Numerical Relativity Simulations for Highly Eccentric Black Holes Mergers

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Abstract: The precise modelling of gravitational waves has been crucial for their detection by the LIGO-Virgo-Kagra Collaboration. While most of the detected mergers fit into a quasi-circular description, some challenging events do not seem to fit in this category, and seem to be more accurately interpreted as a highly eccentric merger of black holes. The aim of this project is to study the gravitational waves emitted by highly eccentric black hole binaries. This research has been conducted by performing simulations of Einstein's equations (Numerical Relativity) using the open software *Einstein Toolkit* in high-performance computers including the supercomputer Mare Nostrum. After post-processing the output data, which is necessary in order to compute the gravitational waveform, an analysis has been carried out on the obtained results so as to evaluate the accuracy of the current methods of post-processing in the different scenarios of black holes mergers.
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I. INTRODUCTION

The detection and characterisation of gravitational waves (GW) in the recent years by the LIGO-Virgo-Kagra (LVK) Collaboration has required a highly precise newtork of interferometers along with sophisticated data analysis techniques.

One of the major motivations for performing numerical relativity simulations is the accurate calculation of gravitational waveforms from promising sources in order that these theoretically computed signals can be compared with observational data from GW detectors.

Such comparison will be needed not only for the physical interpretation of any observational data, but also to increase significantly the probability of a detection. Since measured GW are extremely weak, foreknown knowledge of the expected signals will greatly aid the initial detection and subsequent understanding of measurements.

The predominant type of detections made so far in the LVK catalog have been categorized as binary black holes (BBHs). While most of the mergers fit into a quasi-circular (QC) description (which means that their orbits have small or negligible eccentricity), some events do not easily match with this characterization, and are more likely to be interpreted as dynamical captures, which are highly eccentric mergers of binary black holes.

Dynamical captures have a completely different phenomenology from the QC ones. Therefore, in order to detect and adequately characterize such events, detailed modeling of the waveforms is requiered. Although they have not been a majority in the detections up to now, these events are expected to be relevant for next-generation detectors such as LISA and the Einstein Telescope.

In this project we have focused on the dynamical capture regime and performed several simulations of BBH mergers through Numerical Relativity, which consists on the exact evolution dictated by Einstein's equations. For this purpose, it has been necessary to use high-performance computers such as Mare Nostrum, given that NR demands a large computational cost.

Even if it provides the most detailed description of BBH mergers, NR is too computationally expensive and it is impractical to directly employ it for GW searches. That is why, in practice, approximate solutions of the full general-relativistic two body problem (known as "approximants") are used as data analysis tools. Thus, matched filtering techniques are performed by comparing the observational data to this (semi-)analytical models that are fast to evaluate at expense of loss of accuracy.

The final purpose of performing NR simulations is to make an assessment of the range of validity of these approximants in different regimes. In particular, this project is framed in the goal of making an evaluation of one of the most popular approximants, the Effective One Body (EOB) models, which needs a re-calibration in the dynamical capture regime in order to increase its accuracy.

To accomplish that, in this project we have performed a number of NR simulations and analysed the obtained post-processed results so as to evaluate the accuracy and performance of the current methods of computing the gravitational waveform. As an important outcome, it is remarkable that the method of post-processing currently used in dynamical captures has been seen not to be appropriate for mergers with three encounters.

II. NUMERICAL RELATIVITY

The theoretical background on Numerical Relativity simulations is of a huge importance in order to be able to adequately develop them. We will assume the basics on General Relativity are known, although we will briefly go over its main points as far as GW are concerned.

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A. Physics of Gravitational Waves

First of all, it is crucial to clearly understand the basis on General Relativity, in concrete, the origin and meaning of gravitational waves.

