvers.

5.2. 1D Riemann problems with non-zero tangential velocity

While velocities tangential to the initial discontinuity v^t do not affect the evolution of Riemann problems in classical hydrodynamics, they do have a severe impact on the emerging wavefan in relativistic hydrodynamics because of the non-linear coupling introduced by the Lorentz factor. We demonstrated that these effects are also correctly handled by our implementations by solving the Riemann problem

$$(\rho, v^x, v^t, p) = \begin{cases} (1, 0.5, 0, 1) & \text{for } x < 0.5 \\ (0.125, 0, v_R^t, 0.1) & \text{for } x > 0.5 \end{cases} \quad (51)$$

for different values of the right-sided, tangential velocity v_R^t in analogy to the ones in Sect. 5.1. Exact semi-analytic solutions with non-zero tangential velocities¹ are again available in the literature (see Pons et al. 2000; Rezzolla et al. 2003), which were used to produce the reference solutions shown in Fig. 2.

We investigated two scenarios with $v_R^t = 0.7$ and $v_R^t = 0.9$ and show the numerical solutions in Fig. 2. The numerical results agree well with the exact solutions and show the transition from a rarefaction-shock to a shock-shock pattern expected at $v_R^t \sim 0.85$ (Rezzolla et al. 2003). The numerical L_1 errors are $L_1^p = 6.20 \times 10^{-3}$; 9.76×10^{-3} for the density and $L_1^\rho = 6.61 \times 10^{-3}$; 9.04×10^{-3} for the pressure, corresponding to $v_R^t = 0.7$; 0.9 , respectively.

5.3. 2D Riemann problem

After the successful tests in one dimension, we now move to tests in higher dimensions. First, we consider a two-dimensional

¹See github.com/cxkoda/srrp for an implementation of an exact Riemann solver for relativistic hydrodynamics in PYTHON.

Fig. 1. Numerical results for one-dimensional Riemann problems at time $t = 0.4$. The density (blue crosses) and pressure (orange plus signs) are shown. The underlying solid black line corresponds to the exact solution. The numerical solutions have been obtained using 400 gridpoints, the minmod slope limiter, the HLLC solver, and CFL = 0.4. To improve visibility, we show only every fourth point of the numerical results and scaled the different quantities as annotated. The parametrisations of the Riemann problems for the numerical test can be found in Table 2.

Fig. 2. Same as in Fig. 1, but for Riemann problems involving non-zero tangential velocities in the right state with $v_R^t = 0.7$ (top) and $v_R^t = 0.9$ (bottom) as parameterised in Eq. (51). The solutions for the tangential velocity (green crosses) and the pressure (orange plus signs) are shown.

Riemann problem, which is posed by the interaction of four different initial states; one in each quadrant of the two-dimensional plane. For the sake of comparison, we solved the same problem as investigated by Del Zanna & Bucciantini (2002) that is parameterised as

$$(\rho, v^x, v^y, p) = \begin{cases} (0.1, 0, 0, 0.01) & \text{for } x > 0, y > 0 \\ (0.1, 0.99, 0, 1) & \text{for } x < 0, y > 0 \\ (0.5, 0, 0, 1) & \text{for } x < 0, y < 0 \\ (0.1, 0, 0.99, 1) & \text{for } x > 0, y < 0. \end{cases} \quad (52)$$

Again, we used extrapolating boundary conditions, the minmod slope limiter, and an ideal EoS with $\Gamma = \frac{5}{3}$.

In Fig. 3, we present the numerical results using the HLL and HLLC solver, respectively. The initial discontinuities separating the two top states and the two right states evolve into curved shock waves that enclose a drop-shaped region in the top-right quadrant. The lower-left region remains confined by two contact discontinuities and forms a jet-like structure. While the contact discontinuities remain sharp and steady using the HLLC solver, they degenerate into spurious waves using the HLL solver because of the increased numerical dissipation of the latter, demonstrating the better performance of the HLLC solver. Our numerical results agree well with the ones in the literature (e.g. Del Zanna & Bucciantini 2002; Mignone & Bodo 2005). Having verified the implementation on Cartesian grids, we moved to curvilinear coordinates in the subsequent test.

5.4. Axisymmetric relativistic jet

In this numerical test, we demonstrate the implementation of geometric source terms arising in non-Cartesian coordinate systems (see Sect. 3.1). For this, we simulated the evolution of an axisymmetric relativistic jet in 2D cylindrical geometry. The jet was set up by initialising the computational volume with an ambient, background medium (respective quantities are denoted with an index m) and injecting the supersonic beam material (denoted with an index b) by imposing constant boundary conditions at $z = 0$ for radii $r < 1$. At the symmetry axis of the jet $r = 0$, we imposed reflecting boundary conditions and outflowing boundary conditions everywhere else. The computational domain covers the region $0 \leq r \leq 12$ and $0 \leq z \leq 35$. For the sake of comparison, we adopted the same set of parameters as Del Zanna & Bucciantini (2002), which are given by the beam density $\rho_b = 0.1$, the beam speed $v_b^z = 0.99$, the ambient medium density $\rho_m = 10$, matched pressures $p_b = p_m = 10^{-2}$, and an ideal EoS with $\Gamma = \frac{5}{3}$. The ambient medium is at rest, $v_m = 0$, and the beam has no radial velocity, $v_b^r = 0$.

The results at time $t = 80$ are shown in Fig. 4 and exhibit typical features of relativistic jets, such as the bow-like shock of the

Fig. 3. Logarithmically equidistant contours of the rest-mass density for numerical solutions of the two-dimensional Riemann problem given in Eq. (52) at time $t = 0.8$. The results using the HLL solver (top) and HLLC solver (bottom) are shown, respectively. The solutions were obtained on a grid with 400^2 cells using a CFL number of 0.4

ambient medium, a hull of shocked material, a central relativistic stream, and turbulence excited by the Kelvin-Helmholtz instability due to the high velocity shear. Simulations using the HLLC solver show more small-scale fluctuations than those using the HLL solver because of the latter's higher numerical dissipation. This again demonstrates the superior performance of the HLLC solver. The results are in good qualitative agreement with the numerical solutions obtained by Del Zanna & Bucciantini (2002) and Mignone & Bodo (2005). The slight extension of the head using the HLLC solver is potentially caused by the carbuncle problem, which usually manifests itself as an extended nose on the jet axis (Quirk 1994) and has also been seen in other implementations of this test (e.g. see Lamberts et al. 2013).

Fig. 4. Rest-mass density for the relativistic jet given in Sect. 5.4 at time $t = 80$. The results using the HLL solver (left half) and HLLC solver (right half) are shown, respectively. The numerical solutions were obtained on a grid with 512×1536 cells in cylindrical axisymmetry using a CFL number of 0.4.

Table 3. Ambient medium densities and one-dimensional estimates for the jet speed according to Eq. (53) for the jets considered in Sect. 5.5.

	$\Gamma = \frac{5}{3}$	$\Gamma = \frac{4}{3}$	TM
ρ_m	27.7424	2.19394	10.3337
V_j	0.30354	0.57883	0.39243

Here, we exclusively considered a single ideal EoS. The evolution of relativistic jets, however, is heavily affected by the particular choice of the EoS, which is exploited in the next tests.

5.5. Equation of state

Here we verify the different EoSs implemented in CRONOS (see also Sect. 2). For this, we again simulated the propagation of relativistic jets in analogy to the setup in Sect. 5.4. For a given equation of state, the properties of a jet are determined by three parameters: the density ratio $\eta = \rho_b/\rho_m$, the beam's Lorentz factor u_b^0 , and its Mach number $M_b = v_b/c_s$. Following the tests performed in Mignone et al. (2007), we adopted the same jet parameters $\eta = 10^{-3}$, $u_b^0 = 10$, $M_b = 1.77$ and investigated the jet

Fig. 5. Rest-mass densities for the jets simulated with different equations of state (as annotated) at $t = 60$. The computations were performed on a grid with 512×1536 cells in cylindrical symmetry using the HLLC solver and $\text{CFL} = 0.4$. The jets were set up using the parameters given in the text and Table 3.

Fig. 6. Position of the head of the jet over time for different equations of state: $\Gamma = \frac{5}{3}$ (orange, circles, dashed), $\Gamma = \frac{4}{3}$ (blue, squares, dash-dotted), TM-EoS (green, triangles, dotted). Markers correspond to numerical results and lines to one-dimensional estimates given by Eq. (53). The simulated jets correspond to the ones depicted in Fig. 5.

evolution under three different EoSs: two ideal ones with $\Gamma = \frac{5}{3}$ and $\Gamma = \frac{4}{3}$ and the TM EoS. We further chose the pressures $p_b = p_m = 10^{-2}$ resulting in the ambient medium densities ρ_m listed in Table 3, which were used together with $\rho_b = \eta \rho_m$ and $v_b = 0.995$ to specify the setup for the simulation.

In Fig. 5 we show the resulting densities for the simulated jets at $t = 60$. Owing to the different EoSs, the head of the jets propagate at different speeds along the z -axis, which is visible from the different jet extents in the simulation. In one dimension, the propagation of relativistic jets was investigated by Martí et al. (1997) who derived the following analytical

expression for the speed of the head of a jet:

$$V_j = \frac{u_b^0 \sqrt{\eta h_b/h_m}}{1 + u_b^0 \sqrt{\eta h_b/h_m}}. \quad (53)$$

The values corresponding to our setups can again be found in Table 3, which serve as a test for our implementations. In Fig. 6 we show the locations of the jet heads in our numerical simulations, which are in good agreement with the analytical estimates from Eq. (53). As expected from similar simulations performed by Mignone et al. (2007), the simulated jets become slower and start to deviate from the linear propagation in one dimension for later times, which follows from the two-dimensional nature of the numerical tests.

5.6. Spatial order

Finally, we verified the order of our scheme using similar tests as those performed for classical hydrodynamics with CRONOS (see Ryu & Goodman 1994; Kissmann et al. 2018). These tests investigate the decay of two-dimensional standing sound waves by the numerical dissipation of the scheme.

In analogy to classical hydrodynamics, also in special relativity, acoustic waves can be excited by adding velocity perturbations to a constant background state, owing to the similar structure of the eigenvectors of the linearised equations (see Rezzolla 2013). We initialised sinusoidal sound waves using

$$\delta u^x = \delta u^y = \delta_{\text{amp}} \sin(k_x x + k_y y), \quad (54)$$

with the perturbation amplitude $\delta_{\text{amp}} = 10^{-5}$, the wavenumbers $k_x = k_y = \frac{2\pi}{L}$, and the side length of the computational domain $L = 1$. This produces two acoustic waves that propagate with velocities $\lambda_{\pm}(w_0)$ into opposite directions, which can be computed from Eq. (28) for a given constant background state w_0 . For the purpose of this test, we chose the background density $\rho_0 = 1$ and the four-velocity $u_0^x = u_0^y = 0, u_0^z = \text{const.}$ to ensure that both waves travel at the same speed, yielding

$$\lambda_{\pm} = \pm c_s \sqrt{\frac{1 - (v_0^z)^2}{1 - (v_0^z)^2 c_s^2}}, \quad (55)$$

where $v_0^z = \frac{u_0^z}{\sqrt{1 + (u_0^z)^2}}$ is the three-speed in z -direction and c_s the sound speed of the background medium, respectively.

In a periodic domain, this produces a standing wave that oscillates with frequency $f = \frac{\sqrt{2}}{L \lambda_{\pm}}$. To introduce relativistic effects, we set the background speed to a relativistic value of $u_0^z = \frac{2}{\sqrt{3}}$. Choosing $c_s = \frac{1}{2}$, which implies $p_0 = \frac{3}{4\rho_0}$ for an ideal EoS with $\Gamma = \frac{4}{3}$, therefore leads to one oscillation in two units of time. By simulating until $t = 20$, we thus captured ten full oscillations.

From the simulations, we retrieved the spatial root-mean-squared average of the velocity perturbation that oscillates with the double frequency. Due to the presence of numerical viscosity, its amplitude decreases exponentially $\propto \exp(-\Gamma_{\text{decay}} t)$. The decay rate Γ_{decay} was determined from the simulation results as a function of spatial resolution and is shown in Sect. 5.6. The second-order nature of our scheme is obvious from $\Gamma_{\text{decay}} \propto N^{-2}$. As expected, the HLLC solver introduces less numerical viscosity as compared to the HLL solver. In both cases we used the minmod slope limiter and $\text{CFL} = 0.4$.

Fig. 7. Damping rate Γ_{decay} for the decaying, sound-waves test (see Sect. 5.6) as a function of the number of grid cells N using the HLL (blue circles) and the HLLC solver (orange triangles), respectively. The black dotted line indicates a N^{-2} dependence to guide the eye.

Fig. 8. Scaled speedup of simulations performed using Cronos as a function of the number of computation cores in a weak-scaling test. The dotted line indicates perfect scaling.

6. Parallel performance

6.1. Weak scaling

The relativistic extension of CRONOS has been successfully employed in various computational environments using up to $\sim 10^4$ computing cores. The code was parallelised using a halo-communication approach that was realised employing the Message Passing Interface (MPI) library.

To test the parallel efficiency of our code, we performed a weak-scaling test on the Joliot-Curie Rome HPC environment with AMD Rome (Epyc) 7H12 2.6GHz bi-processor compute nodes. As a test setup, we considered the colliding winds of two spherically symmetric, static sources similar to the simulation of gamma-ray binaries in Huber et al. (2021a). Initially, the system was divided into two regions, each filled by one of the winds, using an approximate curve for the contact discontinuity in the system. The simulation was run sufficiently long to obtain a representative average of the time step duration. While the domain size was increased with each test, the workload handled by each computation core was kept constant at 64^3 cells. The results are shown in Fig. 8. As expected, the parallel efficiency drops with an increasing number of cores, but remains above 93% for more than 1.6×10^4 cores.

7. Summary

We have presented and verified an extension to the CRONOS code treating special relativistic hydrodynamics for astrophysical applications. The code is based on a semi-discrete finite-volume framework, ensuring the conservation of relevant quantities to efficiently capture shocks. CRONOS employs a second-order spatial reconstruction combined with a second-order Runge-Kutta time-integrator. The extension was developed with a focus on robustness, providing the user with additional interfaces to prevent, detect, and possibly counteract failures.

Our implementation was verified against a set of standard problems, for which either an analytical solution or established numerical solutions from the literature are available. Parallel scaling for up to $\sim 10^4$ cores has been demonstrated.

As the rest of the CRONOS framework, this extension was also developed with modularity in mind, making it easy to consider additional physics supplied by the user. This was, for example, used to simulate an additional transport of energetic particles governed by a Fokker-Planck type equation alongside the fluid dynamics (as demonstrated in Huber et al. 2021a,b).

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Table A.1. Coordinate variables x^i , scale factors h_i , and geometrical source terms G_{mj} for the different coordinate systems implemented in CRONOS.

	Cartesian	Cylindrical	Spherical
(x^1, x^2, x^3)	(x, y, z)	(r, ϕ, z)	(r, θ, ϕ)
(h_1, h_2, h_3)	$(1, 1, 1)$	$(1, r, 1)$	$(1, r, r \sin \theta)$
G_{m^1}	0	$\frac{p+m^\phi v^\phi}{r}$	$\frac{2p+m^\theta v^\theta+m^\phi v^\phi}{r}$
G_{m^2}	0	$\frac{-m^\phi v^r}{r}$	$\frac{-m^\theta v^r+(p+m^\phi v^\phi) \cot \theta}{r}$
G_{m^3}	0	0	$\frac{-m^\phi (v^r+v^\theta \cot \theta)}{r}$

Appendix A: Geometrical source terms

The geometrical source terms G_{mj} arising in Eq. (7) can be obtained using the anholonomic connection symbol Ω_{ik}^j in the given coordinate system as

$$G_{mj} = -\Omega_{ik}^j T^{ik}, \quad (\text{A.1})$$

where $T^{ij} = m^i v^j + p \delta^{ij}$ denotes the stress-tensor components. The connection symbol corresponds to the anholonomic components of the Christoffel symbol of second kind Γ_{ik}^j (also known as natural connection) in physical units and can be computed by (see Altman & de Oliveira 2011)

$$\Omega_{ik}^j = \frac{h_j}{h_i h_k} \Gamma_{ik}^j - \frac{h_j}{h_k} \partial_k (1/h_i) \delta_i^j. \quad (\text{A.2})$$

This yields the geometrical source terms

$$G_{mj} = - \sum_{i,k} \frac{h_j}{h_i h_k} \Gamma_{ik}^j T^{ik} + \sum_i \frac{\partial_i h_j}{h_i h_j} T^{ij}. \quad (\text{A.3})$$

The Christoffel symbol can be readily obtained from the metric tensor $g_{ij} = h_i h_j \delta_{ij}$ and its derivatives via

$$\Gamma_{bc}^a = \frac{1}{2} g^{ai} (\partial_b g_{ci} + \partial_c g_{ib} - \partial_i g_{bc}). \quad (\text{A.4})$$

For orthogonal coordinates (Stone & Norman 1992), the only non-zero entries are given by

$$\Gamma_{ii}^i = \frac{\partial_i h_i}{h_i}; \Gamma_{jj}^i = \frac{h_j}{h_i^2} \partial_i h_j; \Gamma_{ij}^i = \Gamma_{ji}^i = \frac{\partial_j h_i}{h_i}. \quad (\text{A.5})$$

The resulting source terms for the implemented coordinate systems are summarised in Table A.1. We note that the source terms arising in special relativistic hydrodynamics are formally identical to the ones in Newtonian hydrodynamics. This is intuitive since both sets of equations are also formally identical except for different definitions of the conserved variables.