A weak gravitational field is one in which the metric can be written as the flat space-time metric, $\eta_{\mu\nu}$, plus a perturbation, h: $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$. For such a metric, Einstein's equations written in a convenient gauge (the Lorenz gauge) lead to the following solution for the trace reversed perturbation, $\bar{h}_{\mu\nu} \equiv h_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu}h$:

$$\bar{h}_{\mu\nu}(t, \mathbf{x}) = 4G \int \frac{1}{|\mathbf{x}-\mathbf{y}|} T_{\mu\nu}(t - |\mathbf{x}-\mathbf{y}|, \mathbf{y}) d^3y \ . \quad (1)$$

This solution has the following interpretation: the disturbance in the gravitational field at $(t, \mathbf{x})$ is a sum of the influences from the energy and momentum sources at the point $(t_r, \mathbf{x}-\mathbf{y})$ on the past light cone, with $t_r \equiv t - |\mathbf{x}-\mathbf{y}|$ the retarted time [4]. In vaccuum, a particular wave-like solution arises:

$$\bar{h}_{\mu\nu} = A_{\mu\nu}\exp(ik_\alpha x^\alpha) \ . \quad (2)$$

Regarding the physical meaning of gravitational waves, we understand their propagation to cause a perturbation in the proper distances between objects, that is, not in their coordinates, but in the meshing of space-time itself [6].

B. The 3+1 Decomposition of Einstein's equations

Our interest, as far as gravitational waves, is performing simulations for the purpose of obtaining the waveform h, so that it can be compared with detected signals. In order to do so, we encounter two problems in our way.

1. *Time evolution*

To begin with, simulations, by their nature, need some variables to evolve in time so as to calculate their dynamical evolution. The problem in Einstein field equations (EFE) is that they are written in a fully covariant way, i.e., there is no distinction between space and time. Therefore, it is necessary to split the roles of time and space clearly to be able to formulate Einstein's equations as a Cauchy problem, that is, given adequate initial (and boundary) conditions, the fundamental equations must predict the future (or past) evolution [1].

This problem is solved using a 3+1 Decomposition of the Einstein's equations. Not entering into too much detail, the clue step relies on assuming that space-time (a manifold $\mathcal{M}$, with a metric $g_{\mu\nu}$) can be foliated into a family of non-intersecting spacelike 3-surfaces which arise, at least locally, as the level surface of a scalar function t, which can be interpreted as a global time function. Then, within this formalism, we will be able to define all sorts of magnitudes from the EFE (metric, energy-momentum tensor, Riemann tensor, ...) in their spatial (3-component) version [2].

This formulation leads the Einstein field equations to split into two different types of equations: the constraint equations and the evolution equations. The former impose conditions on the gravitational fields at any instant of time, including an arbitrary initial time, while the latter determine the time evolution of the fields.

Ideally, the constraint equations are first solved by using the so called *conformal* techniques, and the solutions of the evolution equations must fulfill the constraints at any time if they do at an initial time. Still, numerical simulations have some error, and can therefore lead to solutions that do not satisfy the constraints at all times. This and other problems we may encounter in performing NR simulations can be solved with reformulations of the 3+1 decomposition, that is, finding a formulation in which the error behaves better and the implementation is stable [3].

2. *Extraction of waveforms*

The second issue in performing NR simulations is as follows. Our main aim from a NR perspective is the extraction of gravitational waveforms in a numerical simulation, in order that, as it has been previously commented, they can be compared with detected signals. However, we encounter the next problem: in constructing templates, natural observable is the one which is also measured by detectors: the GW strain, $h \equiv h_+ + ih_\times$, decomposed into '+' and '×' polarizations in the TT gauge, but this is not typically the quantity directly computed in NR simulations.

Far from sources, gravitational radiation is weak and can be described in the linearised formulation, in which the wave information can be expressed in terms of the two polarization amplitudes, h_+ and $h_\times$.

Nevertheless, NR simulations focus on strong-field regimes and compute 3+1 decomposed magnitudes. In this formalism, it is not trivial to extract in a gauge-invariant way the linearized wave quantities we have mentioned (h_+ and $h_\times$).