A similar procedure can also be used to derive the source terms for co-rotating coordinate systems in special relativistic hydrodynamics. This has been done in Huber et al. (2021a) in the context of simulation of gamma-ray binaries and is also available in CRONOS.

ARTICLE II

RELATIVISTIC FLUID MODELLING OF GAMMA-RAY BINARIES.
I. THE MODEL

which appeared as

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Relativistic fluid modelling of gamma-ray binaries

I. The model

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ABSTRACT

Context. Gamma-ray binaries are systems that radiate the dominant part of their non-thermal emission in the gamma-ray band. In a wind-driven scenario, these binaries are thought to consist of a pulsar orbiting a massive star, accelerating particles in the shock arising in the wind collision.

Aims. We develop a comprehensive numerical model for the non-thermal emission of shock-accelerated particles including the dynamical effects of fluid instabilities and orbital motion. We demonstrate the model on a generic binary system.

Methods. The model was built on a dedicated three-dimensional particle transport simulation for the accelerated particles that were dynamically coupled to a simultaneous relativistic hydrodynamic simulation of the wind interaction. In a post-processing step, a leptonic emission model involving synchrotron and inverse-Compton emission was evaluated based on resulting particle distributions and fluid solutions, consistently accounting for relativistic boosting and $\gamma\gamma$ -absorption in the stellar radiation field. The model was implemented as an extension to the CRONOS code.

Results. In the generic binary, the wind interaction leads to the formation of an extended, asymmetric wind-collision region distorted by the effects of orbital motion, mixing, and turbulence. This gives rise to strong shocks terminating the pulsar wind and secondary shocks in the turbulent fluid flow. With our approach it is possible for the first time to consistently account for the dynamical shock structure in particle transport processes, which yields a complex distribution of accelerated particles. The predicted emission extends over a broad energy range, with significant orbital modulation in all bands.

Key words. radiation mechanisms: non-thermal – gamma rays: stars – methods: numerical – relativistic processes – hydrodynamics – binaries: general

1. Introduction

Gamma-ray binaries are composed of an early-type massive star in orbit with a compact object, either a neutron star or a black hole. They are characterised by a dominant radiative output in the gamma-ray regime >1 MeV (see Dubus 2013; Paredes & Bordes 2019, for a review). They exhibit broadband non-thermal emission ranging from radio through low-energy (LE, 1–100 MeV) up to high-energy (HE, >100 MeV) and very high energy (VHE, >100 GeV) gamma-rays. For most systems, observations show flux variations with the orbital phase. At the time of writing, nine gamma-ray binaries emitting in the HE regime are confirmed: 1FGL J1018.6-5856 (Fermi LAT Collaboration 2012; H.E.S.S. Collaboration 2015a), 4FGL J1405-6119 (Corbet et al. 2019), HESS J0632+057 (Aharonian et al. 2007), HESS J1832-093 (H.E.S.S. Collaboration 2015b; Martí-Devesa & Reimer 2020), LMC P3 (Corbet et al. 2016; H.E.S.S. Collaboration 2018), LS 5039 (Paredes et al. 2000; Aharonian et al. 2005a), LS I +61 303 (Kniffen et al. 1997; Albert et al. 2006), PSR B1259-63 (Aharonian et al. 2005b), and PSR J2032+4127 (Abeysekara et al. 2018).

In the literature, two possible mechanisms are proposed to explain the non-thermal emission (see e.g. Mirabel 2006; Romero et al. 2007): A jet-related emission scenario, where the compact object accretes matter from its stellar companion, releasing the accretion energy in the form of relativistic jets with

high-energy particles (see e.g. Bosch-Ramon & Khangulyan 2009); or a wind-driven scenario, in which the compact object is commonly assumed to be a pulsar, whose rotational energy is dissipated as a relativistic pair plasma interacting with the wind of the early-type companion star (see Maraschi & Treves 1981; Dubus 2006). In close-orbit binaries, this interaction leads to the formation of an extended wind-collision region (WCR) that terminates both the pulsar and stellar wind by shocks (see e.g. Bogovalov et al. 2008; Bosch-Ramon et al. 2012). At these sites, particles can be accelerated to ultra-relativistic energies through diffusive shock acceleration and other processes (Sironi & Spitkovsky 2011), which then produce the observed radiation. For many systems, a wind-driven interpretation seems favoured. This has been investigated using a variety of different approaches ranging from simple few-zone models to more complex numerical models including different emission mechanisms (see e.g. Khangulyan et al. 2007; Bosch-Ramon et al. 2008; Cerutti et al. 2010; Bednarek 2011; Zabalza et al. 2013; Takata et al. 2014; Dubus et al. 2015; Barkov & Bosch-Ramon 2018; Molina & Bosch-Ramon 2020). However, while the explored approaches succeed at modelling some observed features, they fail at reproducing others. In this work, we also focus on a wind-driven scenario and aim to alleviate some of the encountered issues.

In analogy to gamma-ray binaries, extended WCRs can also be formed in colliding-wind binaries (CWBs). These systems

are very similar in terms of wind interaction, but they harbour a second early-type star instead of the neutron star. CWBs can therefore be viewed as a non-relativistic analogue of gamma-ray binaries in the wind-driven scenario. The HE emission of such systems has been successfully described by [Reitberger et al. \(2017\)](#) employing a dynamically coupled treatment of the particle transport and the fluid. The corresponding numerical model was implemented as an extension to the CRONOS code (see [Kissmann et al. 2018](#)) solving a Fokker-Planck type particle transport equation for protons and electrons simultaneously to the equations of magneto-hydrodynamics.

In this work, we extend this approach to gamma-ray binaries by translating the previous simulations into a relativistic framework, but we neglect the possible effect of the pulsar and stellar magnetic field on the fluid flow at this stage ([Dubus et al. 2015](#); [Bogovalov et al. 2019](#)). This allows a production of emitting particle distributions that is consistent with the dynamics of the wind interaction; this has not been attempted in the case of gamma-ray binaries before. In turn, this enables the prediction of the non-thermal emission from gamma-ray binaries in a self-consistent framework.

This is the first in a series of papers. With this first paper, we establish the governing equations, describe their numerical treatment, and demonstrate the approach on a generic binary system. In a second paper ([Huber et al. 2020](#)), the developed model is specifically applied to the LS 5039 system, and we compare the predicted emission to observations.

The paper is structured as follows: In Sects. 2.1 and 2.2 we introduce the governing equations for the coupled fluid and particle transport simulation, respectively, together with their numerical treatment and their implementation within CRONOS. In Sect. 2.3 we present the emission model involving synchrotron and inverse-Compton emission with additional modulations by relativistic boosting and $\gamma\gamma$ -absorption. In Sect. 3 we demonstrate the general properties of our model on a generic binary system and present the resulting fluid structure, particle distributions, and emission spectra and light curves. A concluding summary and outlook are given in Sect. 4.

2. Numerical model

The numerical model can be conceptually split into three distinct parts: the fluid model formulated in special relativity treating the interaction of the winds (see Sect. 2.1), the particle transport treating the evolution of the particle distributions embedded in the fluid (see Sect. 2.2), and the emission model predicting the radiation from the system (see Sect. 2.3). The first two are treated simultaneously in the simulation, whereas the radiation is computed in a post-processing step using previously obtained particle and fluid solutions.

2.1. Fluid model

Owing to the relativistic pulsar wind, a classical treatment does no longer suffice and a special relativistic hydrodynamic framework has to be employed to accurately simulate the stellar and pulsar wind interaction. In this section we briefly summarise the necessary ingredients that are treated in an extension of the CRONOS code ([Kissmann et al. 2018](#)), which will be described in more detail in a future paper. The governing equations can be cast into a set of hyperbolic conservation equations that in Cartesian coordinates take the form

$$\partial_t U + \partial_i F^i(U) = S, \quad (1)$$

where U denotes the conserved quantities, F^i its respective flux, and S an additional source term. The first two can be expressed through primitive fluid variables such as the mass density ρ , the pressure p , the four-velocity u^μ , and specific enthalpy h as

$$U = \begin{pmatrix} D \\ E \\ m^j \end{pmatrix} = \begin{pmatrix} \rho u^0 \\ Dhu^0 - p \\ Dhu^j \end{pmatrix} \quad (2)$$

and

$$F^i(U) = \begin{pmatrix} D u^i / u^0 \\ m^i \\ m^j u^i / u^0 + p \delta^{ij} \end{pmatrix}. \quad (3)$$

In this paper we use the normalisation $c = 1$ and notate the three spatial components of the fluid four-velocity vector as $\mathbf{u} = u^i$ and its Lorentz factor as u^0 . The presented system of five equations in six unknowns is closed by an additional equation of state. For now we employ an ideal equation of state,

$$h(\rho, p) = 1 + \frac{\Gamma}{\Gamma - 1} \frac{p}{\rho}, \quad (4)$$

where $\Gamma = 4/3$ is the constant adiabatic exponent of the fluid, as this was found to have only a negligible effect on the resulting fluid structure with respect to more sophisticated ones ([Bosch-Ramon et al. 2015](#)).

In our simulation, we employed the HLLC solver ([Mignone & Bodo 2005](#)) alongside a second-order sub-grid reconstruction using a MINMOD slope limiter. To further increase the stability and robustness of our simulation, we directly evolved $\tau = E - D$, which replaces the energy equation, and solved an additional conservation equation for the specific entropy $s = p/\rho^\Gamma$ used in smooth flows,

$$\partial_t(sD) + \partial_i(sDu^i/u^0) = 0. \quad (5)$$

2.1.1. Wind injection

The stellar and pulsar wind were injected in the simulation by prescribing a solution in a spherical region with radius r_{inj} of the domain. Inside each wind injection volume, we prescribed the solution as

$$\rho(\mathbf{r}) = \frac{\dot{M}}{4\pi r^2 u}, \quad \mathbf{u}(\mathbf{r}) = u \mathbf{e}_r, \quad p(\mathbf{r}) = 10^{-6} \rho(\mathbf{r}), \quad (6)$$

where $\mathbf{r}$ denotes the vector originating at the injection centre to a given point in space, $\dot{M}$ the mass injection rate, and u the four-speed of the injected wind. We kept the wind speed constant at its terminal velocity over the whole injection volume. The density gradient was scaled such that the prescribed mass-loss rate was recovered for every spherical shell inside the injection region. Because the effect of thermal pressure is neglected in our simulation, it was set to a low value scaled with the density gradient in order to keep the corresponding temperature constant.

In simulations of gamma-ray binaries, it is common practice to prescribe the pulsar mass-loss rate through the ratio η of the total momentum. The pulsar mass-loss rate can hence be obtained by

$$\dot{M}_p = \eta \frac{\dot{M}_s u_s}{u_p}, \quad (7)$$

where quantities indicated with p and s belong to the pulsar and star, respectively.

In practice, the injection was realised by resetting the states of the respective cells after every time-step with those computed from the prescribed solution. A cell was treated as part of the star or pulsar, respectively, when its centre was within a spherical volume of given radius r_{inj} around the star or pulsar location.

2.1.2. Orbital motion

To account for the orbital motion, the wind injection volumes were relocated after every step of the simulation to their respective position on the Keplerian orbit. In standard approaches, the system is treated in the laboratory frame (see e.g. [Bosch-Ramon et al. 2012](#)). In our approach, we treat the binary in a frame corotating with the average angular velocity of the system as described in Appendix A. This has the advantage that the vector connecting the two companions remains fixed for circular orbits instead of performing full rotations. For mildly eccentric orbits, this translates into an oscillation in a narrow angular range. Consequently, the wind injection volumes have to be relocated by a smaller amount than in the laboratory frame, which increases the stability of the simulation by avoiding unphysical conditions upon relocation.

Furthermore, because the binary motion is restricted, the orientation of the WCR is also restricted. This allows saving computational effort by reducing the simulation volume behind the star as seen from the centre of mass because we are mostly interested in the cometary tail-like downstream of the WCR behind the pulsar.

2.2. Particle transport

The particle transport equation for cosmic rays has been presented in the relativistic case by [Webb \(1989\)](#). It takes the following form:

$$0 = \nabla_\mu (u^\mu f'_0 + q^\mu) + \frac{1}{p^2} \frac{\partial}{\partial p'} \left[-\frac{p'^3}{3} \nabla_\mu u^\mu f'_0 + p' \dot{\text{loss}} p'^2 f'_0 - \Gamma_{\text{visc}} p'^4 \tau \frac{\partial f'_0}{\partial p'} - p'^2 D_{pp} \frac{\partial f'_0}{\partial p'} - p' (p'^0)^2 \dot{u}_\mu q^\mu \right], \quad (8)$$

where $f'_0(x^\mu, p')$ is the isotropic part of the particle phase space density. All primed quantities are given in the fluid frame. The first term describes passive advection with the fluid bulk motion u^μ and spatial diffusion with the heat flux q^μ . The other terms in square brackets describe the transport in momentum space. From left to right, they correspond to adiabatic losses or gains, generic momentum losses (e.g. from radiative processes), viscous shear acceleration, the second-order Fermi process, and losses due to non-inertial frame changes. Following [Vaidya et al. \(2018\)](#), we neglected (for the purpose of this paper) spatial diffusion ($q^\mu = 0$), viscous shear-acceleration ($\Gamma_{\text{visc}} = 0$), and momentum diffusion ($D_{pp} = 0$). Because we assume the ultra-relativistic limit, the particle Lorentz factor can be readily obtained as $\gamma \approx p'/m$, leading us to define $N'(x^\mu, \gamma') = 4\pi p'^2 f'_0 m$, with $N' dV' d\gamma'$ corresponding to the number of particles within a volume dV' in the range $[\gamma', \gamma' + d\gamma']$. According to our assumptions and substitutions, we obtain the simplified transport equation

$$\nabla_\mu (u^\mu N') + \frac{\partial}{\partial \gamma'} \left[\underbrace{\left(-\frac{\gamma'}{3} \nabla_\mu u^\mu + \dot{\gamma}'_{\text{rad}} \right)}_{=\langle \frac{d\gamma'}{dt} \rangle} N' \right] = 0, \quad (9)$$

with $\langle \frac{d\gamma'}{dt} \rangle$ being the total energy loss rate in the fluid frame. We now consider electrons and positrons in the particle

transport because accelerated nuclei are thought to not contribute efficiently to the overall emission (e.g. [Bosch-Ramon & Khangulyan 2009](#)).

2.2.1. Implementation

Following [Reitberger et al. \(2014\)](#), we implemented the transport equation Eq. (9) within CRONOS by employing a splitting scheme that separates the problem into a spatial and an energy part,

$$\partial_t (u^0 N') + \nabla_i (u^i N') = 0 \quad (10)$$

$$\partial_t (u^0 N') + \partial_{\gamma'} \left(\left\langle \frac{d\gamma'}{dt} \right\rangle N' \right) = 0. \quad (11)$$

Both parts are treated independently and sequentially one after the other. The particle density was discretised in space in the same manner as the fluid variables, while its spectrum was subdivided into spectral bins $[\gamma'_{l-1/2}, \gamma'_{l+1/2}]$. In our implementation, we allow the user to specify the limits of the simulated spectral range, that is, the first and the last edge $\gamma'_{-1/2}, \gamma'_{N_\gamma-1/2}$, and the number of spectral bins N_γ . The range was then subdivided into logarithmic bins with

$$\gamma'_{l-1/2} = \gamma'_{-1/2} \left(\frac{\gamma'_{N_\gamma-1/2}}{\gamma'_{-1/2}} \right)^{l/N_\gamma}, \quad \text{for } l \in \{0, \dots, N_\gamma\}. \quad (12)$$

The cell centre γ'_l is then obtained as the arithmetic mean of its limits.

Averaging Eq. (10) over the l -th energy bin yields the finite-volume version of the spatial particle transport,

$$\nabla_\mu (u^\mu N'_l) = 0 \quad (13)$$

with the cell averages $N'_l = \Delta \gamma'^{-1}_l \int_{\gamma'_{l-1/2}}^{\gamma'_{l+1/2}} N' d\gamma'$ and $\Delta \gamma'_l = \gamma'_{l+1/2} - \gamma'_{l-1/2}$. The spatial particle distribution corresponding to a given spectral bin can therefore be represented by an additional three-dimensional scalar field N'_l . The spatial transport, amounting to a mere spatial convection, is solved directly by the hydrodynamic solver similar to the mass continuity equation (the first component in Eq. (1)).

Averaging Eq. (11) over a spatial cell with index i, j, k , and treating the fluid variables as constant in time yields

$$\partial_t N'_{i,j,k} + \partial_{\gamma'} \left(\frac{1}{u^0} \left\langle \frac{d\gamma'}{dt} \right\rangle N'_{i,j,k} \right) = 0, \quad (14)$$

where $N'_{i,j,k}$ is the spatial cell average of the differential particle number density at a certain energy. The spectral evolution of the particle distribution can therefore be viewed as an advection in energy with energy-dependent velocity $\dot{\gamma}' = \langle \frac{d\gamma'}{dt} \rangle / u^0$.