In order to address that, there are different strategies. We will just comment on the Weyl formalism [2], the one that is implemented in most NR simulations, in particular in the *Einstein Toolkit* (see section III). In this formalism, the information of the GW that is obtained in a simulation is ψ_4, which has the following expression:

$$\begin{aligned}\psi_4 = -\tfrac{1}{4}\Big({}^{(4)}R_{\hat{t}\hat{\theta}\hat{\theta}\hat{\theta}} - 2i\,{}^{(4)}R_{\hat{t}\hat{t}\hat{t}\hat{\phi}} - 2\,{}^{(4)}R_{\hat{t}\hat{\theta}\hat{\theta}\hat{\theta}} + \\ 2i\,{}^{(4)}R_{\hat{t}\hat{\phi}\hat{\theta}\hat{\theta}} - {}^{(4)}R_{\hat{t}\hat{\phi}\hat{\phi}} + {}^{(4)}R_{\hat{\theta}\hat{\theta}\hat{\theta}\hat{\theta}} + 2i\,{}^{(4)}R_{\hat{t}\hat{\theta}\hat{r}\hat{\phi}} + \\ 2\,{}^{(4)}R_{\hat{t}\hat{\phi}\hat{\phi}\hat{\phi}} - 2i\,{}^{(4)}R_{\hat{r}\hat{\phi}\hat{\theta}} - {}^{(4)}R_{\hat{f}\hat{\phi}\hat{\phi}\hat{\theta}}\Big)\end{aligned} \quad (3)$$

We note that computing ψ_4 involves the covariant four-dimensional Riemann tensor ${}^{(4)}R_{abcd}$, while many numerical simulations employ a 3+1 formalism based on working on 3D quantities. Before we can compute ψ_4, it is necessary to reconstruct ${}^{(4)}R_{abcd}$ from these spatial quantities, reversing steps done in the 3+1 formalism.

It is not hard to verify that ψ_4 provides a measure of outgoing radiation, since to linear order in small deviations from flat space-time expression 3 can be written:

$$\psi_4 = \ddot{h}_+ - i\ddot{h}_\times \ . \quad (4)$$

This way, we have found how to compute h_+ and $h_\times$ in terms of ψ_4. Moreover, knowing the relation between ψ_4 and h, it is also possible to calculate the radiated energy and momentum.

III. OBTAINING DATA: *EINSTEIN TOOLKIT*

Einstein Toolkit (ET) is an open source software of core computational tools for relativistic astrophysics and gravitational physics. It is an enormously powerful tool to perform Numerical Relativity simulations.

Performing a simulation with ET involves the following steps. First, one needs to download and build ET in the cluster where the simulations are going to be carried out.

After the ET is installed, simulations require an executable to be compiled. This executable has one mandatory argument: a *parameter file*. It is a simple text file which contains all the variables and the desired settings for the simulation in the form of key-value pairs: symmetries, time stepping, thin of the grid, initial data (spins, masses, etc), boundary conditions, gauge fixing, and a huge list of other parameters. Given this parameter file, *Einstein Toolkit* performs the simulations and we obtain as a result the output data.

We will just give a brief inside on how ET works. Solving partial derivatives equations numerically involves approximating the fields by their values on a Cartesian 3D computational grid. This way, derivatives are approximated by finite differences (when working on evolution) or spectral operators (when working on initial data). Time evolution is performed by the method of lines, with an iterative integrator, usually Runge-Kutta4.

In order to improve efficiency, *Einstein Toolkit* uses what is called adaptive mesh refinement (AMR): it works with grids that are finer (with smaller steps of time and distance) near the black holes, since it is where we need more precision, and a coarser grid at larger distances [7]. The accuracy of the solution is adapted dynamically while it is being calculated. This helps on reducing the number of point updates in an order of 10^8.

Another improvement included is implementing system symmetries, such as reflection symmetries by an axis or 180° rotational symmetry. Since ET performs a full simulation of the Einstein equations, with no approximations, its computational cost is huge, and therefore all these improvements of efficiency are vital.

IV. POST-PROCESSING DATA

Now we move on to the final part of performing a Numerical Relativity simulation, and the main focus of this work, as it will be shown in the following section: extracting physical information from the data obtained thanks to *Einstein Toolkit*. So as to do so, it is necessary to analyze in depth the obtained data, and work on codes that let us read its physical meaning.