The evolution in energy was treated independently for each spatial cell by a semi-Lagrangian solver in analogy to the one presented by [Zerroukat et al. \(2006\)](#), which we detail in the following. For better readability, we omit in the following the prime and the indices on the particle number density $N \equiv N'_{i,j,k}$ and the particle Lorentz factor $\gamma \equiv \gamma'$. We can show that the absolute number of particles in the energy range $[\gamma_-(t), \gamma_+(t)]$ remains constant if the limits $\gamma_\pm(t)$ satisfy the characteristic equation

$$\frac{d}{dt} \gamma = \dot{\gamma}(\gamma), \quad (15)$$

which can be exploited to construct a conservative and explicit update scheme for the particle number densities.

We obtained the particle number density N_l^{n+1} at the next timestep t^{n+1} by first considering where the particles inside the bin were advected from, that is, in which γ -range they were at time step t^n . This was done by performing a backward integration of the bin edges $\gamma_{l\pm 1/2}$ following Eq. (15) to identify the corresponding values $\gamma_{l\pm 1/2}^n$ at time t^n (denoting propagated edges with a superscript). Equation (15) was solved numerically using a second-order explicit Runge-Kutta method, for example Ralston's method, with the time step provided by the RHD solver.

After the interval edges $\gamma_{l\pm 1/2}^n$ were identified, the updated number density was obtained using particle conservation

$$\Delta\gamma_l N_l^{n+1} = \int_{\gamma_{l-1/2}^n}^{\gamma_{l+1/2}^n} N^n d\gamma = I^n[\gamma_{l+1/2}^n] - I^n[\gamma_{l-1/2}^n], \quad (16)$$

where $I^n[\gamma]$ denotes the cumulative particle count up to a value γ , for the spectrum at time t^n (see also Eq. (19)). To approximate the integral, we considered a second-order, piece-wise linear reconstruction in energy in each cell, in analogy to the spatial reconstruction in the hydrodynamics part,

$$N^n(\gamma) = N_l^n + \delta_l^n(\gamma - \gamma_l), \quad (17)$$

with $\gamma_{l-1/2} < \gamma < \gamma_{l+1/2}$. Here, δ_l^n denotes the slope of the reconstruction obtained after applying the van Leer limiter (van Leer 1977),

$$\delta_{\text{vanLeer}} = \frac{\max(\delta^+ \delta^-, 0)}{\delta^C}, \quad (18)$$

to the right-, left-, and two-sided finite differences, denoted by δ^+ , δ^- , and δ^C , respectively. With this, the integral can be approximated directly as piecewise parabolas by

$$\begin{aligned} I^n[\gamma] &= \int_{\gamma_{-1/2}}^{\gamma} N^n(\tilde{\gamma}) d\tilde{\gamma} \\ &\approx I^n[\gamma_{l-1/2}] + (N_l^n - \delta_l^n \gamma_l) h_\gamma + \frac{\delta_l^n}{2} h_\gamma^2, \end{aligned} \quad (19)$$

with $\gamma_{l-1/2} < \gamma < \gamma_{l+1/2}$, $h_\gamma = \gamma - \gamma_{l-1/2}$, and the exact integrals at the cell edges,

$$I^n[\gamma_{l-1/2}] = \int_{\gamma_{-1/2}}^{\gamma_{l-1/2}} N^n d\gamma = \sum_{j=0}^{l-1} \Delta\gamma_j N_j^n, \quad (20)$$

where $\gamma_{-1/2}$ is the lower edge of the first spectral bin $l = 0$.

On either end of the energy grid, we employed outflowing boundary conditions, ensuring that particles cannot be gained but only lost through the boundaries. This was realised by setting the particle number density to zero outside the energy domain, which amounts to a constant extrapolation of I^n in the evaluation of the right-hand side of Eq. (16). To determine the slope of the first and last spectral bin according to Eq. (18), we added a ghost-cell at either end of the spectrum (with $l = -1$ and $l = N_\gamma$, using Eq. (12)), and set the cell values to zero.

2.2.2. Magnetic field model

For the purpose of this work, we employed a simplified magnetic field model. We assumed the magnetic field to be amplified by plasma instabilities to a fraction ζ_b of the available internal

energy. This fraction was kept constant throughout the simulation (see also Dubus et al. 2015; Barkov & Bosch-Ramon 2018). The strength of the post-shock magnetic field B' in the fluid frame can therefore be expressed as

$$\frac{B'^2}{2\mu_0} = \zeta_b \frac{p}{\Gamma - 1}. \quad (21)$$

We assumed no direction on the magnetic field.

2.2.3. Radiative losses

As energy-loss processes for the accelerated electron-positron pairs we considered synchrotron and inverse-Compton losses. The energy-loss rates are given by

$$\dot{\gamma}'_{\text{syn}} = \frac{4}{3} \frac{\sigma_T}{m_e c} w'_B w'_\gamma \gamma'^2 \quad (22)$$

$$\dot{\gamma}'_{\text{ic}} = \frac{4}{3} \frac{\sigma_T}{m_e c} w'_{\text{rad}} \gamma'^2 F_{\text{KN}}(\epsilon'_0, \gamma'), \quad (23)$$

with w'_B and w'_{rad} being the magnetic and radiative energy densities in the fluid frame, respectively, and F_{KN} the Klein-Nishina factor.

The magnetic field in the fluid frame can be readily obtained by the transformation

$$\mathbf{B}' = \frac{1}{u^0} \left[\mathbf{B} + \frac{\mathbf{B} \cdot \mathbf{u}}{u^0 + 1} \mathbf{u} \right]. \quad (24)$$

The corresponding magnetic field strength is therefore given by

$$B' = \frac{1}{u^0} \sqrt{B^2 + (\mathbf{B} \cdot \mathbf{u})^2}, \quad (25)$$

yielding the magnetic energy density $w'_B = \frac{B'^2}{2\mu_0}$. For disordered magnetic fields, that is, when no information on the magnetic field orientation is available, we dropped the term containing $\mathbf{B} \cdot \mathbf{u}$ in Eq. (25) (see Dubus et al. 2015).

For the inverse-Compton losses, we assumed the radiation field to be monochromatic and mono-directional. The energy density of a beam of photons with direction Ω_0 is given in the fluid frame by Doppler boosting the laboratory energy density,

$$w'_{\text{rad}} = \mathcal{D}_{u\Omega_0}^{-2} w_{\text{rad}}, \quad (26)$$

with the Doppler factor $\mathcal{D}_{u\Omega_0} = (u^0 - \mathbf{u} \cdot \Omega_0)^{-1}$. The radiation field relevant for the inverse-Compton losses emerges from the stellar binary companion,

$$w_{\text{rad}} = \frac{L_{\text{star}}}{4\pi r_{\text{star}}^2 c}, \quad (27)$$

where r_* is the distance to the star and L_* its luminosity. We employed the Klein-Nishina factor following Moderski et al. (2005),

$$\begin{aligned} F_{\text{KN}}(\tilde{b}') &= \frac{9}{\tilde{b}'^3} \left[\left(\frac{1}{2} \tilde{b}' + 6 + \frac{6}{\tilde{b}'} \right) \log(1 + \tilde{b}') + 2\text{Li}_2(-\tilde{b}') \right. \\ &\quad \left. - \left(\frac{11}{12} \tilde{b}'^3 + 6\tilde{b}'^2 + 9\tilde{b}' + 4 \right) \cdot (1 + \tilde{b}')^{-2} - 2 \right], \end{aligned} \quad (28)$$

assuming an isotropic seed photon and electron distribution for simplicity, with $\tilde{b}' = 4\epsilon'_0 \gamma' (m_e c^2)^{-1}$ and $\epsilon'_0 = \mathcal{D}_{u\Omega_0}^{-1} \epsilon_0$ denoting the Doppler-boosted photon energy of the stellar radiation field.

2.2.4. Particle injection

Strong shocks are commonly regarded as sites for particle acceleration, where we expect a fraction of pairs from the pulsar wind to be accelerated to high energies. However, because the converging fluid flow is the principal driver for several acceleration processes, we generally consider that strongly compressive flows participate in the acceleration. In the simulation, we identified these sites using the criterion

$$\nabla_\mu u^\mu < \delta_{\text{sh}}, \quad (29)$$

with a typical value of $\delta_{\text{sh}} = -10 \text{ c/AU}$ to ignore weakly converging flows (see also Appendix C for a comparison to a common shock-identification criterion).

In the identified cells we injected two populations of pairs: thermal pairs from the cold pulsar wind that are isotropised, following a Maxwellian distribution; and non-thermal accelerated pairs, following a power-law spectrum (similar to Dubus et al. 2015), which are parametrised as

$$\mathcal{N}^{\text{MW}} = K^{\text{MW}} \gamma^2 \exp(-\gamma/\gamma_t) \quad (30)$$

$$\mathcal{N}^{\text{PL}} = K^{\text{PL}} \gamma^{-s} \quad \text{for } \gamma_{\text{min}}^{\text{PL}} < \gamma < \gamma_{\text{max}}^{\text{PL}} \mathcal{N}^{\text{MW}} \quad (31)$$

The maximum Lorentz factor $\gamma_{\text{max}}^{\text{PL}}$ for the power law is determined by the balance between acceleration and radiative losses. The acceleration timescale is given by a multiple of the gyration time of the particle $\tau_{\text{acc}} = 2\pi R_L / c\xi_{\text{acc}}$ with the Larmor radius $R_L = \frac{\gamma m}{eB'}$ and the acceleration efficiency ξ_{acc} . We assumed synchrotron losses to be dominant for the particles at highest energies. Together with the loss timescale $\tau_{\text{loss}} = \gamma'/\dot{\gamma}'$ given by Eq. (22), this yields the maximum particle Lorentz factor expected at the current location,

$$\gamma_{\text{max}}^{\text{PL}} = \sqrt{\frac{3}{4\pi} \frac{\mu_0 e c}{\xi_{\text{acc}} \sigma_T B'}} \approx 4.65 \times 10^7 \sqrt{\frac{1 \text{ G}}{\xi_{\text{acc}} B'}}. \quad (32)$$

Because the dominant particle acceleration mechanism in gamma-ray binaries could not be clearly identified, we took a generic phenomenological approach and treated both the spectral index s and the acceleration efficiency ξ_{acc} as free parameters of the model (similar to Dubus et al. 2015; Molina & Bosch-Ramon 2020).

The average Lorentz factor of the Maxwellian γ_t , the lower cutoff of the power-law spectrum γ_{min} , and both normalisations K^{PLMW} were determined from fluid properties. This was controlled by three free parameters: ζ_n^{PL} the fraction of accelerated non-thermal pairs, ζ_e^{PL} the fraction of internal energy converted to non-thermal pairs, and ζ_p to account for the pulsar wind speed, which might be too low in our simulation and result in an over-estimation of the particle number density in the pulsar wind. The respective fractions for the Maxwellian are then readily given by $\zeta_n^{\text{MW}} = 1 - \zeta_n^{\text{PL}}$ and $\zeta_e^{\text{MW}} = 1 - \zeta_e^{\text{PL}}$. In our simulation, we kept all injection parameters constant in time and space. The injected spectra are therefore related to fluid quantities by

$$\int_{\gamma_{\text{min}}^{\text{PLMW}}}^{\gamma_{\text{max}}^{\text{PLMW}}} \mathcal{N}^{\text{PLMW}}(\gamma) d\gamma = \underbrace{\zeta_n^{\text{PLMW}} \zeta_p \psi_p \rho / m_e}_{=: \mathcal{N}^{\text{PLMW}}} \quad (33)$$

$$\int_{\gamma_{\text{min}}^{\text{PLMW}}}^{\gamma_{\text{max}}^{\text{PLMW}}} \gamma m_e c^2 \mathcal{N}^{\text{PLMW}}(\gamma) d\gamma = \underbrace{\zeta_e^{\text{PLMW}} \psi_p e_{\text{thermal}}}_{=: e^{\text{PLMW}}}, \quad (34)$$

where $0 < \psi_p < 1$ is a passive tracer indicating the fraction of pulsar wind material and the thermal energy density $e_{\text{thermal}} = \frac{p}{\Gamma-1}$ given by the fluid pressure.

For the non-thermal particles, the above expressions yield an implicit equation for $\gamma_{\text{min}}^{\text{PL}}$, which was solved numerically by a standard root-finding algorithm. The injection normalisation K^{PL} was then determined from Eq. (33). When the internal fluid energy was too low,

$$\int_{\gamma_{\text{min}}^{\text{PL}}}^{\gamma_{\text{max}}^{\text{PL}}} \gamma m_e c^2 \mathcal{N}^{\text{PL}}(\gamma) d\gamma > e^{\text{PL}}, \quad (35)$$

we did not inject particles in the given cell.

For the Maxwellian, Eqs. (33) and (34) can be inverted analytically in the limit $\gamma_t \gg 1$ using $\gamma_{\text{min}}^{\text{MW}} = 1$ and $\gamma_{\text{max}}^{\text{MW}} = \infty$, yielding

$$\gamma_t = \frac{1}{3} \frac{e^{\text{MW}}}{n^{\text{MW}} m_e c^2}, \quad K^{\text{MW}} = \frac{n^{\text{MW}}}{2\gamma_t^3}. \quad (36)$$

2.3. Emission

The particle distributions resulting from a joint hydrodynamic and particle-transport simulation (as detailed in Sects. 2.1 and 2.2) were used in a post-processing step to predict the expected emission. In this section, we elaborate on the calculations of the emission and their implementation.

The involved radiative processes are again synchrotron (Sect. 2.3.1) and inverse-Compton emission (Sect. 2.3.2). Furthermore, the produced fluxes were modified by $\gamma\gamma$ -absorption on photons of the stellar radiation field depending on the location of the emitter (Sect. 2.3.3). For the sake of better readability, we omit the dependence on the location $\mathbf{x}$ when it is not imperative.

We formulated the emission in the fluid frame, represented by primed quantities, and then related it to the laboratory frame with a Doppler boost. The spectral emissivity j_ϵ , that is, the emitted power per unit photon energy per unit solid angle per unit volume, for a given emitted photon energy ϵ and direction Ω is hence given by

$$j_\epsilon(\epsilon, \Omega) = \mathcal{D}_{u\Omega}^2 j'_\epsilon(\epsilon', \Omega'), \quad (37)$$

where $\mathcal{D}_{u\Omega} = (u^0 - \Omega \cdot \mathbf{u})^{-1}$ is the corresponding Doppler factor. The respective energy and direction of the emitted photons are given in the fluid frame by

$$\epsilon' = \mathcal{D}_{u\Omega}^{-1} \epsilon, \quad \Omega' = \mathcal{D}_{u\Omega} \left[\Omega + \left(\frac{\Omega \cdot \mathbf{u}}{u^0 + 1} - 1 \right) \mathbf{u} \right]. \quad (38)$$

Furthermore, it is convenient to express the spectral emissivity in terms of the emission produced by a single electron $\mathcal{P}'(\epsilon', \Omega', \gamma')$, that is, the emitted power per unit photon energy per unit solid angle per electron under the assumption of an isotropic distribution of particles in the fluid frame. The spectral emissivity can then be formulated as

$$j'_\epsilon(\epsilon', \Omega') = \int \mathcal{P}'(\epsilon', \Omega', \gamma') \mathcal{N}' d\gamma'. \quad (39)$$

2.3.1. Synchrotron emission

The total power emitted by a single electron in a magnetic field B' can be expressed as

$$\mathcal{P}'^{\text{tot}}_{\text{syn}}(\epsilon', \gamma') = \frac{\sqrt{3}e^3}{8\pi^2 \epsilon_0 m_e c \hbar} B'_{\perp} F\left(\frac{\epsilon'}{\epsilon'_c}\right), \quad (40)$$

which is peaked around the critical photon energy,

$$\epsilon'_c = \frac{3e\hbar}{2m_e} B'_\perp \gamma'^2 = 1.74 \times 10^{-8} \text{ eV} \frac{B'_\perp}{1 \text{ G}} \gamma'^2. \quad (41)$$

$B'_\perp = B' \sin(\alpha)$ denotes the magnetic field component perpendicular to the electron motion, which gyrates with a pitch angle α around the magnetic field lines. For ultra-relativistic electrons, the emission is strongly beamed in their instantaneous direction of motion (within a cone of angle $1/\gamma'$). Only particles whose pitch angle coincides with the angle between the magnetic field $\mathbf{B}'$ and the line of sight $\mathbf{\Omega}'$ therefore contribute to the emission, effectively yielding $B'_\perp = |\mathbf{B}' \times \mathbf{\Omega}'|$. Together with the assumption of an isotropic particle distribution, this yields

$$\mathcal{P}'_{\text{syn}}(\epsilon', \mathbf{\Omega}', \gamma') = \frac{\sqrt{3}e^3}{32\pi^3 \epsilon_0 m_e c \hbar} B'_\perp F\left(\frac{\epsilon'}{\epsilon'_c}\right). \quad (42)$$

In many cases, we approximated the magnetic field to be disordered, that is, we have no information on the direction of the field lines. In this case, we approximated the $B'_\perp$ in Eqs. (41), (42) by its pitch-angle average $\bar{B}'_\perp = \frac{\pi}{4} B'$.

2.3.2. Inverse-Compton emission

Through the inverse-Compton process, photons of the stellar radiation field are scattered to gamma-ray energies by highly energetic particles. Following the description of [Moderski et al. \(2005\)](#), the power emitted through this process is given by

$$\mathcal{P}'_{\text{ic}}(\epsilon', \mathbf{\Omega}', \gamma') = \epsilon' \frac{\partial \dot{N}'_{\text{sc}}}{\partial \epsilon' \partial \mathbf{\Omega}'}, \quad (43)$$

where $\frac{\partial \dot{N}'_{\text{sc}}}{\partial \epsilon' \partial \mathbf{\Omega}'}$ is the scattering rate of photons on isotropically distributed electrons. The scattering rate was presented by [Aharonian & Atoyan \(1981\)](#) in the case of $\epsilon' \gg \epsilon'_0$ and $\gamma' \gg 1$ taking the form

$$\frac{\partial \dot{N}'_{\text{sc}}}{\partial \epsilon' \partial \mathbf{\Omega}'} = \frac{3}{16\pi} c \sigma_T \frac{1}{\gamma'^2} \iint_{\epsilon'_{0,\min}}^{\infty} f_{\text{ic}}(\epsilon', \epsilon'_0, \gamma', \mu') \frac{n'_{\epsilon'_0}(\epsilon'_0, \mathbf{\Omega}'_0)}{\epsilon'_0} d\epsilon'_0 d^2\Omega'_0, \quad (44)$$

where $n_0(\epsilon_0, \mathbf{\Omega}_0)$ is the density of the seed photons with energy ϵ_0 and direction $\mathbf{\Omega}_0$ and $\epsilon'_{0,\min}$ the lowest seed photon energy that is still scattered to a given energy ϵ' and direction $\mathbf{\Omega}'$

$$\epsilon'_{0,\min} = \epsilon' \left[2(1 - \mu')(1 - \frac{\epsilon'}{\gamma' m_e c^2}) \right]^{-1}. \quad (45)$$

The scattering kernel f_{ic} is given by

$$f_{\text{ic}}(\epsilon', \epsilon'_0, \gamma', \mu') = 1 + \frac{w'^2}{2(1 - w')} - \frac{2w'}{b'_\mu(1 - w')} + \frac{2w'^2}{b'^2_\mu(1 - w')^2}, \quad (46)$$

with $b'_\mu = 2(1 - \mu')\epsilon'_0\gamma'(m_e c^2)^{-1}$, $w' = \epsilon'(\gamma' m_e c^2)^{-1}$ and the cosine of the scattering angle $\mu' = \mathbf{\Omega}' \cdot \mathbf{\Omega}'_0$, which can be expressed in terms of laboratory quantities by

$$\mu' = 1 + \mathcal{D}_{\mathbf{\Omega}\mathbf{\Omega}_0} \mathcal{D}_{\mathbf{\Omega}\mathbf{\Omega}'} (\mu - 1). \quad (47)$$

Together with the relativistic invariant $\frac{n'_{\epsilon'_0}}{\epsilon'^0} d\epsilon'_0 d^2\Omega'_0 = \frac{n_{\epsilon_0}}{\epsilon_0} d\epsilon_0 d^2\Omega_0$ Eq. (44) can be expressed directly in terms of the seed photon field in the laboratory frame,

$$\frac{\partial \dot{N}'_{\text{sc}}}{\partial \epsilon' \partial \mathbf{\Omega}'} = \frac{3}{16\pi} c \sigma_T \frac{1}{\gamma'^2} \iint_{\epsilon_{0,\min}}^{\infty} f(\epsilon', \epsilon_0, \gamma', \mu') \frac{n_{\epsilon_0}(\epsilon_0, \mathbf{\Omega}_0)}{\epsilon_0} d\epsilon_0 d^2\Omega_0. \quad (48)$$

Applying the factorisation of the target photon field (Appendix B) yields

$$\frac{\partial \dot{N}'_{\text{sc}}}{\partial \epsilon' \partial \mathbf{\Omega}'} = \frac{3}{16\pi} c \sigma_T \frac{1}{\gamma'^2} g_n(\mathbf{x}) \int g_{\Omega}(\mathbf{\Omega}_0) \int_{\epsilon_{0,\min}}^{\infty} f(\epsilon', \epsilon'_0, \gamma', \mu') \frac{g_{\epsilon}(\epsilon_0)}{\epsilon_0} d\epsilon_0 d^2\Omega_0, \quad (49)$$

which can be further simplified depending on the employed radiation field model.

2.3.3. $\gamma\gamma$ -absorption

As a result of the strong stellar photon field, parts of the VHE gamma-ray flux produced through inverse-Compton scattering are significantly attenuated by $\gamma\gamma$ -pair creation. This effect depends strongly on the geometry of the system and the location of the observer, yielding strongly modulated spectra with the binary orbit. For a consistent model of gamma-ray binary emission, this attenuation has to be taken into account for every cell in our simulation.

The absorption opacity $\tau_{\gamma\gamma}$ of photons with energy ϵ originating at $\mathbf{x}$ in direction $\mathbf{\Omega}$ can be expressed by a three-fold integration of the differential absorption opacity given by [Gould & Schröder \(1967\)](#),

$$d\tau_{\gamma\gamma} = (1 - \mu) \sigma_{\gamma\gamma}(\beta) n_{\epsilon_0}(\mathbf{x}, \epsilon_0, \mathbf{\Omega}_0) dl d^2\Omega_0 d\epsilon_0, \quad (50)$$

over the line of sight l , the solid angle Ω_0 , and the seed photon energy ϵ_0 . Here, $\mu = \mathbf{\Omega} \cdot \mathbf{\Omega}_0$ denotes the scattering angle cosine between a VHE photon with direction $\mathbf{\Omega}$ and a seed UV photon with direction $\mathbf{\Omega}_0$, $\beta^2 = 1 - \frac{m_e^2 c^4}{\epsilon \epsilon_0} \frac{2}{1 - \mu}$ the speed of the created $e^\pm$ pair normalised to c and $\sigma_{\gamma\gamma} = \frac{3}{16} \sigma_T f_{\gamma\gamma}(\beta)$ the scattering cross-section with

$$f_{\gamma\gamma}(\beta) = (1 - \beta^2) \left[(3 - \beta^4) \log\left(\frac{1 + \beta}{1 - \beta}\right) - 2\beta(2 - \beta^2) \right]. \quad (51)$$

The lower bound of the energy integration is provided by the lowest seed photon energy $\epsilon_{0,\min} = \frac{m_e^2 c^4}{\epsilon} \frac{2}{1 - \mu}$ to create an $e^\pm$ pair under a given scattering angle. The stellar seed photon density n_{ϵ_0} is defined in the same way as in Sect. 2.3.2.

For numerical purposes, it is more suitable to transform the occurring improper integrals into proper ones. For the line-of-sight integration, we therefore used the transformation $l = d_0 \frac{\sin(\psi - \psi_0)}{\sin(\psi)}$ (as detailed in [Dubus 2006](#)). The integration over target photon energy ϵ_0 was transformed into an integral over the speed of the created pairs β . Together with the radiation field factorisation (Appendix B), this yields

$$\tau_{\gamma\gamma} = \frac{3}{16} \sigma_T \int_{\psi_0}^{\pi} \frac{dl}{d\psi} g_n(\mathbf{x}') \int (1 - \mu) g_{\Omega}(\mathbf{x}', \mathbf{\Omega}_0) \int_0^1 \frac{d\epsilon_0}{d\beta} g_{\epsilon}(\mathbf{x}', \epsilon_0) f_{\gamma\gamma}(\beta) d\beta d^2\Omega_0 d\psi, \quad (52)$$

which can be further simplified depending on the stellar radiation field model.

The integration over solid angle Ω_0 is approximated by a nested quadrature rule with equidistant points in azimuth and a Gauss-Legendre quadrature in the polar angle (see [Hesse & Womersley 2012](#)). For the integrals over ψ and β , we employed standard Gauss-Legendre quadratures. The necessary routines are provided by the GSL.

3. Application to a generic binary

In the following section, we apply the presented numerical model to a generic binary system. We focus on exploring the general properties of our model.

The considered binary is composed of an O-type star in a circular ($e = 0$) 1 d orbit with a pulsar at an orbital separation of $d = 0.2$ AU. We adopted a stellar mass-loss rate of $\dot{M}_s = 2 \times 10^{-8} M_\odot \text{ yr}^{-1}$ launched at a velocity of $v_s = 2000 \text{ km s}^{-1}$. The pulsar wind was injected at a speed of $v_p = 0.99c$ and a mass-loss rate scaled with $\eta = 0.1$ in Eq. (7).

The simulation was performed on a Cartesian grid in corotating coordinates (as detailed in Sect. 2.1.2). The computational volume has the dimensions $[-0.4, 0.4] \times [-0.2, 0.6] \times [-0.2, 0.2] \text{ AU}^3$ and is homogeneously subdivided into $256 \times 256 \times 128$ spatial cells. The binary orbits in the $x-y$ plane, with the stellar companion residing at the coordinate origin.

The stellar and pulsar winds are injected as described in Sect. 2.1.1 with an injection radius of four cell widths. Initially, both injection volumes were placed in a vacuum. We ran the simulation for 0.58 d giving the slow stellar wind time to populate the computational domain.

3.1. Fluid structure

In Fig. 1 we show the resulting fluid mass, bulk four-speed, and magnetic field strength in the fluid frame, using the magnetic field model as described in Sect. 2.2.2 with $\zeta_b = 0.5$. The interaction of the stellar and pulsar wind gives rise to an extended WCR delimited by shocks on both the stellar and the pulsar side. Through the Coriolis force in the rotating system, the WCR is highly asymmetric and bends in the direction opposite to the orbital motion. This leads to the termination of the pulsar wind on the far side of the system, forming another shock at the Coriolis turnover (hereafter Coriolis shock). The location of the Coriolis shock was noted previously and is consistent with previous studies (see e.g. Bosch-Ramon et al. 2015; Dubus et al. 2015). In the wings of the WCR, the shocked pulsar wind is reaccelerated to a Lorentz factor ~ 3 , again in agreement with previous simulations by Bogovalov et al. (2008).

The strong velocity shear between the shocked winds at the contact discontinuity and the steep density gradient at the stellar wind shock leads to the development of fluid instabilities (see also Bosch-Ramon et al. 2012). As a consequence, many secondary shocks are formed in the turbulent regions.

3.2. Particle distribution

To economise on computation time, we did not perform a particle transport simulation for the full time span used in Sect. 3.1. Instead, we restarted such a simulation on a preconverged fluid solution and ran it for a shorter time span $t = 0.029$ d, allowing the accelerated electron-positron pairs to populate the system, which we also refer to as electrons for brevity.

The simulation presented in this section was carried out using 50 logarithmic bins in energy ranging from $\gamma \in [200, 4 \times 10^8]$. The particle injection was controlled as detailed in Sect. 2.2.4 using $\zeta_p = 5 \times 10^{-4}$, $\zeta_n^{\text{PL}} = 5 \times 10^{-3}$, $\zeta_e^{\text{PL}} = 0.5$, $s = 2$, and $\xi_{\text{acc}} = 1$, assuming the maximum acceleration timescale at the Bohm limit.

In Fig. 2 we present the resulting electron distributions at two energies. The shock structure leaves a clear imprint on the particle distribution. This is especially visible for higher energetic electrons, which remain much more confined to their accelera-

Fig. 1. Resulting fluid structure for a generic binary system in the orbital plane. *From top to bottom:* fluid mass density, bulk speed, and magnetic field strength in the fluid frame. An extended WCR is formed by interaction of the pulsar (blue) and stellar (orange) wind. The reference frame is corotating with counter-clockwise orbital motion. The location of the most relevant shocks is annotated.

tion site due to increased energy-loss rates, as compared to lower energetic electrons. Next to the bow and Coriolis shocks, the secondary shocks arising in the turbulent flow are clearly visible, which are for the first time consistently accounted for in the particle transport.

In Fig. 3 we show the spectral energy distribution of electrons integrated over the computational volume. The contributions of the Maxwellian and the power-law electrons can be easily distinguished, with Maxwellian electrons dominating the low-energy part ($\gamma \lesssim 2 \times 10^4$) and the non-thermal electrons the high-energy part. For the chosen set of parameters, Maxwellian electrons were on average injected with $\gamma_i \sim 1.0 \times 10^3$ and

Fig. 2. Differential particle number density for the energy bin centred at $\gamma = 4.2 \times 10^3$ (upper panel) and $\gamma = 1.1 \times 10^7$ (lower panel) in analogy to Fig. 1. The lower energetic distribution is mainly populated by Maxwellian electrons, whereas the higher energetic distribution is dominated by power-law electrons. For clarity we show only five orders of magnitude below the highest value. The blue regions correspond to those with lower values.

Fig. 3. Spectral energy distribution of accelerated electrons integrated over the computational domain for different orbital phases.

non-thermal electrons within the limits of $\gamma_{\min} \sim 1.1 \times 10^5$ and $\gamma_{\max} = 2.4 \times 10^7$.

The number and extent of particle acceleration sites identified in the turbulent Coriolis shock downstream region were determined by the chosen compression threshold in Eq. (29) (see also Appendix C). The particles accelerated in this region reach higher energies because the magnetic field is lower than in regions near the bow shock. Choosing a more restrictive thresh-

Fig. 4. Spectral energy distribution of the emission predicted by our model for a generic binary with a system inclination of 30° . The results are shown for the sampled orbital phases (grey) and their average (black). The average spectral distribution is further split into the individual radiative processes: synchrotron (green) and inverse Compton attenuated by $\gamma\gamma$ -absorption (orange). Inferior (dashed red, $\phi = 0$) and superior conjunction (dashed blue, $\phi = 0.5$) emissions are highlighted.

old, that is, one with higher compression, would thus decrease the total number of particles at higher energies in the simulation.

3.3. Emission

In this section, we present the predicted emission for the generic binary. The involved computations were performed in a post-processing step as detailed in Sect. 2.3, using the previously obtained particle distribution (see Sect. 3.2) and fluid solution (see Sect. 3.1).

We chose the observer to be located at a distance of $d_{\text{obs}} = 2.5$ kpc along the $+y$ -axis of the system for the orbital phase $\phi = 0$. The phases $\phi = 0$ and $\phi = 0.5$ therefore correspond to inferior and superior conjunction, respectively. As a result of the employed corotating coordinates, the observer rotates clockwise with respect to the simulation frame. For the present purpose, the underlying particle and fluid solutions were kept constant for all orbital phases.

To compute the inverse-Compton emission, we treated the stellar photon field as monochromatic, whereas for the $\gamma\gamma$ -absorption, a full blackbody spectrum was considered. In both cases, the source was treated as an extended sphere with luminosity $L_\star = 2 \times 10^5 L_\odot$, temperature $T_\star = 40\,000$ K, and resulting radius $R_\star = 9.3 R_\odot$. The emission was computed for a system inclination of $i = 30^\circ$ and 20 equidistant orbital phases.

In Fig. 4 we show the resulting spectral energy distribution of emitted photons. Ranging from X-rays up to LE gamma-rays, the spectrum is dominated by synchrotron emission from electrons at the power-law tail of the spectrum. The same population of electrons is responsible for the inverse-Compton scattering of stellar UV photons to the VHE gamma-ray regime, which are heavily attenuated by $\gamma\gamma$ -absorption in the 0.1–10 TeV range, depending on the orbital phase. Again, the emission in the HE gamma-ray regime is produced through the inverse-Compton process, but by the low-energy Maxwellian electrons.

In our model, the predicted spectra can be tuned most directly by varying the parameters that regulate the emerging electron distributions, that is, the unknown injection parameters and the magnetic field model. Here, the acceleration efficiency ξ_{acc} limits the maximum energy reached $\gamma_{\max}$ (see Eq. (32)), hence affecting the location of the LE and VHE cutoff. The

Fig. 5. Emission light curves predicted by our model for a generic binary for different energy bands and a system inclination of 30° . Inferior and superior conjunction correspond to $\phi = 0$ and $\phi = 0.5$, respectively. For better visualisation, we show the data for two full orbits.

shape of the injected electron spectrum, and consequently, the main emission features, are determined by the electron specific energy density given by the ratio $\zeta_e^{\text{PL,MW}} / (\zeta_\rho \zeta_n^{\text{PL,MW}})$. In the case of the Maxwellian electrons, this can be used to shift the inverse-Compton bump at HE in energy. For the non-thermal power-law electrons, their specific energy density affects the low-energy cutoff of the spectrum. The overall normalisation of the spectrum is given by the amount of energy deposited in the respective populations, determined by $\zeta_e^{\text{PL,MW}}$. The index of the injected electrons translates into the spectral index of the X-ray synchrotron emission and affects the spectral index at VHE gamma-rays. ζ_b is used to control the magnetic field strength in the simulation that affects the amplitude of the synchrotron emission, the VHE cutoff, and the evolution of the electron distribution itself with more subtle consequences for the emission spectra. Because the compression threshold δ_{sh} mostly affects the particle density at highest energies in the turbulent Coriolis shock downstream, this parameter can affect the synchrotron fluxes produced in the LE gamma-ray band, depending on the magnetic field in this region, and the VHE gamma-ray flux at superior conjunction.

In Fig. 5 we show the predicted light curves for different energy bands, which exhibit a significant orbital modulation in all bands. The X-ray and LE gamma-ray light curves show a clear correlation, which is expected because both bands are dominated by synchrotron emission generated by the same particle population. Because we assumed no direction for the magnetic field, the synchrotron emissivity is isotropic in the fluid frame of our model. The driver for the orbital modulation in these bands is accordingly solely given by relativistic boosting. Because the WCR is bent by orbital motion, relativistic boosting is at its maximum at $\phi \sim 0.1$, while deboosting is most significant for $\phi \sim 0.6$.