Since, as it has been previously commented, the output data of ET is not directly the natural observable of gravitational waves, h, but is instead ψ_4, it is necessary to post-process this data.

From equation 4 one may think that by directly integrating twice the obtained ψ_4 we should get h_+ and $h_\times$ from its real and imaginary part. Still, when doing that for quasi-circular orbits (the first type of simulations that were studied), integrating ψ_4 lead to a waveform with deviations from the expected h. In particular, h was seen to be different from 0 for times quite after the encounter has happened, which has no physical meaning, since there is no more emission of GW long later than the merger. These deviations are known as "drifts" in the signal.

Another method of integration was then used, known as fixed frequency integration (FFI) [5], which consists in integrating a function in the frequency domain. In this domain, derivating is equivalent to multiplying by $i\omega$:

$$f(t) = \int e^{i\omega t} f(\omega) dt \rightarrow \quad \dot{f}(t) = \int e^{i\omega t} (i\omega f(\omega)) dt \ .$$

Thus, integrating amounts to dividing by $i\omega$. In order to avoid divergences, FFI defines a minimum frequency, ω_0, so that when $\omega < \omega_0$, the integral is calculated by dividing by $i\omega_0$, while in any other case it is calculated by dividing by $i\omega$. For QC orbits, this method has been proven to avoid the drifts obtained by direct integration.

However, when working with dynamical captures, that is, higher eccentric orbits than the QC ones, FFI is not very well-defined, since the minimum frequency ω_0 that has to be chosen to avoid drifts is so big that it erases all physical meaning of the wave. It has been decided, hence, to return to direct time integration (DTI), implemented with polynomial substraction, which consists of choosing the integration constants so that the formerly commented drifts are avoided and $h = 0$ is obtained when the encounter has finished.

It should also be analyzed if $h = 0$ at the beginning of the simulation, since, before the encounter, the emission of GW must also be zero. This is a point being currently examined, and no systematization has still been found to ensure it. In fact, I have taken part in assessing the error obtained regarding these initial drifts, as it will be later explained.

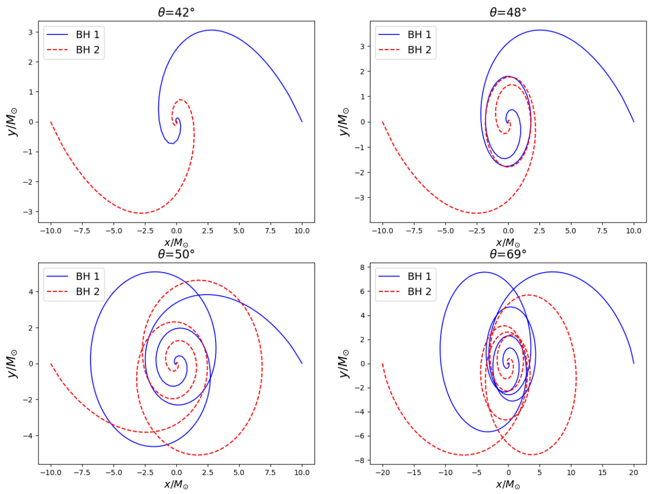

Figure 1: Plot of the trajectories for the collision of four different black holes mergers.

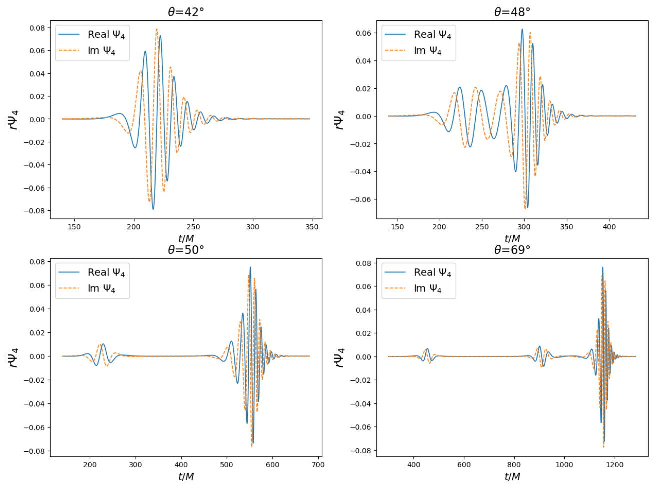

Figure 2: Plot of ψ_4 for the collision of four different black holes mergers.