At HE gamma-rays, the anisotropic inverse-Compton scattering cross-section introduces a further line-of-sight-dependent modulation. The scattering process is most efficient for large

scattering angles, which are achieved at superior conjunction ($\phi = 0.5$). This is reflected in the respective light curve, which reaches its maximum shortly before superior conjunction through the onset of relativistic deboosting, yielding an anti-correlation of the HE gamma-ray band and the previously discussed one.

The VHE gamma-ray emission is again produced by inverse-Compton process, but the upscattered photons are attenuated by $\gamma\gamma$ -pair creation with the stellar photon field. This once more introduces a line-of-sight-dependent modulation that reaches its maximum attenuation at superior conjunction, where the produced VHE photons have to propagate through the entire stellar radiation field. Consequently, the maximum photon flux can escape the system at inferior conjunction, with a slight shift to $\phi = 0.1$ due to relativistic boosting, leaving the VHE correlated with the X-ray to LE gamma-ray band and therefore anti-correlated to HE gamma-rays.

4. Summary and outlook

We presented a novel numerical model for gamma-ray binaries treating the transport of shock-accelerated electron-positron pairs dynamically coupled to the relativistic fluid dynamics of the stellar and pulsar wind interaction. With this, it is possible for the first time to obtain self-consistent three-dimensional particle distributions and fluid solutions while consistently accounting for dynamic fluid instabilities, mixing, and the effects of orbital motion. The proposed emission model is purely leptonic, thus we inferred the expected emission through the synchrotron and inverse-Compton process acting on accelerated pairs from the pulsar wind obtained through the particle transport simulation. Together with the simultaneously obtained fluid solution, it is therefore possible to consistently account for relativistic boosting and $\gamma\gamma$ -absorption. The model was implemented as a relativistic extension to the CRONOS code (Kissmann et al. 2018).

The capabilities of the presented model were demonstrated on a generic binary system. The wind interaction yields an extended asymmetric wind collision region bent by the effects of orbital motion, exhibiting a strong bow-like pulsar-wind shock and a Coriolis shock behind the pulsar. The expressed features are in qualitative agreement with previous works (see e.g. Bosch-Ramon et al. 2015).

The developing fluid instabilities give rise to the formation of secondary shocks. Our model naturally includes the reacceleration of cooled particles at these shocks, which has not been done before in the case of gamma-ray binaries. In our generic simulation, parts of the turbulence are damped by numerical diffusion due to our choices of spatial resolution. More highly resolved simulations might hence yield a more turbulent fluid and consequently more secondary shocks.

The emission predicted for the generic binary was extended over a broad range in energy reaching up to VHE gamma-rays. Our results are consistent with the simulations performed by Dubus et al. (2015), showing a strong resemblance because the investigated models are similar.

Our model predicts significant orbital modulation in every energy band. The main driver for the modulation in the X-ray to LE gamma-ray synchrotron emission is given by relativistic boosting in the wings of the WCR. In addition to the modulation introduced by the anisotropic inverse-Compton scattering producing the HE and VHE gamma-ray emission, the VHE band is further modulated by $\gamma\gamma$ -absorption. For the investigated general binary, the model naturally predicts a correlated X-ray to LE gamma-ray and VHE gamma-ray emission, while being

anti-correlated to the HE band, as is seen in the observations of many gamma-ray binaries (e.g. LS 5039, [Chang et al. 2016](#)).

Because many of the observed gamma-ray binaries are known to host Be stars, a possible extension of the model foresees the inclusion of more complex, anisotropic stellar wind structures, such as adding an equatorial disc. In the forthcoming second paper of this series, we will apply the presented model specifically to the well-studied LS 5039 system ([Huber et al. 2020](#)), for which no stellar disc has been found. The wealth of available data means that the comparison of our model predictions with observations will provide valuable insights into gamma-ray binaries and a calibration of our model, pointing out potential aspects that might need more modelling effort in the future.

This might, for example, consist of an inclusion of the pulsar and stellar magnetic fields in the dynamics of the wind interaction by extending the model to relativistic magnetohydrodynamics. This might be used to obtain a self-consistent picture for the magnetic field strength and direction, which could further enable the incorporation of more sophisticated particle acceleration models in the future, for example including the obliquity of magnetised shocks (e.g. [Vaidya et al. 2018](#), and references therein).

Another possible extension of this model could consist of easing some simplifications made in the particle transport model, for example by including spatial diffusion. Next to the obvious changes in the spatial particle distribution, an additional effect is provided by the loss term accounting for non-inertial frame changes. This effect has not been studied in the context of gamma-ray binaries.

In future, our model can further help to shed light on dynamical phenomena that can now be addressed with a higher level of sophistication. This could involve investigations of the role of turbulence and the variability it introduces in the radiative output of gamma-ray binaries. Particularly, it remains to be investigated in which way the emission from these systems may vary from one orbit to the next. In a broader context, this might also yield implications for and connect to transient phenomena, such as flaring events in otherwise regular gamma-ray binary emissions (e.g. PSR B1259-63 [Johnson et al. 2018](#)).

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Appendix A: Corotating frame

We considered a reference frame that corotates with the mean angular velocity of the binary Ω in the x - y plane. The corotation velocity is in this case given by the orbital period of the system as $\Omega = 2\pi/P_{\text{orb}}$. The set of new coordinates, indicated by a bar, can be readily expressed as

$$\bar{t} = t \quad (\text{A.1})$$

$$\bar{x} = x \cos(\Omega t) + y \sin(\Omega t) \quad (\text{A.2})$$

$$\bar{y} = y \cos(\Omega t) - x \sin(\Omega t) \quad (\text{A.3})$$

$$\bar{z} = z. \quad (\text{A.4})$$

Transforming the flat Cartesian Minkowski metric into the corotating system yields

$$g_{\bar{\mu}\bar{\nu}} = \begin{pmatrix} -1 + \Omega^2(\bar{x}^2 + \bar{y}^2) & -\Omega\bar{y} & \Omega\bar{x} & 0 \\ -\Omega\bar{y} & 1 & 0 & 0 \\ \Omega\bar{x} & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{A.5})$$

$$g^{\bar{\mu}\bar{\nu}} = \begin{pmatrix} -1 & -\Omega\bar{y} & \Omega\bar{x} & 0 \\ -\Omega\bar{y} & 1 - \Omega^2\bar{y}^2 & \Omega^2\bar{x}\bar{y} & 0 \\ \Omega\bar{x} & \Omega^2\bar{x}\bar{y} & 1 - \Omega^2\bar{x}^2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (\text{A.6})$$

Generic metric tensors can be accounted for in the broader framework of general relativistic hydrodynamics. Here, the equations for energy and momentum conservation are given by $\nabla_\mu T^{\mu\nu} = 0$ with the energy-momentum tensor $T^{\mu\nu} = \rho h u^\mu u^\nu + p g^{\mu\nu}$. Because of the non-vanishing, off-diagonal terms in the metric, the SRHD schemes can no longer be applied without modification.

In a 3+1 decomposition (Misner et al. 1973), the line element is expressed as $ds^2 = -(\alpha^2 - \beta_i \beta^i) dt^2 + 2\beta_i dx^i dt + \gamma_{ij} dx^i dx^j$, with α the lapse, β^i the shift, and γ_{ij} the spatial metric. These gauge functions can be directly obtained from the metric tensor Eqs. (A.5) and (A.6). For the presented corotating system, they are given by

$$\bar{\alpha} = 1 \quad (\text{A.7})$$

$$\bar{\beta}^i = \bar{\beta}_i = (-\Omega\bar{y}, \Omega\bar{x}, 0)_i \quad (\text{A.8})$$

$$\bar{\gamma}_{ij} = \mathbb{1}. \quad (\text{A.9})$$

In our approach, we relied on the so-called 3+1 *Valencia* formulation of general relativistic hydrodynamics (Banyuls et al. 1997), and chose the conserved variables

$$U = \begin{pmatrix} D \\ E \\ m_j \end{pmatrix} = \begin{pmatrix} \rho W \\ DhW - p \\ DhWw_i \end{pmatrix}, \quad (\text{A.10})$$

consisting of the rest-mass density D , the momentum density in the j -direction m_j , and the total energy density E , measured by a family of Eulerian observers. In their respective frames, the fluid three-velocity is given by w^i , which is related to the four-velocity in the rotating system by $w^i = (u^i/u^t + \beta^i)/\alpha$. The corresponding Lorentz factor is given by $W = (1 - w_i w^i)^{-1/2}$ with $w_i = \gamma_{ij} w^j$.

The chosen variables closely resemble those in SRHD Eq. (2) up to the usage of covariant momentum densities instead of contravariant ones, which are equivalent and interchangeable in our case because $\gamma_{ij} = \mathbb{1}$. This allows an effective reuse of the variable inversion scheme developed for the special relativistic case that is already implemented in CRONOS.

The evolution equations take the generic form

$$\partial_t(\sqrt{\gamma}U) + \partial_i(\sqrt{\gamma}F^i) = \sqrt{\gamma}S, \quad (\text{A.11})$$

with $\gamma = \det(\gamma_{ij})$ and the fluxes

$$F^i = \begin{pmatrix} \alpha w^i D - \beta^i D \\ \alpha m^i - \beta^i E \\ \alpha(m_j w^j + p \delta_j^i) - \beta^i m_j \end{pmatrix}. \quad (\text{A.12})$$

The system of equations again closely resemble those in special relativity Eq. (1) up to the additional fluxes introduced by $\beta^i \neq 0$. We treated the equations using the scheme presented by Pons et al. (1998), describing how special relativistic Riemann solvers can be used with general metrics. The required transformations between the Eulerian and the local inertial frames in our case take the especially simple form

$$M^i_{i|\Sigma_{\bar{x}}} = \mathbb{1}, \quad M^i_{i|\Sigma_{\bar{y}}} = \mathbb{1}, \quad M^i_{i|\Sigma_{\bar{z}}} = \mathbb{1}. \quad (\text{A.13})$$

The source terms in Eq. (A.11) are given by (Banyuls et al. 1997)

$$S = \begin{pmatrix} 0 \\ \alpha^2 (T^{\mu t} \partial_\mu \ln \alpha - \Gamma_{\mu\lambda}^t T^{\mu\lambda}) \\ \alpha T^{\mu\nu} (\partial_\mu g_{\nu j} - \Gamma_{\nu\mu}^\lambda g_{\lambda j}) \end{pmatrix}, \quad (\text{A.14})$$

and reduce to

$$S = (0, 0, \Omega m_{\bar{y}}, -\Omega m_{\bar{x}}, 0)^\top \quad (\text{A.15})$$

in our case. This result may seem counter-intuitive at first glance because the terms formally do not correspond to their Newtonian analogue for the centrifugal and Coriolis force in a rotating system. However, we recall that the conserved quantities are measured by the Eulerian observers instead of in the rotating frame.

Finally, our approach is equivalent to others such as Papadopoulos & Font (2000), who chose $T^{0\nu}$ as conserved variables and evolved the quantities directly in the rotating frame, which recovers the well-known terms for the fictitious forces. This formulation, however, is less efficient in practice because the involved fluxes are more complex, and the whole metric has to be considered for contractions, for example in the computation of Lorentz factors, instead of just the spatial metric in the 3+1 Valencia formulation, which is unity in our case. Furthermore, the chosen conserved variables formally differ from Eq. (2), prohibiting the reuse of already developed SRHD variable inversion schemes (e.g. Mignone & McKinney 2007).

Ultimately, we are interested in quantities measured in the stationary laboratory frame to compute the radiative output of the system. This amounts to a Lorentz transformation of the corotating velocity field $u^{\bar{\mu}}$, which is obtained from the velocities measured by the Eulerian observers to the stationary u^μ . For our case, we find after some algebra that the Eulerian velocities directly correspond to those in the stationary system up to a rotation in space. This rotation is accounted for in the computation of relativistic boosting described in Sect. 2.3.

Appendix B: Radiation fields

Depending on the radiation field at hand, the integrals in the computation of inverse-Compton emission or $\gamma\gamma$ absorption can be simplified. For example, for monochromatic seed photon fields, the energy integration reduces to a trivial substitution. To be able to map these properties over to our implementation,

we employed a factorisation of the radiation field. In general, a radiation field can be described as the number of photons n per unit volume, unit energy, and unit solid angle, depending on the location $\mathbf{x}$, the photon energy ϵ , and the direction $\mathbf{\Omega}$. For our purposes, however, the spectral shape is direction independent, which allows the following factorisation of the photon density

$$n(\mathbf{x}, \epsilon, \mathbf{\Omega}) = \frac{dN}{dV d\epsilon d\mathbf{\Omega}} = g_n(\mathbf{x}) \cdot g_\epsilon(\mathbf{x}, \epsilon) \cdot g_\Omega(\mathbf{x}, \mathbf{\Omega}), \quad (\text{B.1})$$

with a factor g_n describing the total photon density, a factor g_ϵ describing the energy dependence, and a factor g_Ω describing the directional profile,

$$g_n(\mathbf{x}) := \frac{dN}{dV} \quad (\text{B.2})$$

$$g_\epsilon(\mathbf{x}, \epsilon) := \left(\frac{dN}{dV} \right)^{-1} \frac{dN}{dV d\epsilon} \quad (\text{B.3})$$

$$g_\Omega(\mathbf{x}, \mathbf{\Omega}) := \left(\frac{dN}{dV} \right)^{-1} \frac{dN}{dV d\mathbf{\Omega}}. \quad (\text{B.4})$$

We note that g_ϵ and g_Ω are normalised with respect to ϵ and $\mathbf{\Omega}$, respectively.

When we consider spherically expanding photons injected at a location $\mathbf{x}_\star$ with a given rate $\dot{N}_\star$, the photon number density is given by

$$g_n^{\text{spherical}}(\mathbf{x}) = \frac{1}{r^2} \frac{\dot{N}_\star}{4\pi c}, \quad (\text{B.5})$$

where $r = \|\mathbf{x} - \mathbf{x}_\star\|$.

A mono-directional or beamed radiation field in a given direction $\mathbf{\Omega}_{\text{beam}}$ is in general described by

$$g_\Omega^{\text{beamed}}(\mathbf{x}, \mathbf{\Omega}) = \delta(\mathbf{\Omega} - \mathbf{\Omega}_{\text{beam}}). \quad (\text{B.6})$$

The radiation field of a point-like source can therefore be viewed as a special case of a field beamed in the radial direction $\mathbf{\Omega}_{\text{beam}} = \mathbf{e}_r = \mathbf{r}/r$. An extended spherical source is approximated as a disc with constant brightness and angular extent limited by the source radius R ,

$$g_\Omega^{\text{extended}}(\mathbf{x}, \mathbf{\Omega}) = \begin{cases} (2\pi(1 - \mu_{0,\min}))^{-1} & \mu_0 > \mu_{0,\min} \\ 0 & \text{else} \end{cases}, \quad (\text{B.7})$$

where μ_0 is the cosine of the angle enclosed between $\mathbf{\Omega}$ and $\mathbf{e}_r$ and $\mu_{0,\min} = (1 - R^2/r^2)^{1/2}$.

The radiation field of the companion star can be approximated as a blackbody spectrum with temperature T ,

$$g_\epsilon^{\text{blackbody}}(\mathbf{x}, \epsilon) = \frac{1}{2\zeta(3)k_b T} \frac{(\epsilon/k_b T)^2}{\exp(\epsilon/k_b T) - 1}. \quad (\text{B.8})$$

This can be further approximated as a monochromatic spectrum with the average photon energy $\bar{\epsilon} = k_B T \frac{\pi^4}{30\zeta(3)}$,

$$g_\epsilon^{\text{mono}}(\mathbf{x}, \epsilon) = \delta(\epsilon - \bar{\epsilon}). \quad (\text{B.9})$$

In our simulation, the radiation field of the star was parametrised by its luminosity $L_\star$ and its temperature $T_\star$. The extent of the source is therefore given by $R_\star^2 = L_\star / (\frac{4\pi}{3} \sigma T_\star^4)$ and its photon injection rate by $\dot{N}_\star = L_\star / \bar{\epsilon}_\star$.

Appendix C: Comparison to a common shock-identification criterion

In the literature, particle acceleration is thought to occur at strong shocks, which are usually identified by a diverging fluid flow and a jump in pressure (see e.g. [Vaidya et al. 2018](#)). As described in Sect. 2.2.4, we employed a less restrictive criterion on the fluid compression alone because a jump in pressure might not yet have developed for a given instance in time.

For the generic binary system considered in Sect. 3, we found both sets of criteria to identify the same main shock features, that is, the bow and Coriolis shock, with reflected shocks at their encounter and secondary shocks. In comparison to our criterion, the usual approach identifies fewer and less extended acceleration sites in the turbulent Coriolis shock downstream region because of the additional pressure constraint. This introduces a slight decrease in the emission at all wavelengths through the reduced particle injection, which could be compensated for by a different set of injection parameters. Because the magnetic field in the Coriolis shock downstream region is lower, the effect becomes more relevant for particles at higher energies, leading to a decrease in the synchrotron emission in the LE gamma-ray band. The temporal behaviour remains unaffected in all bands. For a compression threshold of $\delta_{\text{sh}} \sim -50 c/\text{AU}$, we found that our criterion identified the same acceleration sites as the classical approach. We treated the threshold as a free parameter of the simulation, which might be constrained for a given system compared with observations.

ARTICLE III

RELATIVISTIC FLUID MODELLING OF GAMMA-RAY BINARIES.
II. APPLICATION TO LS 5039

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Relativistic fluid modelling of gamma-ray binaries

II. Application to LS 5039

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ABSTRACT

Context. In the first paper of this series, we presented a numerical model for the non-thermal emission of gamma-ray binaries in a pulsar-wind-driven scenario.

Aims. We apply this model to one of the best-observed gamma-ray binaries, the LS 5039 system.

Methods. The model involves a joint simulation of the interaction between the pulsar wind and the stellar wind and the transport of electron pairs from the pulsar wind accelerated at the emerging shock structure. We compute the synchrotron and inverse Compton emission in a post-processing step while consistently accounting for relativistic beaming and $\gamma\gamma$ -absorption in the stellar radiation field.

Results. The wind interaction leads to the formation of an extended, asymmetric wind collision region that develops strong shocks, turbulent mixing, and secondary shocks in the turbulent flow. Both the structure of the collision region and the resulting particle distributions show significant orbital variation. In addition to the acceleration of particles at the bow-like pulsar wind and the Coriolis shock, the model naturally accounts for the re-acceleration of particles at secondary shocks that contribute to the emission at very-high-energy (VHE) gamma-rays. The model successfully reproduces the main spectral features of LS 5039. While the predicted light curves in the high-energy and VHE gamma-ray band are in good agreement with observations, our model still does not reproduce the X-ray to low-energy gamma-ray modulation, which we attribute to the employed magnetic field model.

Conclusions. We successfully model the main spectral features of the observed multi-band, non-thermal emission of LS 5039 and thus further substantiate a wind-driven interpretation of gamma ray binaries. Open issues relate to the synchrotron modulation, which might be addressed through a magnetohydrodynamic extension of our model.

Key words. radiation mechanisms: non-thermal – gamma rays: stars – methods: numerical – relativistic processes – hydrodynamics – stars: individual: LS 5039

1. Introduction

Gamma-ray binaries are composed of an early-type, massive star in orbit with a compact object, either a neutron star or a black hole, and are distinguished from X-ray binaries by a dominant radiative output in the gamma-ray regime >1 MeV (see [Dubus 2013](#); [Paredes & Bordas 2019](#), for a review). They exhibit broadband non-thermal emission, which is modulated with the orbital phase for most systems.

In the literature, two possible mechanisms are proposed to explain their non-thermal emission (see e.g., [Mirabel 2006](#); [Romero et al. 2007](#)): a microquasar scenario, where high-energy particles are produced in relativistic jets powered by the accretion of stellar matter onto the compact object (see e.g., [Bosch-Ramon & Khangulyan 2009](#)); or a wind-driven scenario, where the compact object is commonly assumed to be a pulsar, accelerating particles at the shocks formed in the wind collision region (WCR) through the interaction between the stellar wind and the relativistic pulsar wind (see [Maraschi & Treves 1981](#); [Dubus 2006](#)).

In this work, we will specifically focus on the LS 5039 system, one of the most closely studied gamma-ray binaries, which constitutes a suitable test bed for different modelling approaches thanks to well-known orbital parameters and a wealth of available broadband data. The LS 5039 system is composed of a

massive O-type star in a mildly eccentric ($e = 0.35$) $\sim 3.9 d$ orbit with a compact object ([Casares et al. 2005](#)). This system is widely assumed to be a representative of the wind-driven scenario, where the compact object is assumed to be a pulsar, which is supported by the available data that show regular orbital modulations in X-rays ([Takahashi et al. 2009](#)) as well as low-energy (LE; [Collmar & Zhang 2014](#)), high-energy (HE; [Abdo et al. 2009](#)), and very-high-energy (VHE; [Aharonian et al. 2005](#)) gamma-rays.

The system shows correlated orbital modulations in the X-ray, LE, and VHE bands, peaking at inferior conjunction (when the compact object passes in front of the star as seen by the observer) and reaching its minimum close to superior conjunction (the compact object passes behind the star). In contrast, the HE modulation is anti-correlated with the previously mentioned bands, peaking at superior conjunction.

Most emission models for LS 5039 are purely leptonic, establishing synchrotron emission and anisotropic inverse Compton scattering on the stellar radiation field as the dominant radiative processes (see e.g., [Zabalza et al. 2013](#); [Dubus et al. 2015](#); [Molina & Bosch-Ramon 2020](#)). While inverse Compton scattering is most efficient at superior conjunction, where the stellar photons are back-scattered in the direction of the observer (see e.g., [Dubus et al. 2008](#)), the attenuation of the VHE flux due to the $\gamma\gamma$ pair-production process (see e.g., [Dubus 2006](#))

is also at its highest there since the generated radiation has to propagate through the binary system before it can escape. Since the shocked pulsar wind retains relativistic velocities (see e.g., [Bogovalov et al. 2008](#)), the emission reaching the observer at Earth is modulated by relativistic boosting (see e.g., [Dubus et al. 2010](#)) that depends on the orientation of the system. This interplay between the generation of inverse Compton emission and its absorption by pair production together with the phase-dependent relativistic boosting is commonly used to explain the observed anti-correlation of the HE gamma-ray emission with the X-ray and VHE gamma-ray fluxes.

Due to the high $\gamma\gamma$ -opacity, a one-zone model for LS 5039 with a single emitter at the stellar and pulsar wind standoff predicts non-detectable VHE fluxes at superior conjunction, but a faint source is still clearly detected. This indicates that the VHE emitting region is more extended and located farther away from the star since an alternative explanation involving an electromagnetic cascade initiated by the $\gamma\gamma$ pair production turned out to be incompatible with the observed spectrum (see e.g., [Bosch-Ramon et al. 2008](#); [Cerutti et al. 2010](#)). A plausible second emission region is the Coriolis shock, which is formed due to the orbital motion of the system (see [Bosch-Ramon & Barkov 2011](#); [Bosch-Ramon et al. 2012](#)). Using an analytic approximation to describe its location, the Coriolis shock was established as a viable site for particle acceleration and the subsequent production of VHE gamma-rays (see e.g., [Zabalza et al. 2013](#)). While such an analytic two-zone model still oversimplifies the structure of the WCR, it shows that an approach that contains the precise structure of the WCR can take the extended emission region and the consequent dilution of $\gamma\gamma$ -absorption into account very naturally. To obtain a more realistic picture of the WCR, the pulsar wind–stellar wind (PW-SW) interaction was investigated numerically using dedicated special-relativistic hydrodynamic (RHD) simulations (see e.g., [Lamberts et al. 2013](#); [Bosch-Ramon et al. 2015](#)). These simulations were used in combination with particle transport models to build more comprehensive emission models with various degrees of complexity (see e.g., [Dubus et al. 2015](#); [Molina & Bosch-Ramon 2020](#)). However, these models do not take the complex dynamic structure of the wind interaction into account and rely on simplified simulations or analytic reductions of simulations.

In [Dubus et al. \(2015\)](#), the authors solve a Fokker-Planck-type particle-transport equation for accelerated electron pairs using results from a simplified wind-interaction simulation as a steady-state background. This allows for relativistic and anisotropic effects to be consistently included in the computation of the generated emission. The wind interaction was simulated in a non-turbulent setup, symmetric around the binary axis, which is re-scaled for different orbital phases. While reducing the computational effort, the assumption of axisymmetry prevents orbital motion from being taken into account, implying that a Coriolis shock cannot be formed in such a simulation. Furthermore, with a steady-state fluid background, the impact of fluid dynamics is neglected. However, more complex simulations (e.g., [Bosch-Ramon et al. 2015](#)) have shown that neither the shock structure nor the downstream flow are stationary but depend on the orbital phase and are subject to turbulence arising in the WCR.

In [Huber et al. \(2021\)](#) we presented a novel numerical model for the non-thermal emission of gamma-ray binaries in a pulsar-wind-driven scenario, with which we aim to alleviate some of the approximations in previous modelling efforts while incorporating previous approaches in a self-consistent framework. In the presented approach, the PW-SW interaction is treated in a

dedicated three-dimensional RHD simulation. The novelty of this approach consists of a simultaneous solution of the fluid dynamics and the particle transport for the electron-positron pairs, which are accelerated at the arising shocks. This yields consistent particle distributions, which are used together with the fluid solutions to generate predictions for the non-thermal emission of the system, comprising synchrotron and anisotropic inverse Compton emission with additional modulation by relativistic boosting and $\gamma\gamma$ -absorption.

The present paper is the second in a series. Here, we apply the model presented in [Huber et al. \(2021\)](#) to the LS 5039 system. LS 5039 is a prime candidate for investigating fluid models of gamma-ray binaries, thanks to the well-known and less complex stellar-wind model as compared to other systems with stellar disks. With this application, we aim to identify the relevant emission regions in three dimensions and to assess the impact of fluid dynamics on the radiative output of the system, which has not been possible with previous approaches.

The paper is structured as follows: In Sect. 2 we specify the setup of the simulation; the resulting fluid solution, particle distributions, and predicted emission for LS 5039 are presented in Sect. 3; and a summarising discussion is given in Sect. 4.

2. Simulation setup

The LS 5039 system is composed of a massive O-type star in a mildly eccentric orbit with what we assume to be a pulsar despite the fact that no pulsations have been detected yet. We employed the orbital solution determined by [Casares et al. \(2005\)](#), with a period $P_{\text{orb}} = 3.9$ d and eccentricity $e = 0.35$. We assumed a stellar mass $M_{\text{star}} = 23 M_{\odot}$ and a pulsar mass $M_{\text{pulsar}} = 1.4 M_{\odot}$ (similar to [Dubus et al. 2015](#)), yielding a semi-major axis $a = 0.145$ AU, apastron distance $d_a = 0.196$ AU, and periastron distance $d_p = 0.094$ AU, as depicted in Fig. 1.

To simulate the interacting fluids of the stellar wind and the pulsar wind, we numerically solved the equations of RHD, using a reference frame that co-rotates with the average angular velocity of the system, $\Omega = 2\pi/P_{\text{orb}}$ (see [Huber et al. 2021](#), for more details). The dynamical equations were solved using the CRONOS code ([Kissmann et al. 2018](#)). The simulation was performed on a Cartesian grid with dimensions $[-1.25, 1.25] \times [-0.5, 1.5] \times [-0.5, 0.5] \text{ AU}^3$, which is homogeneously subdivided into $640 \times 512 \times 256$ spatial cells. The binary orbits in the $x - y$ plane, with its centre of mass coinciding with the coordinate origin.

For the simulation of the wind interaction (presented in Sect. 3.1), we adopted a stellar mass loss rate of $\dot{M}_s = 2 \times 10^{-8} M_{\odot} \text{ yr}^{-1}$ and a terminal velocity of $v_s = 2000 \text{ km s}^{-1}$ ([Dubus et al. 2015](#)). The speed of the pulsar wind was set to $v_p = 0.99 c$, corresponding to a Lorentz factor of $\gamma_p^0 = 7.08$. While this is smaller than conventional values, $\gamma_p^0 \sim 10^4 - 10^6$ (see e.g., [Khangulyan et al. 2012](#); [Aharonian et al. 2012](#), and references therein), it is still high enough to capture the relevant relativistic effects ([Bosch-Ramon et al. 2012](#)). The pulsar mass loss rate $\dot{M}_p = \eta \frac{\dot{M}_s u_s}{u_p}$ was scaled with $\eta = 0.1$, yielding a corresponding pulsar spin-down luminosity $L_{\text{sd}} = 7.55 \times 10^{28} \text{ W}$. Both the stellar wind and the pulsar wind were continuously injected within a spherical region with radius $r_{\text{inj}} = 0.08 a$ around each object, which were initially placed in a vacuum. To account for the eccentricity of the orbit, the locations of the injection volumes were updated accordingly after every step of the simulation.

Fig. 1. LS 5039 system as determined by Casares et al. (2005) with an orbital period of $P_{\text{orb}} = 3.9$ d and an eccentricity of $e = 0.35$, assuming a stellar mass $M_{\text{star}} = 23 M_{\odot}$ and a pulsar mass $M_{\text{pulsar}} = 1.4 M_{\odot}$. Periastron, apastron, and the conjunctions are indicated. Matching the choices in Aharonian et al. (2006), the orbit is divided into two parts: INFC, ranging from $0.45 < \phi < 0.9$, and SUPC, for $0.9 < \phi < 1$ and $0 < \phi < 0.45$. We point out that, throughout the paper, the acronyms SUPC and INFC refer to the specified parts of the orbit, whereas the terms superior and inferior conjunction denote specific points on the orbit.

The simulation was performed for approximately 1.6 orbits. The first 0.6 orbits were used to initialise the simulation, allowing the slower stellar wind to populate the computational domain. The stellar wind reaches the farthest corner of the simulation box after $t_{\text{crossing}} \approx 0.45 P_{\text{orb}} \approx 1.75$ d. The subsequent full orbit was used for the scientific analysis.

For the evolution of the accelerated electron-positron pairs, we solved a Fokker-Planck-type transport equation simultaneously with the fluid interaction using an extension to the CRONOS code (Huber et al. 2021). For the particles, we used 50 logarithmic bins in energy covering the range $\gamma \in [200, 4 \times 10^8]$. At the acceleration sites – identified by a strongly compressive fluid flow $\nabla_{\mu} u^{\mu} < -10$ c/AU, where u^{μ} is the fluid four-velocity – we injected two particle populations into the simulation: a power-law component, corresponding to accelerated, non-thermal pairs, and a Maxwellian component, corresponding to isotropised pairs from the pulsar wind (see also Dubus et al. 2015). For the sake of brevity, we refer to these particles only as electrons for the rest of this work. The non-thermal electrons were injected with a spectral index $s = 1.5$ and an acceleration efficiency $\xi_{\text{acc}} = 2$, which determines the maximum energy, $\gamma_{\text{max}} = \left(\frac{3}{4\pi} \frac{\mu_0 e c}{\xi_{\text{acc}} \sigma_T B'} \right)^{1/2}$, reached by balancing the shock acceleration and synchrotron losses with the magnetic field strength B' . We assumed a fraction $\zeta_e^{\text{PL}} = 0.45$ of the local internal fluid energy and a fraction $\zeta_n^{\text{PL}} = 4 \times 10^{-3}$ of the number of available electrons from the pulsar wind to be injected as a non-thermal component. The remaining electrons were injected as a Maxwellian component. Since the pulsar-wind Lorentz factor used in our simulation might be higher in reality, the density of the pair plasma would be overestimated in our simulation. To account for this, we decreased the number

of available electrons considered in the injection by a factor of $\zeta_p = 5.5 \times 10^{-4}$.

In our simulation, we did not evolve the magnetic field explicitly, which makes assumptions on its spatial dependence necessary. Therefore, we conducted the simulations under the assumption that the magnetic field energy density in the fluid frame is proportional to the internal energy density of the fluid, $\frac{B'^2}{2\mu_0} = \zeta_b \frac{p}{\Gamma - 1}$ (in analogy to Barkov & Bosch-Ramon 2018) with $\zeta_b = 0.5$. This approximation is similar to the one used in Dubus et al. (2015) at the location of the shocks. Although the evolution of the magnetic field might differ in the shocked downstream flow, this approximation was expected to yield good values at the shocks, which are the most relevant for the particle injection. For the stellar companion, we assumed a luminosity $L_{\star} = 1.8 \times 10^5 L_{\odot}$, temperature $T_{\star} = 39\,000$ K, and resulting radius $R_{\star} = 9.3 R_{\odot}$ (Casares et al. 2005).

3. Results

3.1. Fluid structure

In Fig. 2 we show the resulting fluid mass density for different orbital phases. An extended WCR is formed from the PW-SW interaction, creating a bow-like shock (hereafter the bow shock) on the pulsar side. The overall shape of the WCR is highly asymmetric and bends in the direction opposite to the orbital motion due to the Coriolis force acting on the rotating system. The additional force leads to a termination of the pulsar wind on the far side of the system, forming another shock at the Coriolis turnover (hereafter the Coriolis shock).

In the downstream region of the Coriolis shock, the shocked pulsar wind is turbulently mixed with shocked stellar-wind material, slowing the flow due to the increased mass load (see also Fig. A.1). Many secondary shocks are formed in the turbulent motion of the fluid, which can re-energise already cooled particles accelerated at other shocks (Bosch-Ramon et al. 2012). In the wings of the WCR, the pulsar wind shocked at the bow is re-accelerated towards its initial Lorentz factor (see also Bogovalov et al. 2008) until it reaches the turbulently mixed fluid behind the Coriolis shock, creating an additional shock (hereafter the reflected shock, in analogy to Dubus et al. 2015) that extends diagonally into the region behind the pulsar (clearly visible at $\phi \simeq 0.3$ in Figs. 2 and A.2). Features visible in our simulation are in qualitative agreement with previous works (see e.g., Bosch-Ramon et al. 2015), validating our fluid model.

While the Coriolis shock location is in agreement with previous works at periastron, its distance from the pulsar becomes too large and leaves the computational domain around apastron. This suggests that the simulation box does not capture enough of the leading edge of the WCR (in front of the pulsar with respect to the anticlockwise orbital motion), which therefore cannot sweep up enough dense stellar-wind material to build up the required pressure to terminate the pulsar wind.