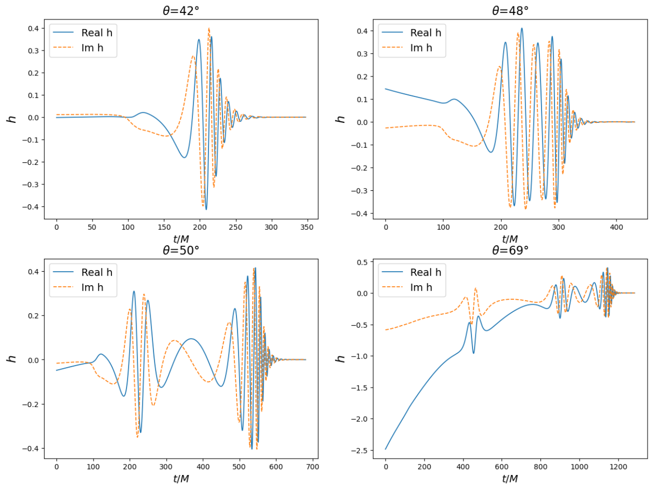

Figure 3: Plot of h for the collision of four different black holes mergers.

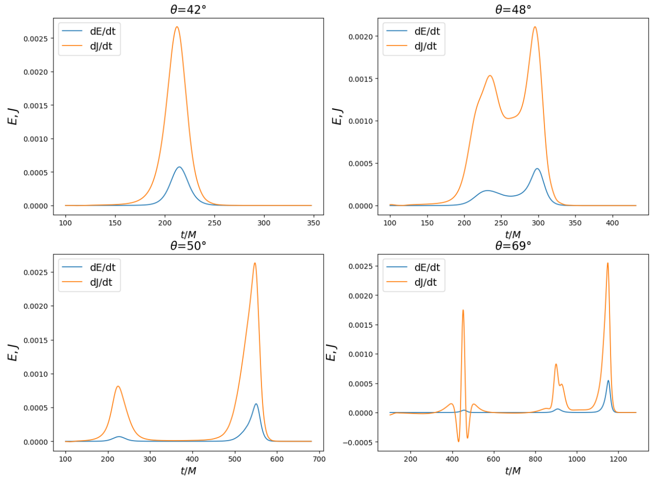

Figure 4: Plot of the radiated energy and momentum for the collision of four different black holes mergers.

V. RESULTS

Here we present four examples of simulations performed using ET both in a cluster at the UB or, if necessary in case of higher computational cost, in the supercomputer Mare Nostrum (as it was the case for the last simulation (69°), which demanded 60 hours running 192 CPUs). They represent a good sample of NR simulations, since they show different possible scenarios expected depending on the type of black holes merger.

For all the simulations, we show the trajectories of the two black holes (figure 1); ψ_4, the directly computed magnitude by *Einstein Toolkit* (figure 2); h, the gravitational waveform (figure 3), computed by direct time integration with polynomial substraction (see section IV); and the radiated energy and momentum (figure 4).

The first simulation (42°), the one with the smallest initial relative angle between black holes (see figure 5), shows just one encounter (the BHs merge the first time they come close to each other). The second simulation (48°) shows an intermediate case between one and two encounters. The third (50°) and fourth (69°) simulations have two and three clear encounters respectively.

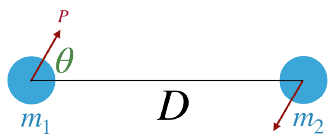

Figure 5: Schematization of the initial data.

Regarding the initial data for the simulations, in addition to the relative angle between trajectories already commented, all simulations have a mass ratio $q \equiv m_1/m_2 = 1$ and a total mass of the system $M \equiv m_1 + m_2 = 1$. The initial distance is $D = 20M$ in units of mass for the first three simulations, while the last one has $D = 40M$. Finally, the last simulation also differs from the others in its initial angular momentum:

$P = 0.061747$ for the former, $P = 0.026224$ for the latter.

It is of particular interest the result obtained for the gravitational waveform of the simulation with $\theta = 69°$. As we can see in figure 3, this simulation shows huge initial drifts in comparison to the other three, that is, the signal h is significantly different from zero at the initial times (contrarily as expected, since the emission of GW is triggered when the two black holes start to accelerate their motion around each other).

As it was explained in section IV, for this type of mergers (with high eccentricity), the most accurate integration method to compute h is the direct integration of ψ_4 with polynomial substraction so that the signal fits the expected zero value at the end of the merger. This procedure has been seen to work for the eccentric mergers with one or two encounters, but when analysing a case with three encounters, we see that the drifts at initial times become so big that it is not possible to consider it anymore an adequate integration method.

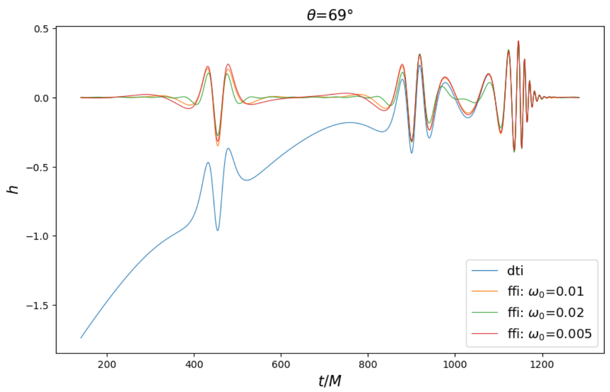

Figure 6: Plot of h for the simulation with $\theta = 69°$ computed with different methods of integration.

In figure 6 we plot the obtained waveform for the $\theta = 69°$ simulation using direct integration and frequency fixed integration with different choices for w_0. Although we have not still found a systematic way of determining the optimal integration method, it is valuable for the project to note that DTI is not working for computing h when we reach three encounters, while FFI integration avoids much better the drifts, with the optimal parameter ω_0 still to be determined.

VI. OUTLOOK AND CONCLUSIONS

In this project there has been an initial task of formation, both on the theoretical background of NR simulations and also on acquiring the skills of remotely working with clusters to run the simulations and later postprocessing the obtained data. These abilities have enabled me to carry an analysis of the dynamical capture regime with some valuable results for the goal of re-calibrating the EOB approximants (see section I).

It is of special interest the discovery that the DTI method, performing well for dynamical captures with one or two encounters, does not work anymore for three encounters. It is still necessary to analyze more in depth these cases and find a systematic way of determining the optimal ω_0 parameter for the FFI method.

Although not shown in this article, it has also been explored how the DTI method works on one and two encounter dynamical captures, changing the initial time of integration of ψ_4 to see how it reflects in the computed h. We have concluded that this initial time does not have great effect on the final h.

All considered, this work has been quite satisfactory and encouraging for my future tasks in this project. First, I expect to make a deeper and more systematic analysis on the best integration method for the different scenarios. Also, I hope for initiating some research in an *Einstein Toolkit* tool that obtains h directly as an output, so it is not necessary to make an integration of ψ_4, which may be very useful in the future of GW modelling, but still needs being investigated in more depth.

Acknowledgments

I would like to thank, first of all, my advisor, for letting me develop such an interesting project and giving to me all his support; it has been enormously enriching to be part of his team and I look forward to continue working in it. I am also really thankful to all the inspiring professors I have encountered in my way here, people that made me believe in myself and made me passionate about science. I as well thank all my colleagues, for taking with me this marvellous and sometimes arduous trip. Finally, I want to express my enormous gratitude to my family, without whom I wouldn't have reached this final project.

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