The structure of the WCR is strongly influenced by turbulence that develops at the contact discontinuity in the WCR. In addition to the Kelvin-Helmholtz (KH) instabilities triggered by the large velocity shear, the arising turbulence is further increased by Rayleigh-Taylor (RT) and Richtmyer-Meshkov (RM) instabilities (Bosch-Ramon et al. 2012). This dominantly occurs at the leading edge of the WCR because there the high-density, shocked stellar wind is pressed against the low-density, shocked pulsar wind by the Coriolis force (see also Bosch-Ramon et al. 2012). We found that the formation of the Coriolis shock is influenced by the arising turbulence (see e.g.,

Fig. 2. Fluid mass density in the orbital plane for different orbital phases, indicated by the inset annotations. An extended WCR is formed due to the interaction of the pulsar (blue) and stellar (orange) wind. The reference frame is co-rotating with the anticlockwise orbital motion. The labels INFC and SUPC correspond to respective parts of the orbit as defined in Fig. 1. The boundaries between the inner and middle regions and between the middle and far regions (further discussed in the text) are indicated by the dashed and dotted lines, respectively.

$\phi \simeq 0.8$ in Fig. 2), which can cause orbit-to-orbit variations in the WCR structure.

The development of KH instabilities is strongly suppressed for highly relativistic flows (see e.g., [Perucho et al. 2004](#); [Bodo et al. 2004](#)). Fluctuations can therefore only efficiently grow in the vicinity of the wind standoff, where the shocked pulsar wind is sufficiently slow with a speed of $\sim c/3$ before being re-accelerated. The timescale for advection out of this region therefore critically determines the largest modes that can be excited in the system since the growth rate for KH instabilities, $\Gamma_{\text{KH}} \propto \lambda^{-1}$, decreases with larger wavelengths (see [Bodo et al. 2004](#); [Lamberts et al. 2013](#)). The maximum wavelength of fluctuations that can be excited in the presented system is of the order of $\lambda_{\text{max}} \sim 0.1$ AU (assuming a region extension of ~ 0.3 AU and an average advection velocity of $\sim 0.5 c$).

The pulsar-wind Lorentz factor used in our simulation is lower than the typically assumed values $\sim 10^4 - 10^6$ due to numerical limitations. A higher pulsar-wind Lorentz factor would yield a faster re-acceleration ([Bosch-Ramon et al. 2012](#)) when the shocked flow is expanding in the wings and might therefore reduce the advection timescale and shift the maximum wavelength of growing fluctuations to smaller values. However, [Bogovalov et al. \(2008\)](#) found that even in the ultra-relativistic limit, the shocked pulsar-wind flow remains slow near the head of the bow shock up to scales of the orbital separation for our choice of η . This is mainly a consequence of the bow-like geometry of the WCR, which causes the upstream incident angle with the shock normal to be small over a wide part of the head of the bow shock, leading to a strongly slowed downstream flow. Furthermore, the flow cannot expand rapidly there, keeping the re-acceleration at a moderate level. The re-acceleration only becomes more important farther out, where the opening angles of the pulsar-wind shock and the contact discontinuity approach their asymptotic values. The extent of the unstable region hence cannot go below the scales of the order of the orbital separation regardless of the pulsar-wind Lorentz factor, thus only slightly changing the estimates from above. Even in the ultra-relativistic limit, KH instabilities are therefore still expected to grow and the overall structure of the WCR should not change significantly.

For our setup, we found in numerical tests (simulating the decay of shear flows as described by [Ryu & Goodman 1994](#)) that damping by numerical viscosity $\Gamma_{\text{damp}} \propto \lambda^{-3}$ dominates over the KH growth rate (estimated from [Bodo et al. 2004](#)) for short-wavelength fluctuations with $\lambda \lesssim 10^{-2}$ AU. The chosen resolution, therefore, allows the growth of fluctuations in the range $10^{-2} \text{ AU} \lesssim \lambda \lesssim 10^{-1} \text{ AU}$ (as seen in Fig. 2), where the larger wavelengths will have the biggest impact on the WCR. This also implies that future higher-resolution simulations will extend the range of turbulence to smaller spatial scales for which the driving by KH instabilities becomes more efficient because $\Gamma_{\text{KH}} \propto \lambda^{-1}$.

In our simulation, we did not consider any feedback of the accelerated particles onto the fluid dynamics. Because the non-thermal electrons contribute a significant fraction of the overall energy density, their cooling will result in a decrease in the fluid's pressure that supports the WCR. Consequently, when taking such feedback into account, the WCR will be less extended and might thus be more susceptible to thin-shell instabilities (as pointed out by [Dubus et al. 2015](#)), as it was seen in the case of colliding-wind binaries by [Reitberger et al. \(2017\)](#). The consideration of such effects is left for future work.

3.2. Particle distribution

Since the timescale for the particle populations to reach a quasi-steady state (by reaching the limits of the computational domain and/or by cooling) is orders of magnitudes smaller than the orbital timescale, we did not perform a particle transport simulation for the full time span of the fluid simulation. Instead, to reduce the computational effort, we restarted a particle transport simulation on previously obtained fluid solutions for the ten chosen orbital phases shown in Fig. 2. We performed these simulations for $t = 1.11$ h, allowing the injected electrons to populate the system.

To simulate the energetic evolution of the electrons, we employed the semi-Lagrangian scheme described in [Huber et al. \(2021\)](#). For this, we used the same time step as for the preceding hydrodynamic step, which is mainly determined by the speed of the un-shocked pulsar wind and the spatial resolution, yielding

Fig. 3. Differential particle number density for electrons with $\gamma = 3.11 \times 10^3$ in analogy to Fig. 2. The arrows indicate the projected direction to an observer at Earth. For clarity, we show only five orders of magnitude below the highest value – the blue regions correspond to those with lower values.

Fig. 4. Same as Fig. 3, but for $\gamma = 1.05 \times 10^7$.

typical values of $\Delta t \sim 0.8$ s. Due to the semi-Lagrangian nature of the scheme, an additional reduction of the time step depending on the energy resolution is not required to maintain stability.

In Figs. 3 and 4 we present the resulting electron distributions for different orbital phases at two energies, which are dominantly populated by Maxwellian and power-law electrons, respectively. The relevant shock structures are imprinted in the electron distributions. This is especially visible for particles at higher energies, which are quickly cooled through synchrotron and inverse Compton losses. Due to increased losses, they remain much more confined to their injection sites. Lower-energetic electrons, in comparison, dominantly lose energy via adiabatic losses and are therefore cooled on longer timescales, populating a much larger spatial domain. In addition to the bow and Coriolis shocks, the reflected shock and the countless secondary shocks in the turbulent downstream region behind the pulsar are also manifestly visible. In our simulation, radiative losses are highest at the wind standoff, which limits the maximum electron energy reached in the acceleration as well as the

length scales over which non-thermal electrons are cooled afterwards. At the Coriolis shock, both the magnetic field and the stellar-radiation field are weaker in comparison and the highest particle energies of the simulation are reached (see Fig. 5).

In Fig. 5 we show the spectral energy distribution of the electrons integrated over the computational volume. The contributions of the Maxwellian and the power-law electrons can be easily distinguished as they dominate the energy range below and above $\gamma \sim 2 \times 10^4$, respectively. It is apparent that not only the normalisation but also the shape of the spectrum are a function of the orbital phase, considering the location of the peak in the Maxwellian electrons, the break in the power-law tail, and the maximum energies reached. Furthermore, it shows that a higher electron density is reached after periastron, which is not intuitive at first glance.

This becomes more apparent in Fig. 6, where we show the temporal evolution of the electron distribution integrated over the computational volume at selected energies. Apparently, the number of electrons in the computational volume lags behind the

Fig. 5. Spectral energy distribution of electrons integrated over the computational domain for different orbital phases (colour-coded solid lines). For $\phi = 0.393$, the contributions of the inner (dashed line), middle (dash-dotted), and outer regions (dotted) are shown as examples.

Fig. 6. Temporal evolution of the spectral energy distribution of energetic electrons integrated over the computational domain for selected energies (colour-coded). For a better visualisation, we show the same data for two orbits.

orbit, that is, the minimum amount of electrons is reached after apastron and the maximum after periastron.

This delay is caused by the inertia of the fluid. The WCR needs a certain amount of time to build up or dissipate its pressure, which critically determines the amount of electrons accelerated at the shocks. This phenomenon can only be seen in approaches that treat the particle transport together with the underlying fluid. The varying size of the shocks counteracts parts of this effect by shrinking and enlarging the acceleration sites at periastron and apastron, respectively; however, this is not dominant in our simulation. The power injected at the shocks reaches its maximum at $\phi \approx 0.2$ in our simulation, suggesting an expected peak in the integrated electron distribution with the same delay.

We find, however, that this delay is energy-dependent. While the number of higher-energetic electrons peaks as expected around $\phi \approx 0.2$, the number of lower-energetic ones peaks earlier, at $\phi \approx 0.1$ (see Fig. 6). This behaviour originates in the turbulent flow behind the pulsar formed earlier around the periastron passage, which leads to a pileup of electrons at lower energies, in turn yielding an earlier peak in their evolution. This effect is not relevant for electrons at higher energies since they are cooled much faster through radiative losses. Consequently,

these particles are more confined to the shocks, preventing a pileup and leaving their number density more directly affected by the acceleration process.

We treated both the spectral slope and the acceleration efficiency as free model parameters since the specifics for particle acceleration in gamma-ray binaries have not yet been firmly identified. In this phenomenological approach, we treated all acceleration sites the same, which might not be the case in reality. For example, in the case of diffusive shock acceleration, both the spectral index and the acceleration timescale depend on the shock's compression ratio, magnetic obliquity, and up- and downstream fluid velocities (see e.g., Keshet & Waxman 2005; Takamoto & Kirk 2015). In future efforts, the current model can be extended to investigate different acceleration mechanisms.

3.3. Emission

In this section, we present the simulation results for the non-thermal emission spectrum and light curves of LS 5039. They were produced in a post-processing step, using the previously obtained particle distributions (see Sect. 3.2) and fluid solutions (see Sect. 3.1). We, therefore, generated direct predictions on the initially spelt-out set of model parameters (see Sect. 2).

For the computation of the inverse Compton emission, we treated the stellar photon field as monochromatic, whereas a full blackbody spectrum was considered for the $\gamma\gamma$ -absorption. In both cases, the source was treated as an extended sphere. We computed the emission for two different system inclinations, $i = 30^\circ$ and $i = 60^\circ$.

In our approach, it is no longer straightforward to separate the emission produced through particles accelerated at the different shocks, like it was possible in previous works (e.g., Dubus et al. 2015), since the downstream flows are turbulently mixed; this had previously been neglected. To obtain a basic understanding of the location dependence of the emission, we subdivided the computational volume into three regions (hereafter the inner, middle, and far regions), the boundaries of which are located at distances of $1.2d$ and $3.5d$ from the binary's centre of mass, where d is the time-dependent orbital distance (see Fig. 2). In Sect. 3.3.1 we present the predicted emission spectra followed by a more detailed discussion for individual energy bands in Sects. 3.3.2–3.3.4. A projection map of the emission is discussed in Sect. 3.5.

3.3.1. Emission spectrum

In Fig. 7 we show the resulting spectral energy distributions of photons emitted for two different inclinations of the system, integrated over different orbital phases: To facilitate a comparison to observations, the orbit has been split into two parts, INFC and SUPC, as defined in Aharonian et al. (2006) (see Fig. 1). To compute the average spectra, we integrated the simulated ones using piece-wise linear interpolations in time.

The spectral features of the particle population leave clear imprints in the emission spectrum. Ranging from X-rays up to LE gamma-rays, the spectrum is dominated by synchrotron emission generated by electrons at the power-law tail of the spectrum, which are dominantly produced in the inner region. The same population of electrons is responsible for the inverse Compton scattering of stellar UV photons into the VHE gamma-ray regime, although the relative contributions of the individual regions to the VHE emission is not constant but varies along the orbit. The emission in the HE gamma-ray regime is also produced through the inverse Compton process, however, by the

Fig. 7. Spectral energy distribution of the emission predicted by our model for LS 5039 for different parts of the orbit and inclinations of the system. Different radiative processes are colour-coded: synchrotron (green lines), inverse Compton (orange), inverse Compton attenuated by $\gamma\gamma$ -absorption (red), and total (black). The contributions to the total emission from the inner (dashed lines), middle (dashed-dotted), and far regions (dotted) are shown separately (for a description of the regions, see the main text). The model predictions are shown together with observations in soft X-rays (Takahashi et al. 2009) as well as LE (Collmar & Zhang 2014), HE (Hadasch et al. 2012), and VHE (Aharonian et al. 2006) gamma-rays. Results are shown for different parts of the orbit as defined in Fig. 1, with INFC on the top and SUPC on the bottom, and for different inclinations i of the orbital plane, with $i = 30^\circ$ on the left and $i = 60^\circ$ on the right.

lower-energetic Maxwellian electrons in the inner region of the system.

3.3.2. X-rays and LE gamma-rays

For the chosen set of parameters, the synchrotron emission predicted by our model is able to explain the observed X-ray to LE gamma-ray emission spectrum (see Fig. 7). This was not possible in previous studies (Dubus et al. 2015; Molina & Bosch-Ramon 2020). Synchrotron emission dominates up to ~ 10 MeV, with a spectral cutoff approximately constant over the orbit. The electrons emitting at the LE cutoff are at the highest end of the power-law tail, accelerated at the apex of the bow shock. These particles are strongly confined to shocks and, thus, rely on our injection model and the conditions directly at the shock. This means that the synchrotron cutoff directly depends on two factors: the maximum electron energy (see Sect. 2) and the maximum photon energy produced through the synchrotron process. Both quantities depend only on the magnetic field, however, counteracting each other and leading to a constant synchrotron cutoff.

While the model predictions closely resemble the X-ray and LE gamma-ray observations at INFC, the X-ray flux is over-predicted at SUPC. This deviation is also manifest in the X-ray light curve (see the first row of Fig. 8). Instead of the observed

correlation with VHE gamma-rays, the predicted X-ray light curve is correlated with the HE gamma-ray flux. This is caused by the still simplistic magnetic field description employed in our model: Since the magnetic field strength scales directly with the fluid pressure, its maximum at the bow shock is reached shortly after periastron. In addition, electron acceleration is also increased in this part of the orbit. The combined effects lead to a modulation of the synchrotron emissivity that dominates over that introduced by relativistic boosting, which was argued to be the dominant source of variability in this band (Dubus et al. 2015). These problems, therefore, highlight the necessity for a more sophisticated magnetic field description in future modelling.

We also investigated the effects of different magnetic field models, such as a passively advected magnetic energy density w_B injected together with the pulsar wind and/or a magnetic field aligned with the fluid bulk motion. The injected magnetic energy density is scaled with the injected kinetic energy density as $w_B = \sigma \frac{\dot{M}_p c^2 u_p^0}{4\pi r^2 u_p}$, where σ is the pulsar wind magnetisation fraction, yielding the magnetic field in the laboratory frame $B = \sqrt{2\mu_0 w_B}$. We found little difference in the resulting emission spectra when using these alternative models for similar magnetic field strengths; they still yielded disagreement for the predicted X-ray light curve.

Fig. 8. Emission light curves predicted by our model for LS 5039 for different energy bands and inclinations of the system. The contributions from the inner (dashed orange lines), middle (dashed-dotted green lines), and far regions (dotted red lines) together with their sum (solid blue lines) are shown (for a description of the regions, see the main text). For better visualisation, we show the same data for two orbits. The results are shown for different energy bands together with observations in individual rows (from top to bottom): soft X-rays (1–10 keV; [Takahashi et al. 2009](#)), HE gamma-rays (0.2–3 GeV; [Hadasch et al. 2012](#)), and VHE (>1 TeV; [Aharonian et al. 2006](#)) gamma-rays. In the left column, results are shown for an inclination $i = 30^\circ$ of the orbital plane, while in the right column the results for an inclination $i = 60^\circ$ are presented. In addition to the orbital phases described in the main text, we show three more light curve points at $\phi \sim 0.55, 0.65$, and 0.85 . The error bars indicate the variability introduced by turbulence (see Sect. 3.4).

For larger inclination angles (see the right column in Fig. 8), relativistic boosting becomes more important. This decreases the X-ray flux at superior conjunction while increasing it at inferior conjunction, which better resembles the features of the observed light curve.

3.3.3. HE gamma-rays

While the overall spectral shape and the flux of the predicted HE emission are in good agreement with observations at SUPC, the predictions prove to be problematic at INFC (see Fig. 7). There, the predicted HE flux drops by approximately one order of magnitude and the spectrum is shifted towards lower energies, leaving the fluxes under-predicted. These changes in the flux are mainly caused by the anisotropic inverse Compton scattering cross-section, which grows with the scattering angle. At phases around superior conjunction, stellar photons have to be scattered by a larger angle to reach the observer as compared to inferior conjunction. Consequently, the highest and lowest inverse Compton fluxes relate to these phases, respectively. The anisotropic scattering further causes the shift in energy, yielding higher scattered photon energies for larger scattering angles. Both effects can also be seen by comparing the different inclination angles (e.g., see Fig. 7).

An additional modulation is generated by the changing stellar seed radiation field density induced by the varying distance of the bow shock apex to the star, with the maximum and minimum stellar photon densities at periastron and apastron, respectively. Due to the geometry of the LS 5039 orbit, the periastron passage occurs very close to superior conjunction, leading this modulation to be added to the former one.

The underestimation of the HE gamma-ray flux at INFC suggests a missing component in our broadband emission model, which could arise from the magnetospheric emission of the pulsar as suggested by, for example, [Takata et al. \(2014\)](#). This process can naturally account for the phase-independent spectral cutoff of the HE emission at energies of a few GeV. To accommodate this emission within our modelling, one would have to find a new set of parameters for the Maxwellian electron distribution to avoid an overestimation of the flux at SUPC.

The discrepancy is also apparent in the predicted HE light curves (see the second row in Fig. 8), which show a phase-independent underestimation with respect to the observations. Disregarding the constant under-prediction, the light curve for an inclination of $i = 30^\circ$ is in good agreement with observations. For the higher inclination angle, the inverse Compton anisotropy leads to a steep rise in emission at superior conjunction, while

Fig. 9. Relative contribution to the radiation emitted at a given orbital phase from spherical shells around the system's centre of mass (with a thickness of 0.05 AU) at two different energies. For clarity, we only present the results for a system inclination of $i = 60^\circ$; the resulting maps qualitatively agree with those for an inclination $i = 30^\circ$. We terminate the analysis at $r = 1.5$ AU, where the farthest edge of the computational volume is reached. Relevant orbital phases are annotated (see also Fig. 1).

it further reduces the flux at phases around apastron and inferior conjunction.

Inverse Compton emission by relativistic Maxwellian pairs in the cold pulsar wind might yield another contribution in this energy band. The current model does not take this contribution into account explicitly since the required ultra-relativistic pulsar wind Lorentz factor, $u_p^0 \sim 5000$, cannot be captured by our numerical methods. The produced spectra, however, strongly resemble the ones produced by the Maxwellian electrons injected at the shocks in our model (see Takata et al. 2014). Due to this degeneracy, the emission produced by the Maxwellian electrons effectively capture this contribution in our modelling.

3.3.4. VHE gamma-rays

In contrast to the HE gamma-ray emission, the flux at VHE is heavily attenuated by $\gamma\gamma$ -absorption, introducing an additional line-of-sight-dependent modulation. The observed spectral features and the temporal characteristics are well recovered by our model, with a high-energy cutoff in excellent agreement with observations and a pronounced anti-correlation with the HE gamma-ray emission, as shown in Fig. 7 and the third row in Fig. 8, respectively.

Due to $\gamma\gamma$ -absorption, the VHE-flux, especially from the inner region, is strongly reduced for all phases (see Fig. 7). At INFC, the larger inclination of $i = 60^\circ$ is favourable because the absorption is weakened by smaller scattering angles as compared

to $i = 30^\circ$. Here, the dominant part of the emission is produced in the middle region with strong relativistic boosting, leading to a hard spectrum, as seen in observations. The increased contribution of this region around inferior conjunction can also be seen more directly in Fig. 9, where we illustrate the relative contribution to the gamma-ray flux as a function of distance from the binary's centre of mass.

In the 100 GeV to 1 TeV range, where the $\gamma\gamma$ -absorption is most pronounced, the flux is underpredicted with respect to observations for SUPC. At phases around superior conjunction, the emission produced in both the inner and middle regions is almost completely attenuated by absorption, as shown in Fig. 9, leaving the radiation to be dominantly produced in the far region of the system. The predicted fluxes, however, are too small to reproduce observations around periastron and superior conjunction (see the third row in Fig. 8) in our simulations. We found that the region that dominates the flux reaching the observer in the energy range most affected by $\gamma\gamma$ -absorption around superior conjunction is extended over a large volume behind the pulsar (see Fig. 9). In particular, it extends to the edges of the computational volume, suggesting that a fraction of the emission is lost by particles leaving the domain. A larger computational domain is required to address this issue, which goes beyond the scope of available computational resources.

For a system inclination of $i = 60^\circ$, we find a sharp peak in the predicted VHE light curve at $\phi \approx 0.55$ (see the third row in Fig. 8). At this phase, the observer's line-of-sight is aligned with the leading edge of the shocked pulsar wind flow, yielding a drastically increased photon flux due to relativistic boosting (which can also be seen at the bottom of Fig. 9) that is incompatible with observations. The trailing edge of the WCR is crossed by the observer between $\phi \approx 0.8$ and $\phi \approx 0.9$ in our simulation, showing no peaked emission.

3.4. Turbulence-induced variability

To assess the impact of short-term variability introduced by turbulence on the system's radiative output, we evolved the particle distributions presented in Sect. 3.2 for a longer time and recomputed the emission. After the initial convergence time of $t_0 = 1.11$ h, we investigated the particle distributions at $t_n = t_0 + n \cdot \Delta t$, with $\Delta t = 0.14$ h and $n = 0, 1, 2, 3, 4$. This time increment, Δt , is sufficiently longer than the growth timescale of KH instabilities (see also Sect. 3.1) for the different solutions to be uncorrelated. For each orbital phase we computed the average and the standard deviation from the five obtained emission solutions; we show the results in Fig. 8.

We found that turbulence introduces variability depending on the orbital phase and photon energy, with typical variability levels of several per cent, though reaching $\sim 17\%$ for the HE flux around superior conjunction and $\sim 12\%$ for the VHE flux around inferior conjunction. Most of the variability is apparent in the inner and middle regions, which is expected since these regions are most directly affected by instabilities formed at the contact discontinuity. Although turbulence introduces visible flux fluctuations, they are still considerably smaller than orbital variations and thus do not dominate the resulting light curves.

Lastly, we found that the pulsar-wind shock structure is influenced by turbulence that develops at the stellar-wind shock on longer timescales (see Sect. 3.1). This has an effect on the variability on orbital timescales and is expected to introduce orbit-to-orbit variations, which will be studied in the future when more computational resources become available.

Fig. 10. Projection of the predicted emission from LS 5039 for different orbital phases with an orbital plane inclination of $i = 60^\circ$. The differential energy flux is shown for distinct energy bands as indicated by the colour bars. For better visualisation, the upper limits of the colour bars have been set two orders of magnitude lower than the maximum HE gamma-ray flux.

3.5. Emission map

For a better visualisation of the emission produced in LS 5039, we show a composite false-colour emission map in Fig. 10 as it would be seen with a perfect angular resolution at Earth. The imprint of the fluid structure is clearly visible, exhibiting the bow shock and the turbulent downstream region behind the pulsar around periastron. At $\phi \approx 0.1$ the star eclipses parts of the emission region, occluding a circular region on the map.

4. Summary and discussion

In this work we present the application of a novel numerical model for gamma-ray binaries (Huber et al. 2021) to the LS 5039 system. We specifically chose this system for its broad observational coverage, known orbital parameters, and comparison to previous modelling efforts.

Our simulations of the wind interaction in this system show an extended asymmetric WCR that is bent by the orbital motion, exhibiting a strong bow-like pulsar-wind shock and a Coriolis shock behind the pulsar. With our approach, it is, for the first time, possible to consistently account for the complex dynamic shock structure in the particle transport model. In addition to the bow and Coriolis shocks, this also includes the reflection shock (formed where the downstream plasma of bow and Coriolis shocks collide) and the secondary shocks (which arise in the turbulent downstream medium of the Coriolis shock). The resulting structures are in agreement with those observed in previous simulations (see Bosch-Ramon et al. 2015), although the Coriolis shock is not formed in the numerical domain at phases around inferior conjunction. This is caused by the computational domain being too small to capture enough of the leading edge of the WCR to reach the required pressure to terminate the pulsar wind at the respective phases. In simulations with a larger computational domain, the Coriolis shock is expected to reappear – possibly so close to the pulsar that it would be within the extents of the current computational domain.

We find that the extrema of the fluid’s internal energy do coincide with orbital extrema, as assumed by previous studies (see e.g., Dubus et al. 2015; Zabalza et al. 2013; Takata et al. 2014). This affects the resulting particle distributions since most of the models, including the presented one, scale the amount and energetics of accelerated electrons with the available internal fluid energy. This results in a delay of the electron density extrema of $\Delta\phi \approx 0.1$ – 0.2 in our model, depending on their energy. This delay also translates to the production of radiation; however, it is compensated for in part by the onset of relativistic de-boosting at superior conjunction (shortly after periastron) in the case of LS 5039.

Our model reproduces the main spectral features of the observed emission from LS 5039, ranging from soft X-rays to VHE gamma-rays, further substantiating a wind-driven interpretation of gamma-ray binaries. In contrast to previous studies (e.g., Dubus et al. 2015), our simulation predicts that the synchrotron emission connects the X-ray emission to the LE gamma-ray emission. We attribute this result to the different WCR geometry, which affects relativistic boosting, and to our improved treatment of the star as an extended photon source, leading to increased $\gamma\gamma$ -absorption. Similar to previous studies (e.g., Dubus et al. 2015; Molina & Bosch-Ramon 2020), we find that a hard spectral index of $s = 1.5$ is required for the electron acceleration to describe the observations. The predicted spectra underestimate the flux in the HE gamma-ray band, presumably lacking a contribution by the magnetospheric emission of the pulsar (Takata et al. 2014).

While the inner region (<1.2 orbital separations d from the system’s centre of mass) provides the bulk of the emission from X-rays to HE gamma-rays, the middle and far regions (1.2 – $3.5 d$ and $>3.5 d$, respectively) are especially relevant for the emission in the VHE band mainly due to relativistic beaming and $\gamma\gamma$ -absorption. Our conclusions contrast the assessment by Molina & Bosch-Ramon (2020), who found the far region to be the dominant emitter for all energies and orbital phases. This directly relates to different assumptions

regarding the injection of non-thermal electrons into the system. While we assume the same fraction of the fluid's internal energy density to be converted to non-thermal electrons at all shocks, Molina & Bosch-Ramon (2020) assume that a significantly larger fraction of the pulsar's spin-down luminosity is converted at the Coriolis shock than at the bow shock; this is not the case in our simulations.

Our model predicts significant orbital modulation in all energy bands, mainly originating via the anisotropic inverse Compton process, relativistic boosting, and the changing properties of the WCR. While the predicted HE to VHE gamma-ray light curves agree with observations, the simulations fail to reproduce the observed orbital X-ray and LE gamma-ray modulation. Instead of the observed correlation with VHE gamma-rays, a correlation with the HE band is predicted. We attribute this to the rather simplistic magnetic field model (i.e. scaling the magnetic energy density with the fluid pressure), which varies strongly across the orbit and is responsible for the dominant modulation in the synchrotron emissivity. Such a model has been employed in previous studies that use a semi-analytical description for the emitting particles (e.g., Barkov & Bosch-Ramon 2018), but it seems to be increasingly incompatible with our more detailed particle transport model, highlighting the need for a more sophisticated approach. This could be realised, for example, via an extension of the presented model to relativistic magnetohydrodynamics. With this, it will be possible to take the impact of the non-negligible magnetic field on the fluid dynamics into account, yielding a more realistic picture of the magnetic field strength and direction, and in turn enabling more realistic injection models and the consideration of anisotropic synchrotron emission.

At INFC, the middle region produces the dominant contribution to the VHE gamma-ray spectrum due to relativistic boosting, allowing a hard spectral index to be maintained. We note that the Coriolis shock is not present in the simulation for most of the corresponding phases, as mentioned previously. Its presence in larger simulations is expected to reduce the size of the bow shock wings, where this relativistically boosted emission originates, which might lead to a softening of the spectrum.

At superior conjunction, a significant part of the VHE gamma-ray emission is produced by electrons in the far region of the system due to the weakened impact of $\gamma\gamma$ -absorption. However, emitting particles are lost at the boundaries of the simulation. We suspect this to be the main reason for the underestimation of the SUPC flux in the 100 GeV to 1 TeV range and the underestimation of the VHE light curve around periastron to superior conjunction. These issues as well as the missing Coriolis shock at some orbital phases can be addressed by employing a larger computational volume.

We found that turbulence formed in the wind interaction introduces sub-orbital variability in the system's radiative output on the levels of several per cent on average, reaching up to ~ 20 per cent for certain orbital phases and photon energies. The introduced variations in the flux, however, are still considerably smaller than those on orbital timescales. On longer timescales, turbulence is expected to introduce orbit-to-orbit variations, which cannot be studied from the single simulated orbit. This shows the need for further investigations on larger timescales and a larger spatial domain.

Both investigated inclinations of the orbital plane yield fluxes that are more or less consistent with observations depending on the considered energy band. The HE gamma-ray light curve slightly favours a lower inclination of $i = 30^\circ$, due to the amplitude of the modulation, whereas the VHE gamma-

ray spectrum prefers the larger inclination of $i = 60^\circ$, due to the hard spectral index. The latter inclination is also favourable because it makes the X-ray light curve more consistent with observations by overcoming parts of the strong internal modulation of the synchrotron emissivity due to the increased relativistic boosting.

Although a larger inclination proves to be favourable due to the later decrease of the VHE flux after superior conjunction, the predicted VHE light curve at $i = 60^\circ$ shows a peak that is incompatible with observations shortly after apastron, arising from relativistic boosting when the leading edge of the shocked pulsar wind flow is crossed by the observer's line-of-sight (see also Dubus et al. 2015). We note again that the amplitude of the VHE peak might be overestimated in the presented work because of the missing Coriolis shock at the phases of the peak.

Since the employed simulations take the naturally arising asymmetric shape of the WCR into account, the trailing edge is considerably wider as compared to the leading edge when the observer's line-of-sight is crossed, smearing out the effects of relativistic boosting. This prevents the formation of the second peak in the VHE light curve around $\phi \sim 0.85$ that has been seen for higher inclinations in previous works that employ a more simplified prescription of the WCR (Dubus et al. 2015). Such a second peak is not visible in related observations.

In this study, we showed the feasibility of a combined fluid and particle-transport simulation for predicting the radiative output of gamma-ray binaries. Future extensions of this model, as discussed, are expected to lead to a better representation of the observations of LS 5039 and will be applied to other well-observed gamma-ray binaries.

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Appendix A: Supplementary material

In this section we provide additional visualisation for the fluid quantities that have been omitted in the main text. In

Figs. A.1–A.3 we show the fluid’s four-velocity, its thermal energy density, and the magnetic field strength in the fluid frame, respectively.

Fig. A.1. Fluid four-speed in analogy to Fig. 2.

Fig. A.2. Fluid thermal energy in analogy to Fig. 2.

Fig. A.3. Magnetic field in the fluid frame in analogy to Fig. 2.

Part III

APPENDIX

CONTRIBUTIONS

This dissertation is composed of three scientific articles, for which I am the corresponding author, handling the scientific work, the compilation of the manuscript, its submission and the peer-reviewing process. In the following sections, I will detail my contributions to the individual articles.

ARTICLE I

[Article I](#) (see [Chapter 4](#)) continues and consummates the efforts started during my Master Thesis (Huber, 2017) to extend the CRONOS code to relativistic hydrodynamics, which is a crucial ingredient for the numerical model presented in this thesis. As the first author of this article, I implemented and validated the numerical code; performing an extensive set of numerical tests. In this context, I joined the CRONOS development team and also contributed to the general maintenance of the code. I produced all the illustrations and the major part of the text in the publication under the supervision of Assoc. Prof. Dr. Ralf Kissmann.

ARTICLE II

As the first author of [Article II](#) (see [Chapter 5](#)), I developed the numerical model and implemented the underlying code dealing with the acceleration and transport

of energetic particles in [HMGBs](#) under a variety of processes and the computation of the subsequently produced emission. Further, I produced all the illustrations and the major part of the text in the publication under the supervision of Univ. Prof. Dr. Olaf Reimer and Assoc. Prof. Dr. Ralf Kissmann.

ARTICLE III

As the first author of [Article III](#) (see [Chapter 6](#)), I applied the developed numerical model to the LS 5039 system. This involves the execution of the code on High-Performance Computing ([HPC](#)) infrastructure, requiring several improvements with respect to scalability, the analysis of the simulated data, and an interpretation and discussion thereof. I produced all the illustrations and the major part of the text in the publication under the supervision of Univ. Prof. Dr. Olaf Reimer and Assoc. Prof. Dr. Ralf Kissmann.

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C

ACRONYMS

AGILE	Astorivelatore Gamma ad Immagini Leggero
AGN	Active Galactic Nucleus
CD	Contact Discontinuity
CGRO	Compton Gamma-Ray Observatory
CMB	Cosmic Microwave Background
COMPTEL	Compton Telescope
CO	Compact Object
CR	Cosmic Ray
CTA	Cherenkov Telescope Array
CWB	Colliding-Wind Binary
DSA	Diffusive Shock Acceleration
EAS	Extensive Air Shower
EGRET	Energetic Gamma-Ray Experiment Telescope
FOV	Field of View
Fermi-LAT	Fermi Large Area Telescope
HAWC	High Altitude Water Cherenkov Observatory
H.E.S.S.	High-Energy Stereoscopic System
HE	high-energy, an observational window for gamma-ray photons in the energy range 0.1 – 100 GeV
HGPS	H.E.S.S. Galactic Plane Survey
HMGB	High-Mass Gamma-Ray Binary
HMXB	High-Mass X-Ray Binary
HPC	High-Performance Computing

IACT	Imaging Atmospheric Cherenkov Telescope
IC	Inverse-Compton
LE	low-energy, an observational window for gamma-ray photons in the energy range 1 – 100 MeV
LHAASO	Large High Altitude Air Shower Observatory
MAGIC	Major Atmospheric Gamma Imaging Telescopes
MHD	Magneto-Hydrodynamics
MSP	Millisecond Pulsar
PSF	Point Spread Function
SNR	Supernove Remnant
SRHD	Special-Relativistic Hydrodynamics
SRMHD	Special-Relativistic Magneto-Hydrodynamics
Tibet AS Array	Tibet Air Shower Array
UV	Ultraviolet
VERITAS	Very Energetic Radiation Imaging Telescope Array System
VHE	very-high-energy, an observational window for gamma-ray photons with energies > 100 GeV
WCR	Wind-Collision Region

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Innsbruck, 2021

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